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Thermodynamic Investigation of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ Cathode, including the Prediction of Defect Chemistry, Electrical Conductivity and Thermo-Mechanical Properties

Shadi Darvish

Florida International University, sdarv003@fiu.edu

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FLORIDA INTERNATIONAL UNIVERSITY

Miami, Florida

THERMODYNAMIC INVESTIGATION OF $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ CATHODE
INCLUDING THE PREDICTION OF DEFECT CHEMISTRY, ELECTRICAL
CONDUCTIVITY AND THERMO-MECHANICAL PROPERTIES

A dissertation submitted in partial fulfillment of the
requirements for the degree of
DOCTOR OF PHILOSOPHY

in

MATERIALS SCIENCE AND ENGINEERING

by

Shadi Darvish

2018

To: Dean John L. Volakis,
College of Computing and Engineering

This dissertation, written by Shadi Darvish and entitled Thermodynamic Investigation of The $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ and $\text{La}_{1-x}\text{Sr}_x\text{Co}_y\text{Fe}_{1-y}\text{O}_{3\pm\delta}$ ($x, y = 0.2-0.4$) As Cathodes of Solid Oxide Fuel Cell; Including Prediction of Defect Chemistry, Electrical Conductivity and Thermo-Mechanical Properties, having been approved in respect to style and intellectual content, is referred to you for judgement.

We have read this dissertation and recommend that it be approved.

Surendra K. Saxena

Arvind Agarwal

Jiuhua Chen

Zhe Cheng

Jean Andrian

Yu Zhong, Major Professor

Date of Defense: February 12, 2018
The Dissertation of Shadi Darvish is approved.

Dean John L. Volakis
College of Engineering and Computing

Andres G. Gil
Vice President for Research and Economic Development
and Dean of the University Graduate School

Florida International University, 2018

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DEDICATION

I dedicate this thesis to my parents, my beloved sister, Neshat, and my best friend, Paniz. Without their patience, understanding, support, and most of all love, the completion of this work would not have been possible.

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I wish to thank the members of my committee, Professor Saxena, Agarwal, Chen, Cheng and Andrian, for their support and patience. Their gentle but firm direction has been most appreciated. Finally, I would like to thank my major professor, Dr. Yu Zhong. From the beginning, he had confidence in my abilities to not only complete a degree, but to complete it with excellence. I have found my coursework throughout the Curriculum and Instruction program to be stimulating and thoughtful, providing me with the tools with which to explore both past and present ideas and issues.

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ABSTRACT OF THE DISSERTATION

THERMODYNAMIC INVESTIGATION OF $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ CATHODE

INCLUDING THE PREDICTION OF DEFECT CHEMISTRY, ELECTRICAL

CONDUCTIVITY AND THERMO-MECHANICAL PROPERTIES

by

Shadi Darvish

Florida International University, 2018

Miami, Florida

Professor Yu Zhong, Major Professor

Fundamental thermodynamic investigations have been carried out regarding the phase equilibria of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ (LSM), a cathode of a solid oxide fuel cell (SOFC), utilizing the CALculation of PHase Diagram (CALPHAD) approach. The assessed thermodynamic databases developed for LSM perovskite in contact with YSZ fluorite and the other species have been discussed. The application of computational thermodynamics to the cathode is comprehensively explained in detail, including the defect chemistry analysis as well as the quantitative Brouwer diagrams, electronic conductivity, cathode/electrolyte interface stability, thermomechanical properties of the cathode and the impact of gas impurities, such as CO_2 as well as humidity, on the phase stability of the cathode. The quantitative Brouwer diagrams for LSM at different temperatures are developed and the detailed analysis of the Mn^{3+} charge disproportionation behavior and the electronic conductivity in the temperature range of 1000-1200°C revealed a good agreement with the available experimental observations. The effects of temperature, CO_2 partial pressure, O_2 partial pressure, humidity level and the cathode composition on the

formation of secondary phases have been investigated and correlated with the available experimental results found in the literature. It has been indicated that the CO₂ exposure does not change the electronic/ionic carriers' concentration in the perovskite phase. The observed electrical conductivity drop is predicted to occur due to the formation of secondary phases such as LaZr₂O₇, SrZrO₃, SrCO₃ and Mn oxides at the LSM/YSZ interface, resulting in the blocking of the electron/ion transfer paths. For the thermomechanical properties of LSM, a new weight loss Mechanism for (La_{0.8}Sr_{0.2})_{0.98}MnO_{3±δ} using the La-Sr-Mn-O thermodynamic database is modeled with respect to the compound energy formalism model. This newly proposed mechanism comprehensively explains the defect formation as a result of volume/weight change during the thermal cycles. According to the proposed mechanism the impact of cation vacancies regarding the volume change of cathode was explained.

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Chapter 1 Introduction

1.1. Objectives

A state-of-the-art fuel cell is considered an electrochemical conversion device, which is able to produce electricity directly from oxidizing a fuel. Fuel cells are mainly classified by their electrolyte material. Solid oxide fuel cells (SOFCs) has a solid oxide or ceramic electrolyte to conduct oxygen ions from cathode side to the anode side. High efficiency, long-term stability, fuel flexibility, low emission, and relatively low cost are all included as advantages of this class of fuel cells. However, besides all these advantages, high operating temperature (500-1000°C), which results in longer start-up times and mechanical and chemical compatibility issues, is the most significant disadvantage of this device. A SOFC is mainly made up of three layers of cathode, electrolyte and anode. There is also a layer of interconnections between them.

A single SOFC, consisting of these three layers stacked together, has dimensions of a few millimeters in thickness and connects hundreds of these cells in series forming an SOFC stack. The electrical and ionic activation of cell parts occurs when the high temperature is reached, and as a consequence, the stacks have to run at temperatures ranging from 500 to 1000°C. The oxygen reduction reaction (ORR), in order to form oxygen ions, occurs at the cathode compartment as illustrated in equation (1). These ions diffuse through the electrolyte to the anode, where they electrochemically oxidize the fuel. In the anode reaction, a water byproduct is given off, as well as two electrons as shown in equation (2). The SOFCs have a wide variety of applications, such as use as auxiliary power units in hybrid or electronic vehicles or stationary power generation with outputs from 100

W to 2 MW. The higher operating temperatures make the SOFCs suitable candidates for applications with heat engine energy recovery devices or combined heat and power, which further increase overall fuel efficiency [1].

1.1.1. Cathode

The cathode is a thin porous ceramic layer on the electrolyte where oxygen reduction reaction (ORR) takes place. The overall ORR is written in Kroger-Vink Notation (equation 3):

Where the e' represents an electron; $V_O^{\bullet\bullet}$, a vacancy of oxygen site with double positive charge; $O_O^{\times}$, an oxygen ion sitting on an oxygen lattice site with a neutral charge.

Cathode ceramics must be electronically conductive. Currently, lanthanum strontium manganite (LSM) is the choice of cathode material primarily for commercial use due to their compatibility with doped zirconia electrolytes. Thermomechanically, LSM has a similar coefficient of thermal expansion (CTE) to yttria-doped zirconia (YSZ) and thus limits stress buildup due to a mismatch in the CTE. Additionally, the LSM has a low level of chemical reactivity with YSZ electrolyte, which avoids degradation of the cathode and electrolyte materials and extends their lifetime. On the other hand, LSM is considered a

poor ionic conductor, and this property results in an electrochemically active reaction which is limited only to the triple phase boundaries (TPBs), where the electrolyte, air, and electrode interact. The LSM works well as a cathode at high temperatures (800-1200 °C). However, its performance quickly drops as the operating temperature is lowered below 800 °C. A potential cathode material must be able to conduct both electrons and oxygen ions in order to increase the reaction zone beyond the TPBs. To address these issues, composite cathode composed of LSM-YSZ has been used to increase the reaction length. Mixed ionic and electronic conducting (MIEC) ceramics, such as perovskite lanthanum strontium cobalt ferrite (LSCF), are also being researched for use in intermediate temperature SOFCs as they are more active and can make up for the increase in the activation energy of the reaction [2].

1.1.2. Electrolyte

The electrolyte in SOFCs is a dense ceramic, which can conduct oxygen anions. The electronic conductivity of electrolyte has to be as low as possible to prevent energy losses. The high operating temperatures of SOFCs allow the kinetics of oxygen ion transport to ensure proper performance. However, as the operating temperature approaches the lower limit for SOFCs, the electrolyte begins to have large ionic transport resistances and affect the performance. Popular electrolyte materials are YSZ (often the 8 mol % yttria-8YSZ), scandia stabilized zirconia (ScSZ) (usually 9 mol% Sc_2O_3 -9ScSZ) and gadolinium doped ceria (GDC) [3]. The electrolyte material has a critical influence on the cell performance [4]. Therefore, it is essential to select a material for the electrolyte, which does not chemically interact with cathode or anode materials. The current target in the related

research areas is to lower the SOFCs functional temperature without reducing the ionic conductivity. This can broaden material choices for SOFC and many existing problems, such as degradation of the cell at high temperature can be potentially solved.

1.1.3. Anode

The ceramic anode layer must be very porous to allow the fuel to flow towards the electrolyte. Similar to the cathode, the anode must conduct electrons, with ionic conductivity, which is considered a positive attribute. The most common anode material used commercially utilized is a cermet made up of nickel mixed with the ceramic material that is used for the electrolyte in that particular cell, typically YSZ nanomaterial-based catalysts. The anode is commonly the thickest and most durable layer in each cell, and is often the layer that provides the mechanical support. One of the functions of the anode allows for the oxygen ions to diffuse through the electrolyte to oxidize the hydrogen fuel. The redox reaction between the oxygen ions and the hydrogen produces heat as well as water and electricity as shown in equation (2) [2].

1.1.4. Current status of SOFC development

All the research efforts are going now in the direction of lower-temperature SOFCs (600 °C). Low-temperature systems can reduce the overall costs by reducing insulation, material design, start-up time and degradation-related expenses. Higher operating temperatures result in temperature gradient increase and the severity of thermal stresses [1]. Another possibility for intermediate temperature (650-800°C) systems is a use of cheaper metallic materials with better mechanical properties and thermal conductivity.

There are a lot of fundamental works, which have been undertaken on the cathode improvement in order to accelerate the ORR and increase the total efficiency of the cell. This extensive research on defect chemistries of the cathode, electrolyte, and anode has been carried out for almost a century as it is closely linked with the thermodynamic equilibria, thermomechanical properties, electrical conductivity, electromechanical properties, superconductivity, catalytic activity, and thermo-electric properties in metal oxides [5]. Even though those efforts were proven successful for specific binary and ternary compounds [6], there is still lack of approach to efficiently understand the accurate defect chemistry, especially for multicomponent metal oxides [7].

The other issue on the cathode side, which is widely being studied, is the formation of new secondary phases on the surface (solid-gas interface) and at the TPBs due to the chemical reactivity of the cathode constituents with the gas species in air, such as CO_2 . The CO_2 is considered the main gas-phase impurity on the cathodic side in SOFCs. Any leakage of exhaust gas from the anode side as a result of anode reaction, which may contain up to 30 vol %. CO_2 , can lead to exposing the cell components, especially the cathode, to high concentrations of CO_2 [8, 9]. The cathode degradation, due to the formation of unwanted secondary phases as a result of reactions among cathode, electrolyte, and certain gas-phase species, would impact the long-term stability of the device and lower its efficiency. Studies have shown that the formation of Sr-containing phases, especially below the operating temperatures, is the main reason for lowering the electronic conductivity and blocking oxygen-transferring path for ORR [10-12].

Most commonly, solid electrolyte materials which are used in SOFCs are YSZ, doped ceria (*e.g.* gadolinium-doped, GDC; and samaria-doped ceria, SDC), stabilized Bi_2O_3 and strontium/magnesium-doped lanthanum gallate (SMLG). A typical SOFC has an electrolyte with YSZ, since YSZ-based SOFCs are required to operate at high temperature of 800-1000°C, researches are underway to replace YSZ with another material, which can be operated at lower temperatures, with at least the same efficiency as YSZ [13]. In the following section, the most prominent experimental and simulation efforts to address the SOFCs current issues have been summarized.

1.2. Thesis Outline

This thesis will be organized into seven chapters.

Chapter 1 provides an introduction to the solid oxide fuel cell and its constituents.

Chapter 2 explains about the CALPHAD approach and thermodynamic assessed databases as well as advantages of this approach.

Chapter 3 describes the defect chemistry analysis of LSM as a cathode of fuel cell utilizing CALPHAD approach. Following that the electronic conductivity predictions have been carried out and comprehensively discussed.

Chapter 4 and 5 present the impact of atmospheric contaminants, *i.e.*, CO_2 and H_2O , on LSM perovskite at the surface and the triple phase boundaries (TPBs) using CALPHAD approach. Secondary phase formation mechanism has been proposed and industrial guidance has been provided.

Chapter 6 discusses the thermomechanical properties of LSM perovskite and related mechanism to volume change and weight loss. New weight change mechanism has been

proposed and represented along with experimental observations and computational predictions.

Chapter 7 summarizes the contribution of the present work and discusses the future work.

Chapter 2 Methodology

2.1. CALPHAD Approach

CALculation of PHase Diagram, known as the CALPHAD approach, is a chronology of what has been achieved and established in the area of phase equilibria by linking thermodynamic principles with mathematical formulations to describe different thermodynamic properties of phases [14]. CALPHAD approach has been developed with consideration of the Gibbs energy minimization of each phase, specie and constituent based on the standard Gibbs energy of pure elements in unary/binary systems. This approach models complex phase equilibria in multicomponent alloys through computer coupling of phase diagrams and thermochemistry. Thermodynamic databases of higher order systems, such as ternary and quaternary systems, can be assessed based on the combination of thermodynamic data of unary/binary systems. The thermodynamic database, containing the description of all phases, is developed, assessed and optimized using Thermo-Calc[®].

There are several significant pros of using CALPHAD approach for thermodynamic assessment of SOFCs;

1. The data from CALPHAD libraries is reliable, because it is assessed based on several experimental measurements on perovskites, but represents the best fit to all experimental data
2. All data is developed in the entire temperature and atmosphere, which SOFCs are being operated.

3. CALPHAD can describe multicomponent systems, which is of great advantage for evaluation of perovskites due to the innumerable possible compositions in solid solutions.

In current work, CALPHAD data of oxygen non-stoichiometry and species concentration, as well as previous existing experimental data are used as input. From this input, defect chemistry analysis, phase stability mapping, electrical and thermo-mechanical properties have been calculated and derived and the outputs of these analyses have been represented and described comprehensively in the following chapters.

2.2. Assessed Thermodynamic Databases

2.2.1. Multicomponent La-Sr-Mn-O Database

The CALPHAD approach models complex phase equilibria in multicomponent systems through computer coupling of phase diagrams and thermochemistry [15, 16]. Its theoretical basis is the thermodynamic description of individual phases. The model used in this work is with respect to the compound energy formalism [17] based on the CALPHAD approach proposed by Grundy [18].

The compound energy formalism is determined to model the thermodynamic features of phases with more than one sublattice. Considering perovskite with ABO_3 formula, three crystallographic sublattices of A, B and oxygen are defined. At least there is one pure component in each sublattice, which is stated as endmember [17].

The most significant advantage of the CALPHAD approach is that it already considered all the possible defect reactions by the modeling choice, which was proved by Grundy for $LaMnO_3$ perovskite [19]. It was proven that only the thermodynamic model, which correctly captured the defect chemistry involved in perovskites, was able to fit the

experimental data, as shown in similar works in La-Co-O [20], La-Ca-Fe-O [21], La-Sr-Co-O [22-24] and La-Sr-Cr-Mn-O [25]. The thermodynamic database of the La-Sr-Mn-O quaternary system was developed based on the overall consideration of the phase stability and thermogravimetry experimental data, and the detailed defect chemistry analysis at different conditions. The accuracy of the database was guaranteed with the model choice and the good agreement with the experimental thermogravimetry data. Consequently, the compound energy formalism model is reliable to expand to the high order system, i.e., the La-Sr-Mn-O system. In according to this model, the Gibbs energy of the perovskite phase is calculated as a mixture of hypothetical endmembers by the following expression [26]:

$$G_m = \sum_{i,j,k} y_i y_j y_k {}^\circ G_{i:j:k}^{Perov} + RT \cdot (\sum y_i \ln y_i + \sum y_j \ln y_j + 3 \sum y_k \ln y_k) + {}^E G_m^{Perov} \quad (1)$$

where y_i is the site fraction of the A-site cations, y_j is the site fraction of the B-site cations, y_k is site fraction of cations in the oxygen site, ${}^\circ G_m^{Perov}$ is the Gibbs energy of perovskite endmembers and ${}^E G_m^{Perov}$ is the excess Gibbs energy of perovskite.

In the La-Sr-Mn-O system, La^{3+} ($\text{La}_A^\times$) will dominate the A site. By doping of the Sr^{2+} , Sr'_A along with the antisite Mn^{3+} ($\text{Mn}_A^\times$), and vacancy (V_A''') will also occupy the A site; Mn with different valence, i.e., Mn^{2+} (Mn'_B), Mn^{3+} ($\text{Mn}_B^\times$), and Mn^{4+} ($\text{Mn}_{Mn}^\bullet$) will dominate the B site. At the same time, vacancy (V_B''') in the B site is also considered. In the O site, O^{2-} ($\text{O}_O^\times$) will dominate while the vacancy ($V_O^{\bullet\bullet}$) in this site is also considered. In according to the defect chemistry analysis, the model based on the compound energy formalism is proposed as:

Since the A site had +3 valence state, the occupation of this site by Sr^{2+} will cause a certain amount of the Mn^{3+} from the B-site move toward the A-site positions, which will decrease the Gibbs energy of LSM. These Mn^{3+} ions were considered as anti-site defects in the A-site. With the Gibbs energy of endmembers and the interaction parameters for the perovskite phase, oxygen nonstoichiometry is modeled as a function of oxygen partial pressure.

The description of equation (8) led to 32 endmembers, e.g. $(\text{La}^{3+})(\text{Mn}^{3+})(\text{O}^{2-})_3$ or $(\text{Sr}^{2+})(\text{Mn}^{2+})(\text{Va})_3$, that Gibbs energy of all of them is required for constructing the basis of the model based on the reciprocal relationship. These Gibbs energy equations of LSM perovskite provided by Grundy [26] pave the way to determine the dominant defect reactions and the electronic conductivity prediction as shown in the current work.

2.2.2. Multicomponent Y-Zr-O Database

Likewise, the La-Sr-Mn-O thermodynamic database, For the Y-Zr-O system proposed by Chen et al. [27], two models were considered based on ZrO_2 crystal structure. The sublattice occupation and the Gibbs energy definition were proposed for monoclinic- ZrO_2 (m- ZrO_2) and tetragonal- ZrO_2 (t- ZrO_2) as $(\text{Y}^{3+}, \text{Zr}^{4+})_1(\text{O}^{2-}, \text{Va})_2$.

$$G_m = y_{\text{Y}^{3+}}y_{\text{O}^{2-}}^{\circ}G_{\text{Y}^{3+};\text{O}^{2-}} + y_{\text{Zr}^{4+}}y_{\text{O}^{2-}}^{\circ}G_{\text{Zr}^{4+};\text{O}^{2-}} + y_{\text{Y}^{3+}}y_{\text{Va}}^{\circ}G_{\text{Y}^{3+};\text{Va}} + y_{\text{Zr}^{4+}}y_{\text{Va}}^{\circ}G_{\text{Zr}^{4+};\text{Va}} + RT[y_{\text{Y}^{3+}}\ln y_{\text{Y}^{3+}} + y_{\text{Zr}^{4+}}\ln y_{\text{Zr}^{4+}} + 2(y_{\text{O}^{2-}}\ln y_{\text{O}^{2-}} + y_{\text{Va}}\ln y_{\text{Va}})] + {}^E G_m \quad (2)$$

Where y_i is the site fraction of species i in the sublattice and the ${}^E G_m$ is the excess Gibbs energy. However, for cubic- ZrO_2 (c- ZrO_2), which is stable in high temperatures, sublattice occupation was defined as: $(\text{Y}, \text{Y}^{3+}, \text{Zr}, \text{Zr}^{4+})_1(\text{O}^{2-}, \text{Va})_2$

According to the sublattice modeling with respect to the compound energy formalism, the Gibbs energy definition for c-ZrO₂ was given as:

$$\begin{aligned}
 G'_m = & y_{\square^{3+}} y_{O^{2-}} {}^\circ G_{Y^{3+};O^{2-}} + y_{Zr^{4+}} y_{O^{2-}} {}^\circ G_{Zr^{4+};O^{2-}} + y_{Y^{3+}} y_{Va} {}^\circ G_{Y^{3+};Va} + \\
 & y_{Zr^{4+}} y_{Va} {}^\circ G_{Zr^{4+};Va} + y_Y y_{O^{2-}} {}^\circ G_{Y;O^{2-}} + y_{Zr} y_{O^{2-}} {}^\circ G_{Zr;O^{2-}} + y_Y y_{Va} {}^\circ G_{Y;Va} + \\
 & y_{Zr} y_{Va} {}^\circ G_{Zr;Va} + RT[y_Y \ln y_Y + y_{Y^{3+}} \ln y_{Y^{3+}} + y_{Zr} \ln y_{Zr} + y_{Zr^{4+}} \ln y_{Zr^{4+}} + \\
 & 2(y_{O^{2-}} \ln y_{O^{2-}} + y_{Va} \ln y_{Va})] + {}^E G'_m
 \end{aligned} \tag{3}$$

In the Y-Zr-O database, solid solution phases, Zr₃Y₄O₁₂ and the liquid phase were modeled as well. The detailed description of the excess Gibbs energy definition and the interaction parameters have been mentioned in Chen et al.'s work [27].

2.2.3. Multicomponent La-Sr-Mn-O-Y-Zr Database

The original La-Mn-O-Y-Zr database was developed by Chen et al. [28] based on the CALPHAD approach. In their work, the thermodynamic descriptions of quaternary subsystems of LaO_{1.5}-YO_{1.5}-ZrO₂, LaO_{1.5}-MnO_x-YO_{1.5}, LaO_{1.5}-MnO_x-ZrO₂, LaO_{1.5}-MnO_x-YO_{1.5}-ZrO₂ were obtained by ideally extrapolation of the ternary systems such as La-Y-O or Y-Zr-O due to the limitation of experimental data for the quaternary systems. Subsequently, the description of La-Mn-O-Y-Zr was obtained based on quaternary subsystems. With the same approach, the La-Mn-O-Y-Zr database was expanded to La-Sr-Mn-O-Y-Zr by Chen [29].

2.2.4. Multicomponent La-Sr-Mn-O-Y-Zr-C Database

In the current work, it is focused on the stability of LSM in the CO₂ containing air atmosphere; However, as 8YSZ is used as an electrolyte in SOFCs and in contact with LSM, as well as CO₂, the whole system is considered for thermodynamic predictions. Instead of assessing all the subsystems, the assessed La-Sr-Mn-O-Y-Zr database is merged

with the SSUB-5 database [30]. The expanded La-Sr-Mn-O-Y-Zr-C is developed by addition of the Gibbs energies of stoichiometric solid phases and also the gas phase from SSUB-5 database. As a result, the assessed La-Sr-Mn-O-Y-Zr-C database can make the predictions of the chemical stability of LSM/8YSZ system in various CO₂ partial pressures with the following major assumptions:

1. LSM perovskite does not have or only has a very limited solubility of C in its lattice.
2. The ionic liquid is not stable in the sintering and operation temperature range.
3. The gas phase is considered an ideal gas in current predictions.

2.2.5. Multicomponent La-Sr-Mn-O-Y-Zr-H-Cr Database

In the current work, the stability of LSM in Cr-containing humid atmosphere is simulated; however, as 8YSZ is used as electrolyte in SOFCs and in contact with LSM as well as Cr and H₂O, the whole system is considered for thermodynamic predictions. For this purpose, the assessed La-Sr-Mn-O-Y-Zr database is merged with the SSUB-5 database [30]. The expanded La-Sr-Mn-O-Y-Zr-Cr-H is developed by addition of the Gibbs energies of stoichiometric solid phases and also the gas phase from SSUB-5 database. As a result, the assessed La-Sr-Mn-O-Y-Zr-Cr-H database is able to make the predictions of the chemical stability of LSM/8YSZ system in various Cr concentration and H₂O partial pressures with the following major assumptions:

1. LSM perovskite does not have or only has a very limited solubility of H in its lattice.
2. The gas phase is considered an ideal gas in current predictions.

Chapter 3 Quantitative Defect Chemistry Analysis and Electronic

Conductivity Prediction of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ Perovskite

3.1. Introduction

The extensive research on defect chemistry has been carried out for almost a century as it is closely linked with the thermodynamic equilibria, thermomechanical properties, electrical conductivity, electromechanical properties, superconductivity, catalytic activity, and thermo-electric properties in metal oxides [5]. Even though those efforts were proven successfully for certain binary and ternary compounds [6], There is still lack of approach to effectively understand the accurate defect chemistry, especially for multicomponent metal oxides.

Analytical defect chemistry analysis, combined with the transport experiments, is the most classic approach used to understand the defect chemistry involved in metal oxides. Over the past two decades, broad efforts have been carried out to quantitatively describe the defect chemistry of metal oxides, including the first principles calculations and analytical and numerical models [31-43]. Precisely, it is well known that the correct defect chemistry analysis should explain both the observations of the electrical conductivity and thermogravimetry behavior. However, such linkage is not well built up, especially for multi-component systems.

On the other hand, extensive efforts were made to develop the thermodynamic databases for metal oxides using the computational thermodynamics approach [19, 44-47]. The primary focus was on the prediction of thermodynamic equilibria in multicomponent systems that typically adopted the compound energy formalism, based on the determination

of the thermodynamic features of phases with more than one sublattice, to describe the ionic species' concentrations and the defect chemistry involved. Despite the fact, no effort has yet been made to directly apply the prediction of the quantitative defect chemistry into the electrical conductivity using the CALculation of PHase Diagram (CALPHAD) approach. The current work represents our initial attempt at the investigation of both the defect chemistry and electronic conductivity of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ with the CALPHAD approach.

3.2. Previous Experimental data

Although the conductivity of $(\text{La}, \text{Sr})\text{MnO}_{3\pm\delta}$ has been studied by different groups, limited data were offered at various temperatures and oxygen partial pressure range. The most prominent works were carried out by Kuo et al. [48] Mizusaki et al. [49], Kamata et al. [50] and Yasuda and Hishinuma [51]. These experiments were mainly different in the powder preparation step. In Kuo et al.'s work [48], powders were prepared by a liquid mix method proposed by Pechini [52] and then sintered at 1400-1500°C to reach high density (relative density $\geq 93\%$). However, the freeze-drying method was employed to acetate aqueous solutions for powder preparation by Mizusaki et al. [49] and Kamata et al. [50]. In Yasuda and Hishinuma's work, powder synthesis was carried out using a high-temperature solid-state reaction of La_2O_3 , SrCO_3 , and MnCO_3 powders [51]. Electrical conductivity in all the studies was measured using the d.c. four-probe technique between 20°C and 1200°C in a furnace as a function of oxygen partial pressure.

In this work, the experimental data from Kuo et al. [48] are adopted to examine the proposed model for the electronic conductivity due to the temperature diversity (1000, 1100, and 1200°C) and also a wide range of oxygen partial pressure (covering both oxygen

excess and oxygen deficient regime) of experiments. The experimental data from Kamata et al. [50], Yasuda and Hishinuma [51] and Mizusaki et al.'s [49] experiments are not adopted for direct comparison with the current investigation, although the same trends are observed in their measurements. The reason is their maximum experiments' temperature is no more than 1000°C, which might be affected more by the slow kinetics inside the perovskite structure especially at low temperature.

3.3. Literature Review on Pervious Defect Chemistry Analysis

The dominant conduction mechanism, which is widely used for perovskite, is shown in equation 1:

$$\sigma_{tot} = \sigma_{ion} + \sigma_e + \sigma_h \quad (1)$$

Where σ_{tot} is the total electrical conductivity, σ_{ion} is the ionic conductivity, σ_e and σ_h are the electronic conductivities due to electrons and electron-holes, respectively. In LSM, σ_{ion} is extremely low and the dominant electronic conductivity is determined by the electron-hole mechanism, i.e., σ_e can be neglected [37, 40, 53].

There are several different conduction mechanisms proposed for LSM from various groups [37, 40, 50, 53, 54]. The overall agreement is the conductivity is closely related to the defect chemistry inside LSM. σ_{ion} is proportional to the $[V_O^{\bullet\bullet}]$, while σ_e and σ_h are proportional to $[Mn'_{Mn}]$ and $[Mn^{\bullet}_{Mn}]$, due to the electron jump between Mn^{2+} and Mn^{3+} states, as well as Mn^{4+} and Mn^{3+} states respectively. It was also agreed that the concentration of Mn^{2+} should be much less than that of Mn^{4+} [37, 40, 53]. However, the critical quantitative concentration of species inside LSM is still not clear.

Since the introduction of the Brouwer diagram in 1954 [55], it is still considered as the most classic method for quickly capturing the involved defect chemistry. In the Brouwer

diagrams, the defect equilibria are divided into several regimes; in each regime, only the dominant equilibria are considered. Although trends in point-defect concentrations can be captured from these diagrams, the quantitative relationships between species' concentrations with various parameters, such as temperature or oxygen partial pressure, are typically not available. To solve this problem, extensive defect chemistry analyses based on some critical assumptions are proposed recently to calculate the species' concentrations quantitatively for further calculations [37, 42, 53].

In the following section, the previous analyses from different groups for the LSM in La-Sr-Mn-O system are reviewed. There were mainly two different models, which can be summarized as the random-defect model and the cluster-defect model. Both of these models assume the various species inside. The difference is that the cluster-defect model assumes that certain clusters may form due to the strong local species' interactions.

In the cluster-defect model proposed by Van Roosmalen and Cordfunke [56], charge disproportionation was also considered. However, it assumed that the neutral defect cluster $\langle Mn'_{Mn} - [V_O^{\bullet\bullet}] - Mn'_{Mn} \rangle$ was formed from Mn'_{Mn} and $V_O^{\bullet\bullet}$ based on the consideration of the MnO_6 octahedron local structure.

In the random-defect model, Sr'_{La} , $Mn^{\bullet}_{Mn}$, and $V_O^{\bullet\bullet}$ were initially considered as the main defects [51] based on the previous effort in the modeling of $LaCrO_3$ [57-59]. It was assumed that the addition of Sr, introduced charge imbalance to the system, which was balanced electronically with the formation of Mn^{4+} as a result of Mn^{3+} ions oxidation and ionically with oxygen vacancies formation. This model was later improved by considering the critical charge disproportionation reaction, i.e. a pair of Mn^{3+} ions decomposed into a pair of Mn^{2+} and Mn^{4+} ions by Kuo et al. [60] to interpret the defect chemistry reactions

for oxygen nonstoichiometry (δ) modeling, as well as electrical conductivity calculation of (La, Sr)MnO₃, which was similar to the one proposed for La_{1-x}Sr_xFeO_{3- δ} [18].

Based on the comparison and also the study of defects mole fraction for the two models by Yasuda and Hishinuma [51], the cluster-defect model was chosen, as it assumed that electrons would be trapped in the cluster and not contribute to the electronic conductivity. The only contribution would come from the electron-hole mechanism, which was associated with the free Mn⁴⁺. The main argument was it had better agreement with the thermogravimetry experimental data in comparison with that from the random-defect model.

However, the later comparisons of these two models were carried out on the other works which proved the random defect-model was able to better reproduce the thermogravimetry data [18]. All the following researchers preferred the random-defect model. For example, Nowotny and Rekas [53] assumed the dominant conduction mechanism was from the Mn⁴⁺ ions, and carefully compared the random-defect model and the cluster-defect model for (La, Sr)MnO_{3 $\pm\delta$} with experimental data from Kuo et al. [48]. It was concluded that the random-defect model matched better with experimental data [53]. Willy Poulsen [37] as well as Zhou and Anderson [40], also investigated the defect chemistry to calculate the electrical conductivity of perovskites. This model is essentially close to Nowotny and Rekas proposed model [53], with the assumption Mn'_{Mn} can be neglected. As a result, $Mn\bullet_{Mn}$ can be considered as the only carrier.

One recent defect chemistry analysis was carried out by Lee and Morgan [42]. The relationships of defect formation enthalpies with defects concentration were obtained from

the calculated *ab initio* defect energies and oxygen non-stoichiometry of LaMnO₃, which also adopted the random-defect model.

It is, in general, agreed that the dominant defect reactions for LSM based on the random-defect model [37, 40, 42, 53] are listed as the following:

$$K_{red} = \frac{[Mn_B^{\times}][V_O^{\bullet\bullet}][P_{O_2}]^{\frac{1}{2}}}{[Mn_{Mn}^{\bullet}][O_O^{\times}]} \quad (3)$$

$$K_{ox} = \frac{[Mn_{Mn}^{\bullet}]^6 [V_A^{'''}][V_B^{'''}][O_O^{\times}]^3}{[Mn_B^{\times}]^6 [P_{O_2}]^{\frac{3}{2}}} \quad (5)$$

Disproportionation)

$$K_{ch.disp} = \frac{[Mn_B'] [Mn_B^{\bullet}]}{[Mn_B^{\times}]^2} \quad (7)$$

which are the same as the dominant defect reactions in LaMnO₃, the addition of Sr will only change the reaction constants.

However, the above defect chemistry analysis and the proposed conduction models on LSM share the following common problems:

1. They were all developed based on certain assumptions on the concentration relationship of different elements or ions, which might be valid only in certain composition ranges;
2. Their models did not consider phases other than the LSM perovskite inside the La-Sr-Mn-O system;

3. The Gibbs energy of LSM perovskite was not considered in their model. Thus, the quantitative concentration of species could be significantly different from the real concentration;
4. None of the non-stoichiometric compositions, i.e., the composition ratio in A-site and B-site away from 1:1, was considered;
5. Extensive defect chemistry analysis with major assumptions is needed for materials with specific compositions. They had difficulty handling the defect chemistry in higher-order multicomponent systems.

In this work, based on our detailed defect chemistry analysis, we also agree with the above dominant reactions, i.e. equations (2), (4), and (6). However, the main difference is considering the CALPHAD approach for conductivity prediction rather than previous approaches, which mainly were based on the calculation of species concentrations in according to oxygen deficiency (δ).

3.4. Result and Discussion

3.4.1. Quantitative Brouwer Diagram

With the correct choice of the thermodynamic model and also the Gibbs energy description, the first quantitative Brouwer diagram for LSM perovskite-based on the CALPHAD approach is developed. It maps out the quantitative concentration of all the species under different conditions as shown in Figure 1. All the defect reactions including the dominant reactions listed in equation 2, 4 and 6 are considered. As a result of quantitative calculation of the concentration of species, especially the ones considered in dominant reactions, the system behavior such as the electrical conductivity could be predicted and tuned based on

the application requirements. Considering the reduction reaction (equation 2), with the increase of oxygen partial pressure, i.e. O_2 (gas) concentration, the reaction is pushed to the left (reactant) side which caused the decrease of $[V_O^{\bullet\bullet}]$ and $[Mn_B^{\times}]$, as well as the increase of $[Mn_{Mn}^{\bullet}]$ and $[O_O^{\times}]$, as shown in Figure 1. It also can be seen that the increase of P_{O_2} in equation 3 will push the reaction to the right (products) side, which will cause the increase of $[V_A^{\bullet\bullet}]$, $[V_B^{\bullet\bullet}]$ and $[Mn_{Mn}^{\bullet}]$ and the decrease of $[Mn_B^{\times}]$.

The Brouwer diagram was calculated for $La_{0.8}Sr_{0.2}MnO_{3\pm\delta}$ by Nowotny and Rekas [53], based on the random-defect model. Since La^{3+} and Sr^{2+} were assigned just on the A-site and Mn ions on the B-site, no Mn^{3+} anti-defects were assumed for the A-site. Furthermore, $V_A^{\bullet\bullet}$ and $V_B^{\bullet\bullet}$ were considered with the same concentration. However, the current calculations based on the CALPHAD approach show different concentration for these vacancies. Increase in cation vacancy concentration in oxygen excess regime is due to the increase in oxygen nonstoichiometry (δ) in this regime. Such differences will greatly affect the equilibrium constants. In addition, off-stoichiometry was considered in their model which would limit their predictions only for the 1:1 ratio in the A: B sites.

Considering all the parameters affecting the electrical conductivity, it is noteworthy that $[V_O^{\bullet\bullet}]$ decreases with the increase of P_{O_2} . The concentration is very low, which is 6.48×10^{-7} per formula at $P_{O_2} = 10^5$ Pa and 2.7×10^{-5} per formula at $P_{O_2} = 1$ Pa. therefore, the ionic conductivity is substantially low in typical operation conditions and can be neglected. Thus, $La_{0.8}Sr_{0.2}MnO_{3\pm\delta}$ is not considered as an oxygen ionic conductor in general.

Figure 1. Quantitative Brouwer Diagrams of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ including all the species in LSM-20 at (a) 1000 °C, (b) 1100 °C and (c) 1200 °C.

3.4.2. Charge disproportionation diagram

The charge disproportionation among the three states of Mn ions, i.e., Mn^{2+} , Mn^{3+} , and Mn^{4+} in manganite perovskite plays the main role in electronic conduction mechanism. Figure 2 illustrates the charge disproportionation (equation 6) in $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ perovskite. It can be seen that with the increase of temperature, the more Mn^{2+} ions form in the whole oxygen partial pressure range as a result of Mn^{3+} disproportionation. Increasing oxygen partial pressure will cause the decrease of the $[\text{Mn}'_{\text{Mn}}]$ and the increase of the $[\text{Mn}^{\bullet}_{\text{Mn}}]$. In the random-defect model proposed by Nowotny and Rekas [53], Mn^{4+} ions are considered as the only charge carriers in LSM perovskites. However, based on the compound energy formalism model, which is close to the random-defect model [53], both Mn^{2+} and Mn^{4+} (charge disproportionation effect) should be considered as carriers in the electrical conductivity calculation. However, Mn^{2+} is not considered in the current work based on the following two reasons:

1. In according to the typical operation condition of LSM-20 ($P_{\text{O}_2} > 1\text{Pa}$), the Mn^{4+} ions, which have a higher concentration than Mn^{2+} , are considered as the main carriers in our calculation. In LSM perovskites by substitution of Sr^{2+} in the A-site, the total A-site valence becomes less than +3, thus the B-site valence increases by the increase of Mn^{4+} ion concentrations.
2. The Seebeck coefficient of LSM was positive in the whole P_{O_2} range, which indicated that LSM was a p-type oxide, i.e., the electronic conductivity was mainly contributed from Mn^{4+} ions [48].

Another significant result achieved from Figure 2 is Mn^{3+} never reaches 100%. It suggests that in the considered temperatures and oxygen partial pressure range, Mn^{3+} is partially disproportionated into Mn^{4+} and Mn^{2+} , as the same reported for LaMnO_3 [19].

At a constant oxygen partial pressure, oxygen deficiency (δ) is decreased with the increase of temperature as exhibited in Figure 3. Consequently, the oxygen-site valence state and $[\text{Mn}'_{\text{Mn}}]$ will increase. It is shown that in $P_{\text{O}_2} < 10^{-15}$ Pa, the oxygen stoichiometry ($3 \pm \delta$) in $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3 \pm \delta}$ is too low, which causes the high $[\text{Mn}'_{\text{Mn}}]$ in this range. The most important outcome, comparing the Figure 2 and Figure 3, is a plateau starting at $P_{\text{O}_2} \sim 10^{-5}$ Pa in δ vs. $\log P_{\text{O}_2}$ which explains the plateaus in the all Mn ions state curves in Figure 2 in the same oxygen partial pressure range. Thus, it is worth noting that the charge disproportionation behavior is affected directly by oxygen non-stoichiometry and temperature.

Figure 2. Charge disproportionation Diagrams of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3 \pm \delta}$ at 1000, 1100, and 1200 °C.

Figure 3. Oxygen stoichiometry as a function of oxygen partial pressure of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3-\delta}$ at 1000, 1100, and 1200 °C.

3.4.3. Equilibrium Constants of Defect Reactions ($K_{\text{red.}}$, $K_{\text{ox.}}$ and $K_{\text{ch.disp.}}$)

One significant thermodynamic parameter discussed mostly [19, 37, 42, 48, 49, 51, 56, 60, 61] for the defect chemistry analysis was the equilibrium constant of the dominant defect reactions. Calculation of this parameter leads to the calculation of further involved thermodynamic parameters as a result of the calculation of the oxygen partial pressure inside the system [60]. Comparison of the calculated equilibrium constant from electrical conductivity with thermogravimetry data was carried out by Kuo et al. [48]. Discrepancies between these two sets of data were mentioned due to the assumption of constant mobility used in conductivity calculation for each oxygen partial pressure, which was actually due to the assumption of the defect model and the summarized relationship among species. One recent effort to calculate the defect reaction equilibrium constants was carried out by Lee and Morgan for lanthanum manganite (LMO) [42]. Based on their assumption, the independency of the equilibrium constant to P_{O_2} in the intermediate region was because of

a small amount of oxygen and cation vacancies, which assumed to be an ideal solution. They concluded that with the change of the oxygen nonstoichiometry (δ), the equilibrium constants would change accordingly. The significant error may occur especially in the intermediate region where δ is close to zero and hard to measure, which may cause the errors in the further calculations on the defect reaction enthalpies and entropies. In most of the previous works [37, 42, 53] the calculation of species concentration was carried out as a function of one or two specific species' concentration, which can be determined from thermogravimetry experimental data. To predict the equilibrium constants, not only δ and cation vacancy concentrations will affect the equilibrium constants of the dominant reactions, the other species' concentration in dominant reactions, e.g. $[Mn_{Mn}^{\bullet}]$ and $[V_O^{\bullet\bullet}]$ should be calculated accurately as well. The defect reactions equilibrium constants based on equation 3, 5, and 7 are plotted in Figure 4-(a) for $La_{0.8}Sr_{0.2}MnO_{3\pm\delta}$ at 1000, 1100, and 1200°C based on the CALPHAD approach. It is shown that with increasing the temperature, the $K_{red.}$ and $K_{ch.disp.}$ will increase. The reason for this increase can be explained in according to defects concentration change as change in temperature at any specific P_{O_2} . According to Figure 1-(a), (b), and (c) and equation 3, with the increase of temperature, $[V_O^{\bullet\bullet}]$ increases while $[Mn_B^{\bullet}]$ decreases, which will cause the increase of $K_{red.}$ (change in $[Mn_B^{\times}]$ and $[O_O^{\times}]$ as a function of temperature is negligible). Considering equation 5 and comparing Figure 1-(a), (b), and (c), shows that with the increase of temperature, the $K_{ox.}$ decreases as a result of the decrease of the cation vacancy concentration in both the A-site and B-site.

Having the exact amount of equilibrium constant for each defect reaction in different temperatures and P_{O_2} ranges helps to find out the exact thermodynamic situation of system

at every point. As an example, the 3-D contour and the 2-D projection for $K_{ch.disp.}$ are mapped out, as shown in Figure 4-(b), in temperature range of 900-1300 °C and 10^{-10} Pa $< P_{O_2} < 10^5$ Pa.

Figure 4. (a) Equilibrium constants of the dominant defect reactions at 1000, 1100, and 1200 °C (b) 2-D projection, (c) and (d) 3-D contour of the charge disproportionation equilibrium constant as a function of oxygen partial pressure and temperature.

3.4.4. Conductivity

The prediction of conductivity for LSM-20 perovskite is carried out using the quantitative Brower diagrams presented in section 5.1. Based on equation 1, the oxygen

vacancy is the carrier for ionic conductivity, while the B site defects concentrations are responsible for electronic conductivity as shown in equation 8,

$$\sigma = e\mu_h[Mn_{Mn}^{\bullet}] + e\mu_e[Mn'_{Mn}] \text{ (S.cm}^{-1}\text{)} \quad (8)$$

where e is the electron charge, $[Mn_{Mn}^{\bullet}]$ and $[Mn'_{Mn}]$ are the carrier concentrations, μ_h and μ_e define electron-hole mobility and electron mobility, respectively.

As discussed in section 5.2, the $Mn_{Mn}^{\bullet}$ is considered as the dominant carrier for the electronic conductivity, considering the LSM operation conditions. Thus, the electron-hole mechanism (the first part of equation (9)) proposed by Nowotny and Rekas [53] for electronic conductivity prediction is used in this work as well. The electron mobility is not discussed in this work due to the neglecting of $[Mn'_{Mn}]$ in this p-type oxide.

μ_h (electron-hole mobility) in equation (8), which is a measure of electron-hole scattering in a system, is presented in the following equation,

$$\mu_h = 2.3 \exp\left(\frac{-0.27 \pm 0.04 \text{ eV}}{kT}\right) \text{ (cm}^2 \cdot \text{s}^{-1}\text{)} \quad (9)$$

As illustrated in equation 9, two constants are considered in the electron-hole mobility calculation from Nowotny and Rekas's work [53]. The energy barrier value from [53] was adopted as the start value and slightly shifted to $(-0.27 \pm 0.04 \text{ eV})$. Figure 5-(a) demonstrates the electronic conductivity (σ) as a function of oxygen partial pressure in the temperature range of 1000-1200°C for $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$. The model matches the experimental data provided by Kuo et al. [48] very well for this perovskite, especially at $P_{O_2} \geq 10^{-6} \text{ Pa}$. The charge disproportionation reaction is considered as the main factor affecting the electronic conductivity. With the increase of $[Mn_{Mn}^{\bullet}]$, the increase of the electronic conductivity in LSM is observed. Since the standard ion in the B site has a

valence of +3, if the Mn^{4+} ion existed in this site, an electron-hole in the B site will be created. Thus, the created electron-hole is directly proportional to the Mn^{4+} concentration, i.e. $[Mn_{Mn}^{\bullet}]$. There are some differences observed in $P_{O_2} < 10^{-6}$ Pa, that might be due to the contribution of $[Mn'_B]$, which increased in this region as shown in Figure 2. The 3-D contours and 2-D projection of electronic conductivity as a function of temperature and P_{O_2} are plotted in Figure 5-(b), (c) and (d). In according to these 3-D contours, the exact amount of conductivity can be predicted in the considered temperature and oxygen partial pressure ranges.

In the case of ionic conductivity, the oxygen vacancies in the third sublattice are determined as the carrier. Since the oxygen vacancy concentration ($[V_O^{\bullet\bullet}]$) has substantially small amount especially in oxygen-deficient region, the ionic conductivity is negligible and the LSM can be considered as pure electronic conductor.

Figure 5. (a) Electronic conductivity (σ) experimental and calculated data of $La_{0.8}Sr_{0.2}MnO_{3+\delta}$ at 1000, 1100, and 1200 °C, vs. P_{O_2} (b) 2-D projection, (c) and (d) 3-D contour of electronic conductivity as a function of oxygen partial pressure and temperature

3.4.5. Effect of A-site deficiency

The two commonly used LSM-20 powders have 2% and 5% A site deficiency. There has been no modeling prediction on the electronic conductivity for perovskite for compositions off stoichiometry. With the CALPHAD approach, the quantitative Brouwer diagrams with the change of composition can be developed. As an example, Figure 6-(a) shows the change of different Mn ions concentration with various A site deficiency at

$P_{O_2} = 1\text{Pa}$ and $T=1000\text{ }^\circ\text{C}$. With that, the 3-D contours and the 2-D projection of $\log \sigma$ vs. $\log P_{O_2}$ with the change in the A-site deficiency are shown in Figure 6-(b), (c) and (d). It is assumed that μ_h is independent of the stoichiometry and only determined by temperature. It predicts that the electronic conductivity of LSM-20 will decrease slightly with the increase of the A-site deficiency, which is directly correlated to the Mn^{4+} concentration in the B-site as shown in Figure 6-(a).

Figure 6. (a) Charge disproportionation Diagrams of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ vs. A site deficiency at $P_{O_2} = 1\text{Pa}$ and $T=1000\text{ }^\circ\text{C}$. (b) 2-D projection, (c) and (d) 3-D contour of conductivity as a function of oxygen partial pressure and A site deficiency.

3.5. Summary

The defect chemistry of LSM-20 was analyzed with the La-Sr-Mn-O thermodynamic database. The quantitative Brouwer diagrams for LSM-20 were developed based on CALPHAD approach. In agreement with the general conduction mechanism (equation 1) with respect to the compound energy formalism theory, the electronic conductivity for $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ was calculated using random-defect model based on CALPHAD approach. It was found the charge disproportionation in the B site played the main role in the electronic conduction mechanism. The calculated electronic conductivity of LSM-20 showed agreement with the experimental data in the literature. In addition, the low ionic conductivity of LSM-20 was explained with the low vacancy's concentration in the oxygen site.

Chapter 4 Thermodynamic Prediction of the Effect of CO₂ to the

Stability of (La_{0.8}Sr_{0.2})_{0.98}MnO_{3±δ} System

4.1. Introduction

Solid Oxide Fuel Cell (SOFC) is regarded as one of the most promising and widely studied state-of-the-art energy resources for the conversion of fossil, bio and hydrogen derived fuels to electrical energy [62]. In a reverse mode, a solid oxide electrolysis cell (SOEC) converts electrical energy to chemical energy in hydrogen [63-65]. Commonly observed degradation of the electrochemically active cell components due to the chemical instability of the cathode surface (solid–gas) and the cathode/electrolyte (solid-solid) interfaces at the TPBs affect the performance of the device during long-term operation [66] in materials systems such as LSM-ScSZ [67, 68], LSCF6428-ScSz [67], LSCF6428-NGO [8], and LSM-8YSZ [69-71]. Many experimental investigations have performed in all probable chemical reactions. Reactions between cell component constituents (cationic species) and atmospheric gases, such as CO₂ or H₂O [64, 72, 73], can be considered as one of the degradation acceleration factors. In addition to the impurity species in the air, any gas leakage from the anode may increase the amount of CO₂ or H₂O in cathode side by more than 30% [8] and leads to the formation of secondary phases such as SrO/SrCO₃ [69, 70, 74, 75], MnO_x oxides [71, 76], La₂Zr₂O₇ (LZO) and SrZrO₃ (SZO) [69, 71, 74], La₂O₃ and La(OH)₃ [68, 71]. It is also suggested that secondary phases impede permeation of oxygen ions (O²⁻) into the cell and could block active oxygen reduction reaction (ORR) sites. These phases are most likely to be electrical insulators that could decrease the electrochemical performance of the cell [70]. Despite the importance of this fact, limited theoretical

investigations have been conducted to determine the exact condition of secondary phase formation and also predict the stability of the cathodes [77]. Current work represents the attempt on the thermodynamic prediction of secondary phase formation for the most classic cathode material, LSM-20, as a result of CO₂ exposure and correlates with the available experimental data.

4.2. Experimental Procedure and Results

LSM-20 electrodes (thickness: ~17 μm , diameter: 1.0 cm) were screen printed on both sides of the 8YSZ electrolyte (Thickness: 185 ± 25 μm) for LSM-20/8YSZ/LSM-20 symmetrical cell fabrication. Similarly, a reference electrode was added above the electrolyte. After drying at room temperature, the electrodes were sintered for 2 h at 1473 K in air and subsequently Pt electrodes (diameter: 6 mm) were applied on both sides of LSM-20 cathodes by using Pt mesh (Alfa Aesar) and Pt paste (Engelhard). The procedure for cell installation has been described completely in Hu et al.'s work [70]. The effect of carbon dioxide on the cell performance was investigated under the range of 0.5-10 vol.% CO₂. The cell was subsequently analyzed for structural and morphological changes by An FEI Quanta 250 FEG SEM.

Figure 7. SEM images of LSM-20 surface in 10% CO₂-air at different temperatures. A: as-fabricated LSM-20 surface in air at 1473 K for 2 h; B, C, and D: exposed at 1023 K, 1073 K, and 1123 K respectively, 100 h, no bias, E: LSM-20 surface cathode at 1023 K with a bias of 0.5 V for 100 h.

The SEM images of the LSM-20 surface before and after exposure to 10 vol.% CO₂ at 1023-1123 K for 100 h are shown in Figure 7. It is observed that particles are segregated on the LSM-20 surface for all the samples either before (Figure 7-(a)) or after (Figure 7-(b, c and d)) exposure to 10 vol.% CO₂. It is observed that introducing 10 vol.% CO₂ to air at 1023 K results in the formation of more and larger particles on the surface. By increasing

temperature to 1073 K and 1123 K, fewer particles are formed and its density decreases (Figure 7- (c and d)). The density of segregated particles for the biased and unbiased samples at 1023 K is essentially the same (Figure 7-(e)).

4.3. Computational Thermodynamics

The CALPHAD approach is developed on the basis of the Gibbs energy minimization of each individual phase in accordance with the standard Gibbs energy of pure elements in unary or binary systems. Accordingly, calculation of higher order systems can be assessed by combination of calculated unary or binary systems. To assess the databases, the Gibbs energies are minimized at equilibrium state under constant temperature and pressure, which are experimentally controlled variables. The thermodynamic databases using in current work were constructed and optimized by Thermo-Calc[®].

The assessed database (See Chapter 1) not only can satisfy the real condition for all the species, phases and constituents, which might form based on the minimization of the Gibbs energy, it can also provide useful information regarding phase formation predictions in LSM/8YSZ/CO₂ system in different conditions.

4.4. Thermodynamic Assumptions

The main aim of the current predictions is to demonstrate the effect of operational parameters, such as temperature, atmosphere and composition, on the secondary phase formation using the CALPHAD approach. Among these parameters, the impact of the atmosphere is more notable due to the two reasons; the first reason is its effect on ORR and the second one is the probability of introducing the impurities like CO₂ to the system, which may lead to the formation of secondary phases.

Better representation of the first impact is demonstrated in Figure 8. There are two main regions responsible for the reactions taking place in SOFCs; region I represents the cathode surface, which is LSM in the current case, and region II shows the TPBs, which is the interface among the cathode (LSM-20)/electrolyte (8YSZ)/atmosphere. In open circuit condition, in both region I and II, oxygen partial pressure (P_{O_2}) is 21 vol.% (air); however, as voltage increases, ORR occurs and P_{O_2} decreases remarkably to 10^{-5} atm or lower in region II [78]. In experimental conditions, cathodic-bias applies to the cell to simulate the effect of long-term reducing atmosphere. The magnitude of P_{O_2} can be estimated for cathodic-bias in current work according to the Nernst equation [79]:

$$\eta_{cath} = RT \ln[p(O_{2-ref})/p(O_{2-interf})]/4F \quad (1)$$

where η_{cath} represents cathodic-bias, $p(O_{2-ref})$ and $p(O_{2-interf})$ define oxygen partial pressure on the surface (region I in Figure 8) as well as TPBs (region II in Figure 8) respectively. R and F are molar gas constant and Faraday constant. Based on the equation (4), considering $P_{O_{2-ref}}=21$ vol.% and applying 0.2 V cathodic-bias, oxygen partial pressure at the interface will be 5.39×10^{-5} atm at $T=1123$ K for typical SOFC operation condition. According to the $p(O_{2-ref})$ calculation, $P_{O_2} = 10^{-5}$ atm is considered as a good estimation of real experimental condition in the current predictions.

As mentioned above, the other issue is the effect of impurities in the atmosphere, which is CO_2 in the current work. The typical CO_2 concentration in air is assumed 400 ppm; however, in current predictions, P_{CO_2} is considered 1 ppm and 0.1 atm (extreme condition) for direct comparison with experimental data provided in current work and also in Hu et

al.'s work [70]. In the following sections, predictions are presented in special atmospheric conditions, which are listed in Table 1, due to the availability of experimental data.

Figure 8. Schematic demonstration of secondary phase formation on the surface and TPBs

Table 1. Atmospheric assumptions representation in current work

Condition #	Experimental Condition	Prediction Condition
C#1	Dry air	$P_{CO_2} = 1 \text{ ppm}$, $P_{O_2} = 0.21 \text{ atm}$
C#2	Air	$P_{CO_2} = 400 \text{ ppm}$, $P_{O_2} = 0.21 \text{ atm}$
C#3	10 vol.% CO ₂ -air	$P_{CO_2} = 0.1 \text{ atm}$, $P_{O_2} = 0.21 \text{ atm}$
C#4	10 vol.% CO ₂ in reducing atmosphere	$P_{CO_2} = 0.1 \text{ atm}$, $P_{O_2} = 10^{-5} \text{ atm}$

4.5. Predictions from Computational Thermodynamics

4.5.1. Secondary Phase Stability at Different Temperatures for LSM-20

It has been observed that secondary phases will form on the surface of LSM. However, various phases were identified ex-situ in different works. Overall, the identified secondary phases have been claimed as either SrO [69, 70, 74, 75] or Mn oxides [71, 76]. The current

work makes an effort for the first time to predict the secondary phases formed on the LSM surface with the CALPHAD approach. Figure 9 shows the thermodynamically stable secondary phases formed in condition (a) C#1, (b) C#3 and (c) C#4 for 1 mole of LSM-20 per formula $((\text{La}_{0.8}\text{Sr}_{0.2})_{0.98}(\text{Mn})_1(\text{O})_{3\pm\delta})$. It is observed from Figure 9-(a), that holding the sample in high temperature at 1500K causes formation of a small amount of Mn_3O_4 (less than 0.5% of 1 mole LSM-20). In the range of 1023-1223 K, which is the typical operation temperature range for SOFCs, LSM-20 is stable and no secondary phase forms. In temperatures lower than 1023 K, precipitation of considerable amount of Mn_2O_3 and/or MnO_2 is predicted. It is worth mentioning that in condition C#2, the results are essentially the same as condition C#1 as shown in Figure 9-(a). Introducing 10 vol.% CO_2 to the previous system (condition C#3) results in the formation of SrCO_3 in low temperatures (<636 K) and also a considerable increase in the amount of MnO_2 as presented in Figure 9-(b). The effect of reducing atmosphere ($P_{\text{O}_2} = 10^{-5}$ atm) with 10 vol.% CO_2 in the atmosphere (condition C#4) is demonstrated on Figure 9-(c). It is observed that the stability temperature of Mn oxides shifts to lower temperature and MnO becomes stable at higher temperatures. Additionally, reducing atmosphere increases the amount of SrCO_3 and also its stability temperature range to 683 K. In current predictions, thermodynamic equilibrium is assumed to occur as sample is annealed for infinite time. However, conditions in experiments could be different due to the limitation of reactions' kinetics as following:

- i. If MnO_x , which could be any of the Mn oxides or mixed type of them depends on the operation condition, forms on the surface, it may remain or dissolve by the change in experimental condition. For instance, Mn_3O_4 formed at sintering

stage (1473 K), may not completely dissolve back into LSM by cooling down the sample and a tiny amount of this phase might remain on the surface.

- ii. In short annealing time, the small amount of high temperature $\text{Mn}_3\text{O}_4/\text{MnO}$ phases, which is precipitated out from LSM-20, might be partially dissociated or changed to other types of Mn oxides (Mn_2O_3 and/or MnO_2) along with a significant decrease in its amount as the sample is cooled down.
- iii. In operation conditions, due to the probability of formation/dissociation of the secondary phases, the existence of a mixed type of MnO_x can be expected after annealing cycles.

Figure 9. Moles of secondary phases of 1 mole LSM-20 within wide range of temperature in condition (a) C#1 (b) C#3 (c) C#4

4.5.2. Secondary Phase Stability at Different Temperatures for LSM-20/8YSZ

In operational condition, the cathode (LSM) is in contact with the electrolyte (8YSZ), and besides the perovskite phase, new phases may form at TPBs. The condition for the cathode/electrolyte interface at typical LSM-20/8YSZ (1:1 molar ratio) operation condition can be simulated in the CALPHAD approach in order to predict the secondary phase formation at TPBs. Addition of 8YSZ to previous sets of conditions at thermodynamic equilibrium results in the formation of c-ZrO₂, La₂Zr₂O₇ and SrZrO₃ as high-temperature phases, as well as m-ZrO₂ and YMn₂O₅ at low temperatures, as illustrated in Figure 10. Although the formation of secondary phases in real condition may be affected by kinetics of reaction, phases such as La₂Zr₂O₇, SrZrO₃ and MnO_x were reported to be formed in high temperature experiments previously [69, 71, 76, 78]. In addition to the formation of secondary phases, 8YSZ in the system increases the stability temperature of SrCO₃ to >700 K. It can be seen that no Mn oxide will form at the interface of LSM-20/8YSZ in temperatures less than ~1429 K in comparison with Figure 9-(c); consequently, it is predicted that Mn oxides would be more favorable to form on LSM-20 surface (region I in Figure 8) than that at the interface or TPBs, because of the lower oxygen partial pressure as a result of more oxygen reduction (region II in Figure 8) [78].

Overall, SrCO₃ forms in low temperatures in regions I and II either in condition C#3 or C#4 as demonstrated in Figure 9 and Figure 10. Formation/dissociation condition of this phase is determined by various parameters including temperature, composition and atmosphere. Therefore, the stability of SrCO₃ as a function of these parameters is examined in the following.

Figure 10. Mole of phases as a function of temperature in $P_{O_2} = 10^{-5}$ atm and $P_{CO_2} = 0.1$ atm for LSM-20/8YSZ system

4.5.3. SrCO₃ Stability

a. Effect of Temperature

The effect of temperature on SrCO₃ stability in the P_{CO_2} range from 10^{-5} – 1 atm for 1 mole LSM-20 is demonstrated in

Figure 11. SrCO₃ is more stable as temperature decreases at constant P_{CO_2} . In addition, by altering P_{CO_2} at the constant temperature, the amount of SrCO₃ increases. For example, current predictions show if T=650 K, SrCO₃ will not form at P_{CO_2} lower than 0.19 atm and it will dissociate at 636 K when $P_{CO_2} = 0.1$ atm in the air.

Figure 11. Mole of SrCO₃ as a function of P_{CO_2} at various temperatures (K) for 1 mole LSM-20 in condition C#2

b. Effect of Oxygen Partial Pressure

Stability of SrCO₃ at different temperatures in the P_{O_2} range from 10^{-5} – 1 atm with 10 vol.% CO₂ in the atmosphere is displayed in Figure 12. This diagram was

plotted to simulate the effect of cathodic-bias applied to the cell as it explained in section 4.

Figure 12 presents that the SrCO_3 stability does not vary considerably in different P_{O_2} , i.e., $10^{-5} - 1$ atm, at the constant temperature, especially at low temperatures. Furthermore, according to the trend for 550 K and 600 K, it is suggested that SrCO_3 is more favorable in lower P_{O_2} due to the higher amount of the phase. Consequently, the higher the temperature is, the more significant effect P_{O_2} will have on the stability of SrCO_3 . By Figure 10, the diagram also illustrates that with the increasing of the temperature in constant P_{O_2} and P_{CO_2} , carbonate amount decreases.

Figure 12. Mole of SrCO_3 as a function of P_{O_2} at 10 vol.% CO_2 and various temperatures for 1 mole LSM-20

c. Effect of LSM Composition

LSMs, which widely used as a cathode in SOFCs, typically contain less than 25% of doped strontium in A-site. Thanks to the CALPHAD approach, predictions can be done in

broad composition range. Therefore, to check the effect of LSM composition on SrCO_3 stability, the mole of SrCO_3 is plotted in the wide range of P_{CO_2} from 10^{-5} – 1 atm for four major LSM compositions (10, 15, 20 and 25% Sr) at 450 K in air. As it is shown in Figure 13, SrCO_3 is more stable as Sr concentration increases, at constant T, P_{CO_2} and P_{O_2} . Considering LSM-20, it is also demonstrated that with increasing P_{CO_2} , mole of the SrCO_3 increases.

Figure 13. Mole of SrCO_3 as a function of P_{CO_2} in different Sr amount of 1 mole LSM at 450 K in air

4.5.4. SrCO_3 Threshold Diagram

The following chemical reaction was considered as dominant reaction introducing the CO_2 to the system based on the thermodynamic equilibrium:

where LSM(reactant) is the sintered LSM which was put in the system initially and LSM(product) is the LSM after CO₂ exposure, which can have a different composition than LSM(reactant) because of the formation of new phases such as SrCO₃. Due to the prediction of the existence of Mn oxides after sintering stage, MnO_x(reactant) is also considered as reactants of the reaction, which may have different composition after CO₂ exposure shown as MnO_x (product). The threshold diagram for the SrCO₃ stability in the air is illustrated in Figure 14-(a) for the first time in the current work. The threshold diagram is established as a unique contribution of mapping of the Gibbs free energy for reaction (2) ($\Delta G_{rxn(2)}$) as a function of temperature, P_{CO_2} and Sr concentration. Such a diagram for stoichiometric phases have been developed previously, however, for the complicated multicomponent system, it can be only developed using the CALPHAD approach. In this diagram, threshold points correspond to the condition where $\Delta G_{rxn(2)} = 0$ (curves in Figure 14) for SrCO₃ formation. If $\Delta G_{rxn(2)} < 0$, which is the lower right corner of the diagram, SrCO₃ will be stable (SrCO₃ stable region) and if $\Delta G_{rxn(2)} > 0$, as defined in the upper left corner of Figure 14, the system is free of SrCO₃ (SrCO₃ free region). As mentioned in previous sections, by decreasing the temperature as well as increasing P_{CO_2} and Sr concentration, the mole of SrCO₃ increases. For example, at constant $P_{CO_2} = 0.1$ atm (red line in Figure 14), LSMs with lower Sr concentration are stable in lower temperatures due to the points having the condition of $\Delta G_{rxn(2)} \leq 0$, or at constant T=450 K (blue line in Figure 14), SrCO₃ is stable for LSMs with higher Sr concentration in lower P_{CO_2} . Furthermore, the effect of P_{O_2} is predicted for SrCO₃ stability threshold diagram in the air and $P_{O_2} = 10^{-5}$ atm as displayed in Figure 14-(a) and (b). At $P_{O_2} =$

10^{-5} atm, the new secondary phase of SrMn_3O_6 at the higher temperature and P_{CO_2} forms for LSM-15 and LSM-20, which may change the dominant reaction. Therefore, reaction (3) could be considered for the Gibbs free energy prediction for the same set of conditions as the reaction (2) except the $P_{\text{O}_2} = 10^{-5}$ atm, as following:

For LSM-10, threshold diagrams are essentially the same in both atmospheres in agreement with the results from Figure 12.

Figure 14. SrCO_3 stability threshold diagram for SrCO_3 stability for various LSM compositions in (a) air (b) $P_{\text{O}_2} = 10^{-5}$ atm

4.6. Discussion

4.6.1. SrO/ SrCO_3 Formation

According to the sets of condition nucleation of various secondary phases was reported [8, 67-71, 80]. Formation of secondary phases, which were predicted to be SrO by first-principles calculations, was predicted for LSM-20/8YSZ/LSM-20 system [70, 74, 75, 81]. It was also claimed that SrCO_3 forms as a result of the reaction between SrO and CO_2 [70,

74]. In order to examine the proposed mechanism for SrO/SrCO₃ formation, a simplified thermodynamic database of Sr-C-O system is considered to determine the formation and dissociation of all the possible phases as demonstrated in Figure 15. Considering one mole LSM-20, i.e. (La_{0.8}Sr_{0.2})_{0.98}(Mn)O_{3±δ}, the maximum amount of Sr can react is 0.2 mole. Thus, the initial Sr concentration is considered 0.2 mole for current prediction and leads to following results:

- i. In condition C#3, SrO is stable at high temperatures, which will react with CO₂ to form SrCO₃ at low temperatures (T<1323 K). Therefore, secondary phase observed in the La-Sr-Mn-O-C system cannot be SrO [69, 70, 74] .
- ii. SrCO₃ has a crystal structure of orthorhombic at temperatures lower than 1323 K, which changes to hexagonal at higher temperatures [82].
- iii. In LSMs, because of the formation of new phases such as perovskite, phase stability will vary from the above Sr-O-C case. Thus, MnO_x is more favorable to form in comparison with the other oxides such as SrO, in both conditions C#3 and C#4 (Figure 9) [71, 76].

Figure 15. Mole of phases as a function of temperature in 10 vol.% CO₂-air having 0.2 mole of Sr

4.6.2. Experimental Investigations vs. Predictions for SrCO₃

Formation of SrCO₃ by current thermodynamic prediction is supported experimentally in current work and also by Hu et al. [70, 74] as a result of the introduction of CO₂ to the system. In their work, it was claimed that the segregated particles might be SrCO₃ due to the high atomic percentage of Sr and C and O on the surface according to Auger electron spectroscopy (AES) data. AES data provides the information regarding the formation of phases from the sample, which was cooled down from 1123 K to room temperature. Based on the current predicted results shown in Figure 9, it is believed that SrCO₃ does not exist at 1123 K. In comparison with the available AES data and the above thermodynamic predictions on the stability of SrCO₃, it is believed that SrCO₃ forms at the lower temperatures and remains stable to room temperature. Therefore, experimental results are in agreement with the current thermodynamic investigations.

The LSM-20/8YSZ/LSM-20 cells were annealed (no bias) at three different temperatures of 1023, 1073, and 1123 K for 100 hours (Figure 7- (b, c and d)) to demonstrate the effect of temperature on the stability of the secondary phase particles on the surface of the LSM-20. It was observed that less amount of secondary phases formed on the surface of the LSM-20 that was annealed at higher temperature. Based on the prediction from Figure 9-(b), it is shown that no secondary phase will be stable in the temperature between 1014 and 1290 K in condition C#3. It successfully explained the experimental observation of the disappearance of the secondary phase particles on the surface of LSM-20 and indicated that the secondary phase particles were dissolved back into LSM-20.

The LSM-20/8YSZ/LSM-20 cells were also tested at 1023 K with bias for 100 hours. It shows that the secondary phase particles are stable on the surface of LSM-20 (Figure 7-(e)). Based on the prediction of Figure 9-(c), it shows that Mn_3O_4 will be stable at the test temperature in condition C#4, which is in agreement with the experimental observations.

4.6.3. LSM Surface vs. TPBs

Formation of $SrCO_3$ on the surface of LSM-20 was discussed in detail in Section 5.1. However, since operation conditions would be different at TPBs (region II in Figure 8) as a result of reaction among the electrolyte (8YSZ), cathode (LSM-20), and atmosphere, new secondary phases form at TPBs as found in section 5.2. Figure 16 demonstrates the $SrCO_3$ stability as P_{CO_2} changes for both region I (air) and region II ($P_{O_2} = 10^{-5}$ atm) at $T=600$ K. Different P_{O_2} were chosen because of the ORR reaction consideration as mentioned above. It shows region II is much more sensitive than region I on the formation of $SrCO_3$,

the threshold for the SrCO_3 formation is as low as 5×10^{-5} atm (50 ppm). This indicates that SrCO_3 may form at the TPBs in typical atmosphere, which has ~ 400 ppm CO_2 .

Figure 16. Mole of SrCO_3 as a function of P_{CO_2} in LSM-20 and LSM/8YSZ system at $T=600\text{K}$ at region I (air) and region II ($P_{\text{O}_2} = 10^{-5}\text{atm}$)

4.6.4. Quantitative Brouwer Diagram and Electrical Conductivity of LSM-

20

Brouwer diagrams are the most classic method for quickly capturing the involved defect chemistry. In the traditional/classic Brouwer diagrams, the defect equilibria are divided into several regimes; in each regime, only the dominant equilibria are considered [55]. the right choice of the thermodynamic model and the optimized Gibbs energy description led to developing the first quantitative Brouwer diagram for LSM perovskite, which can be used for prediction of the electrical conductivity, based on the CALPHAD approach, as shown in our previous work [7]. Figure 17 shows the quantitative Brouwer diagram for LSM-20 in (a) $P_{\text{CO}_2} = 1$ ppm and (b) $P_{\text{CO}_2} = 0.1$ atm. These diagrams map out

the quantitative concentration of 4 species Mn^{2+} , Mn^{3+} , Mn^{4+} and $V_O^{\bullet\bullet}$, which play the main role in electrical conductivity, i.e., electronic and ionic conductivity. The charge disproportionation among Mn^{2+} , Mn^{3+} and Mn^{4+} is shown in equation (4) illustrates that a pair of Mn^{3+} ions decomposed into a pair of Mn^{2+} and Mn^{4+} ions.

Since LSM-20 is a p-type conductor, Mn^{4+} is considered as the main carriers for electronic conductivity as discussed in detail in our previous work [7]. In Figure 17, the concentration of Mn^{4+} is not affected by CO₂ exposure. Furthermore, it is well known that LSM-20 is not a good ionic conductor due to the low concentration of $V_O^{\bullet\bullet}$ as shown in Figure 17. Although $V_O^{\bullet\bullet}$ concentration increases in the more reducing atmosphere (lower P_{O_2}), it is still so low that the ionic conductivity for LSM-20 can be neglected. Additionally, it could be seen that introducing of CO₂ to the system does not alter the $V_O^{\bullet\bullet}$ concentration. As a consequence, since no considerable changes occur in perovskite phase, the formation of La₂Zr₂O₇ and SrZrO₃ at cell operation temperature due to the decomposition of LSM-20 and 8YSZ that is reported in other works [71, 78, 80], can be considered as the main reason for cell's performance degradation.

Figure 17. Quantitative Brouwer Diagrams of $(\text{La}_{0.8}\text{Sr}_{0.2})_{0.98}\text{MnO}_{3\pm\delta}$ at $T=1173\text{ K}$ (a) $P_{\text{CO}_2} = 1\text{ ppm}$ and (b) $P_{\text{CO}_2} = 0.1\text{ atm}$

4.7. Summary

The thermodynamic predictions regarding the phase formation in LSM/8YSZ system in the wide range of temperature, P_{CO_2} , P_{O_2} , and composition have been conducted based on the CALPHAD approach and compared with the experimental observations. It is predicted that MnO_x is the oxide forms on the LSM surface in both biased/unbiased conditions in accordance with current experimental results and in agreement with previous observations [70, 71, 74, 76]. Additionally, in agreement with the previous experimental data in literature [70, 74], formation of SrCO_3 on the surface of LSM-20 in 10 vol.% CO_2 -air is also confirmed and it is concluded that SrCO_3 is more favorable to form at the lower temperatures, the higher concentration of Sr, and the lower P_{O_2} . Quantitative Brouwer diagrams illustrate that introducing 10 vol.% CO_2 to the system would not influence remarkably on LSM electronic/ionic carriers' concentration at $T=1173\text{ K}$, which are responsible of the electronic/ionic conductivity of LSMs. However, the simulation at 600 K at the TPBs shows the possibility of the formation of SrCO_3 even in regular atmosphere

with ~400 ppm CO₂. In temperature range of 1023-1173 K in air containing 21 vol.% oxygen and less than 400 ppm CO₂, no secondary phase will form on the LSM-20 cathode surface. Meanwhile as it was reported in previous studies [78, 80], it is also proposed that the conductivity drop could be as a consequence of formation of the secondary phases at TPBs, such as LaZr₂O₇ or SrZrO₃ as well as the SrCO₃ due to the existence of CO₂ in air, which act as barrier for electron/ion transport.

Chapter 5 Thermodynamic Evaluation of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_{3\pm\delta}$ Cathode in Presence of Cr-Containing Humidified Air

5.1. Introduction

Solid Oxide Fuel Cell (SOFC) is regarded as one of the most promising and widely studied state-of-the-art energy resources for the conversion of fossil, bio, and hydrogen derived fuels to electrical energy [83]. For more efficient performance of SOFCs, it is of significance to acquire knowledge regarding the impact of ambient air on cell durability. Degradation of the cell components, due to the chemical instability of the cathode/gas surface and the cathode/electrolyte interfaces at the Triple Phase Boundaries (TPBs) affect the performance of the device during long-term operation [66] in systems such as LSM-ScSZ [67, 68], LSCF6428-ScSz [67], LSCF6428-NGO [84], and LSM-8YSZ [69-71]. Several experimental and computational investigations have been performed in all possible chemical reactions between cell component constituents (cationic species) and atmospheric gases, such as CO_2 , H_2O and SO_2 [10, 64, 69, 72, 73, 85-95] and agreed that these reactions could be considered as one of the degradation acceleration factors. These reactions lead to the formation of secondary phases such as SrO/SrCO_3 [69, 70, 74, 75, 92], MnO_x oxides [10, 71, 76], $\text{La}_2\text{Zr}_2\text{O}_7$ (LZO) and SrZrO_3 (SZO) [10, 69, 71, 74], and La_2O_3 and $\text{La}(\text{OH})_3$ [68, 71] in different concentration of ambient air contaminants. It has also been proposed that secondary phase formation impede permeation of oxygen ions (O^{2-}) into the cell and could block active oxygen reduction reaction (ORR) sites [90]. Additionally, these phases are most likely to be the electrical insulator, which leads to the lower electrochemical performance of the cell [70]. Due to the presence of humidity in the air surrounding the

cathode the impact of humidity concentration on cathode durability and performance needs further careful and in-depth investigation, especially in the presence of Cr^{6+} gas species [96-99]. Despite the significance of extensive experimental studies, the mechanism of the various secondary phases formation, the roles of operating parameters, and the strategies to suppressing these detrimental phases are not clear and the critical problem in this regard is that slight changes in operation conditions may lead to different observations. Furthermore, previous investigations were conducted in form of accelerated tests (higher concentration of gas species, higher temperature, less time, etc.), which may raise the concern that accelerated condition may differ from the actual operation condition of SOFCs and as a result mixed impact of parameters, such as thermodynamics, kinetics, and microstructural changes were studied. The current work represents an attempt to predict the thermodynamic stability of all the possible secondary phases for the most classic cathode, i.e., Sr-doped Lanthanum manganite (LSM), in humidified Cr-containing air atmosphere, utilizing the CALculation of PHase Diagram (CALPHAD) approach. This work intends to pave the way to unravel the influence of operating parameters from thermodynamics point of view in order to reduce the long-term degradation of Cr-containing SOFCs.

5.2. Previous Experimental Efforts

The most prominent works to investigate the surface segregation criteria and the impact of humidity/ Cr^{6+} poisoning on secondary phase formation has been studied by Kim et al. [68], Chen et al. [100], Nielsen and Mogensen [86], Liu et al. [67], Knöfel et al. [71], Jin and Lu [88], Hu et al. [69, 85], Hardy et al. [87], Heo et al. [99] and Yang et al. [95]. The

latter reviewed the experimental observation from several groups on the impact of humidity and Cr-poisoning of LSM perovskite.

Kim et al. [68] analyzed The impact of water vapor in the air on power generation characteristic of a SOFC by measuring cell voltage at a constant current density, as a function of humidity concentration at 800°C and 1000°C. They also predicted the formation of La_2O_3 and $\text{La}(\text{OH})_3$ on the surface of 2% A-site deficient LSM with the thermochemical computational model using HSC CHEMISTRY. It is predicted that La_2O_3 should be a stable phase at 800°C in both dry and humid air; However, $\text{La}(\text{OH})_3$ should be stable at much higher humidity concentrations or lower temperatures. Chen et al. [100] investigated chromium poisoning of 10% A-site deficient LSM both in dry and humidified (3% H_2O) at 900°C in the presence and absence of Fe-Cr metallic interconnect. ORR electrochemical responses were quite similar for dry and humidified air in the absence of interconnect. However, cell performance gets much poorer performance in humidified air in the presence of interconnect due to the accelerated Cr deposition. Similar to the report from Chen et al. [100], Nielsen and Mogensen [86] carried out impedance spectroscopy tests on LSM-YSZ/8YSZ/Ni-YSZ cell, where tests were performed with compressed air (lower than 0.1% humidity) supplied to the cathode, while the anode was supplied with humidified (4–33%) hydrogen. They didn't observe the apparent change in the surface composition of the LSM samples treated in dry and 70% humidified nitrogen. Enrichment of strontium was detected both on the samples treated in dry nitrogen and 70% humid nitrogen. Additionally, 50% Manganese concentration loss at the surface of perovskite in samples treated in the humidified atmosphere, which may be due to the existence of Mn^{2+} species. Liu et al. [67] performed durability experiments on the LSM and LSCF cathodes

at 800°C up to 1000 h. They also described some morphology changes on LSM samples treated at 3 vol.% humidified air at 800°C; however, the formation of any secondary phases couldn't be characterized. Meanwhile, after 200 hours of treatment in 20 vol.% humidified air, XRD analysis revealed the existence of Mn_2O_3 and Mn_3O_4 . La_2O_3 formation was reported on LSM samples treated in 40 vol.% humidified air at 800°C, as well. In Knöfel et al.'s work [71], there are two types of anode-supported SOFCs tested: one consists of Ni-YSZ/YSZ/LSM-YSZ and the other one has a LSM current collector layer on top of the LSM-YSZ cathode. The samples were first heat-treated at 1050°C in air for 10 hours and then at 1000°C in the different atmosphere for 13 days. Sr enrichment and the decrease of Mn concentration on the surface of LSM, in addition to the formation of monoclinic zirconia and zirconate phases at TPBs were described in Knöfel et al.'s work [71]. Lower oxygen partial pressure leads to more precipitation of Mn oxides. Jin and Lu [88] tested the tri-layer cell, i.e., yttria-stabilized zirconia electrolyte (YSZ)/ strontium-doped lanthanum manganite electrode (LSM)/AISI 441 alloy interconnect structure, in various humidified air concentration at 800°C for up to 500 hours. More Cr- deposition was observed in the samples thermally treated in the humidified air, but no major difference was observed between the samples treated at 10 vol.% and 25 vol.% humidity. The formation of $\text{La}_2\text{Zr}_2\text{O}_7$ at the LSM/YSZ interface and $\text{SrMn}_3\text{O}_{6-x}$, $\text{Mn}_{1.5}\text{Cr}_{1.5}\text{O}_4$ at the LSM grain was observed for all the treatment conditions. At 800°C, the volatile Cr species are affected by the water vapor in the air. In the humidified air, the amount of the volatile $\text{CrO}_2(\text{OH})_2$ gas species is higher than which of the CrO_3 . Hu et al. have done two separate works to investigate the impact of humidity on LSM cathode in absence and presence of Cr [69, 85]. In their first research work, SrO segregation was proposed on the surface of

LSM as well as Mn_2O_3 and $\text{La}_2\text{Zr}_2\text{O}_7$ formation at the interface, which leads to the formation of low-temperature $\text{Sr}(\text{OH})_2$. In their second research work, calculation revealed that LSM remains stable for the whole range of CrO_3 partial pressure and temperature condition. Hardy et al. [87] carried out extensive research on the impact of humidity on LSM/YSZ SOFC by testing at 3vol.% humidified air and dry air at temperatures below 950°C . they claimed from XRD analysis that La_2O_3 and Mn-oxides were also present on the cathode in the quantities of less than 4vol.%. Heo et al. [99] studied chromium poisoning of LSM cathode in a half-cell configuration (Air-3% H_2O - CrO_xH_y /LSM/YSZ/Ag/Air). For the Cr free exposure, no phase segregation was observed at the LSM surface and LSM/YSZ interface. However, for Cr containing humidified air, chromium deposition, claimed in the form of Cr_2O_3 , was observed at the LSM/YSZ interface. Overall, various experimental observation is claimed, especially on the formation of secondary phases such as La_2O_3 , SrMn_3O_6 , and $\text{Mn}_x\text{Cr}_x\text{O}_4$. Therefore, A systematic investigation of the phase equilibria on the cathode is needed to be carried out to investigate the phase formation mechanism.

5.3. Computational Thermodynamics

The CALPHAD approach has been developed originally based on the Gibbs energy minimization of each individual phase according to the standard Gibbs energy of pure elements in unary or binary systems. Consequently, calculation of higher order systems can be assessed by combination of calculated unary or binary systems. In order to construction of the databases, the Gibbs energies are minimized at equilibrium state under constant temperature and pressure, which are experimentally controlled variables. The

thermodynamic databases using in current work were constructed and optimized by Thermo-Calc[®]. comprehensive description of databases is found in Chapter 1.

In the following sections, predictions are presented in special atmospheric condition, which are listed in Table 1, due to the availability of experimental data.

Table 2. Atmospheric assumptions representation in current work

Condition #	Experimental Condition	Prediction Condition
C#1	Air	$P_{O_2} = 0.21 \text{ atm}$
C#2	Humidified Air	$P_{H_2O} = 3 \text{ vol. \%}, P_{O_2} = 0.21 \text{ atm}$
C#3	Reducing Atmosphere	$P_{O_2} = 10^{-5} \text{ atm}$
C#4	Humidified Reducing Atmosphere	$P_{H_2O} = 3 \text{ vol. \%}, P_{O_2} = 10^{-5} \text{ atm}$

5.4. Results

5.4.1. Stability of Secondary Phases at LSM Surface

As it was illustrated in our previous work [10], various Mn oxide species, including MnO_2 , Mn_2O_3 , Mn_3O_4 , and MnO , may form on the surface of LSM in different oxygen partial pressure and temperature in the absence of any contaminants. The main secondary phases predicted to form at C#1, and C#2 conditions are MnO_2 , and Mn_2O_3 , Mn_3O_4 at C#3 and C#4 conditions at the LSM surface as shown in Figure 18. These phases In higher temperature at reducing atmosphere, Mn_2O_3 evaporates and condensates as a form of Mn_3O_4 [101].

The current prediction on the formation of Mn oxides is in agreement with experimental observation [10, 67, 69, 71, 87], which was characterized as Mn_2O_3 and Mn_3O_4 in some

ex-situ experimental observations. It is worth mentioning that stability and amount of these Mn oxides are thermodynamically predicted and may differ from the real experimental observations.

Interesting observation from the diagrams in Figure 18, is that no change has been seen for all the phases as introduction of 3 vol.% humidity to the system in air, which means humidity doesn't make evident significant change in surface composition as previously claimed experimentally [86, 99]. As it will be discussed in detail in the following section, it is suspected that the primary role of the humidity is to increase the kinetics, which causes more severe phase separation as claimed from Hardy et al. [87]. In various research studies, the formation of several other phases, such as La_2O_3 , SrO , $\text{Sr}(\text{OH})_2$, and SrMn_3O_6 , was reported with ex-situ characterization at different humidity concentration and operation temperature [10, 67, 69, 71, 87]. Thanks to the CALPHAD approach, the tendency of the formation of these secondary phases from the main perovskite phase, could be examined by considering their activities. These secondary phases have higher tendency to form when their activity is closer to 1. A small energy perturbation due to surface energy, interface energy, stress may stabilize the phase.

Figure 18. Mole of phases of LSM as a function of temperature at different atmospheric condition (a) C#1 and C#2, (b) C#3 and C#4.

Figure 19 shows the activities of (a) SrO, (b) SrMn_3O_6 , and (c) La_2O_3 in a wide range of temperature at four defined conditions (C#1-C#4). The activity of SrO is increasing with the increase of temperature. However, its activity is very low, and it is unlikely to form at operation condition of SOFC, i.e., 800-1100°C, or lower temperatures. Although humidity may increase the formation chance of this phase comparing to the dry air or dry reducing atmospheres, the current prediction reveals that this phase could not remain stable in operation condition range.

The possible formation temperature for SrMn_3O_6 is predicted to be around 450°C in air (activity close to 1) and even more feasible in reducing atmosphere (temperature lower than 300°C). It is believed that SrMn_3O_6 is favorable in lower temperatures and thermal cycles play a significant role in its stability. While it was claimed SrMn_3O_6 would form at high humidity (> 10% vol.) [88], current prediction shows no apparent change in SrMn_3O_6 activity as humidity exposure (C#2 and C#4 are identical as C#1 and C#3, respectively).

Figure 19. Phase stability vs. temperature change at different C#1-C#4 conditions for (a) SrO, (b) SrMn_3O_6 , (c) La_2O_3 .

Lanthanum oxide (La_2O_3), similar to SrO, is unlikely to form as it is shown in Figure 19-(c) due to its way too low activity (~ 0.03) and similar to SrMn_3O_6 , humidity does not affect its stability. Formation of La_2O_3 was reported in the quantities of less than 4 wt.% in 3 vol.% humidified air [87] and under 40 vol. % humidified air condition at 800 °C [67]. It is worth noting that the secondary phases formed on the surface of the cathode are much less than the concentration predicted by CALPHAD, due to the slow kinetics at low temperature.

5.4.2. The Cr poisoning effect on the Surface of LSM

Gaseous chromium species (Cr^{6+}) is listed as one of the significant hazardous substances. Not only these species are harmful to human health, their presence in cell interconnect (IC) causes cathode poisoning and long-term degradation of the fuel cell [91]. Crofer 22 steel group is mostly used as an interconnect in SOFCs [102, 103]. The continuous flow of the Cr^{6+} gaseous species from the interconnect can significantly increase the Cr^{6+} local concentration at the surface, i.e., 1-10% mol Cr. In Figure 20, phase stability of LSM has been predicted at four defined conditions (C#1 to C#4) for 0.01 mol of Cr. It was found that tiny amount of two new phases, i.e., SrCrO_4 and $\text{Mn}(\text{Mn}, \text{Cr})_2\text{O}_4$ (spinel), form in air and reducing atmosphere; SrCrO_4 as a low-temperature phase (below operation temperature) and spinel as relatively high-temperature phase. It has also been shown that 3vol.% humidity does not affect current phase stabilities. Previously, formation of $\text{Mn}_{1.5}\text{Cr}_{1.5}\text{O}_4$ at 10 and 25 vol.% humidified air [88], $(\text{Mn}, \text{Cr})_3\text{O}_4$ [98] and MnCr_2O_4 at 3% humidified air [96, 98] were reported; which are in agreement with current predictions confirming the formation of a tiny amount of this spinel phase in lower humidity level (3 vol.%). SrCrO_4 was also reported to form on the post-tested LSCF cathode [85]. For LSM cathodes, Cr_2O_3 has been claimed to form at the interface of LSM/YSZ [96, 99]. However, our thermodynamic predictions reveal the formation of a tiny amount of this phase. It is anticipated that SrCrO_4 form as a result of the reaction between Cr and Sr species in long-term operation, but since it forms in a tiny amount, it is suspected that this phase will not be observed on the samples tested in typical operation condition. The tendency of the formation of Mn oxides in air (C#1 and C#2), which were illustrated in Figure 18-(a), has

not been impacted by Cr addition, but interestingly in reducing atmosphere, Mn_3O_4 does not form and the spinel phase stabilizes around 500°C and remains stable till 1100°C.

Figure 20. Mole of phases of LSM as a function of temperature at different atmospheric condition (the mixture of 1 mole per formula of LSM and 0.01 mole of Cr) (a) C#1 and C#2, (b) C#3 and C#4 for 0.01 mole of Cr.

5.4.3. The Cr poisoning effect on the TPBs

Phase stability at the TPBs differs from the cathode surface because of the reduced atmosphere at TPBs. As explained comprehensively in our previous work [10], P_{O_2} has been set at 10^{-5} atm for simulation of TPBs condition due to the polarization. Accordingly, the stability phase at the TPBs of LSM cathode and YSZ electrolyte has been illustrated in Figure 21-(a). Phases such as $\text{La}_2\text{Zr}_2\text{O}_7$ (LZO), SrZrO_3 (SZO), ZrO_2 , YMn_2O_5 , and MnO stabilize as a result of cathode and electrolyte decomposition. Formation of LZO was previously reported broadly in most of the experimental studies at different conditions [69, 85, 87, 88]. Additionally, the formation of zirconate phases, i.e., SZO and LZO, and monoclinic zirconia (ZrO_2 -mono) were claimed by Knöfel et al. [71].

ZrO₂-cubic is the stable phase in 8-YSZ in the whole temperature range we are interested. However, by mixing with LSM, ZrO₂-cubic lost its stability and will partially transform into ZrO₂-mono in the temperature slightly lower than 900°C. as shown in Figure 21. However, it is not expected a significant amount of ZrO₂-mono will form due to the slow kinetics at low temperature. Introduction of Cr to this system leads to the formation of SrCrO₄ at temperatures below 500°C. Similar to the LSM surface, formation of Cr₂O₃ before the formation of SrCrO₄ is possible before reaching equilibrium. Comparing Figure 20-(b) and Figure 21-(b), could be presumed that this phase remains stable until higher temperatures at the TPBs than the cathode surface. Other phases stability has not been altered considering 1% Cr in the system. But with the continues gas flow with Cr species in air, the local concentration of Cr can be significantly increased. As seen in Figure 21-(c), LZO and SZO formation have been impacted considerably and similar to the LSM surface spinel and SrCrO₄ start to form. A phase separation has also been observed for the LSM perovskite phase, which could be due to the decomposition tendency of perovskite and the interdiffusion of Cr to the perovskite lattice.

Figure 21. Mole of Phases of LSM/YSZ as a function of temperature at reducing atmosphere condition containing the mixture of 1 mole per formula of LSM and 1 mole per formula of 8YSZ and (a) 0 mole of Cr (b) 0.01 mole of Cr, (c) 0.1 mole of Cr, (d) Phase amount demonstration of LSM/YSZ as a function of Cr concentration at 900°C in reducing atmosphere.

To comprehensively describe the Cr concentration on affected phases, Figure 21-(d) illustrates the phase stability at TPBs as a function of Cr concentration at 900°C in reducing atmosphere. It is found that Cr concentration less than 0.01 mole, will not impact much to the LSM/YSZ system; however, passing this threshold, a small change in Cr concentration changes the stability of all secondary phases and the perovskite phase. As Cr getting into the LSM lattice, LSCrM perovskite with Cr addition to B-site atoms form $(\text{La}, \text{Sr})\text{Mn}_{1-x}\text{Cr}_x\text{O}_{3\pm\delta}$, which reduces the stability of LZO. This could be helpful for the

performance of the cell, since LZO formation is the dominant mechanism for degradation of the cell. However, more Cr concentration causes the formation of the other secondary phases, such as spinel or SZO at TPBs, which could be harmful to the cell.

5.5. Discussion

Current work predicts the stability of Mn oxides at the LSM surface and SZO, LZO, $\text{Mn}(\text{Mn}, \text{Cr})_2\text{O}_4$ as well as monoclinic zirconia at the interface of LSM/YSZ, in the presence and absence of Cr containing humidified air from the thermodynamic point of view. These results are in agreement with ex-situ experimental observations. However, these predictions are not able to fully support and cover all the previous observations, such as the formation of SrO , La_2O_3 , Cr_2O_3 , and SrMn_3O_6 and it is worthwhile to discuss the discrepancies observed in detail, especially the fundamental mechanism of secondary phase formation.

The first is the phase formation mechanism proposed for the impact of humidity on LSM/YSZ system. For MnO_x formation, previously Mn species evaporation and condensation in the other forms of Mn oxides were reported [86, 101, 104]. The current thermodynamic predictions revealed that La_2O_3 is unlikely to form due to their low activities; however, La_2O_3 was reported to form experimentally [87, 101], which is suspected to be due to the proposed Mn evaporation mechanism. To examine that, La_2O_3 threshold stability diagram has been illustrated in Figure 22, for different B-site deficiency (Mn concentration) at a wide range of temperature in air and reducing atmosphere. In this diagram, threshold points correspond to the condition where $\Delta G = 0$ (curves in Figure 22) for La_2O_3 formation. If $\Delta G < 0$, which is the lower right corner of the diagram, La_2O_3 will

be stable (La_2O_3 stable region) and if $\Delta G > 0$, as defined in the upper left corner of Figure 22, system is free of La_2O_3 (La_2O_3 free region).

Figure 22. La_2O_3 threshold stability diagram for different B-site deficiency ($Mn=0.85$ to 1.05 mol) in air (black) and reducing atmosphere (red).

It can be concluded that in the higher percentage of B-site deficiency ($\text{La}_{0.8}\text{Sr}_{0.2}\text{Mn}_{0.85}\text{O}_{3\pm\delta}$) La_2O_3 is more probable to form in lower temperature range ($\sim 850^\circ\text{C}$) at the surface of perovskite (black curve) and could get stabilized in even the lower temperature at the interface of cathode and electrolyte (red curve). It is believed that the formation of La_2O_3 is due to the evaporation of Mn on the surface of LSM, which greatly increased the B-site deficiency. The same thermodynamic prediction has been carried out for SrO stability evaluation; even though the stability diagrams will change with the change of B-site deficiency, SrO does not reach the stability criteria to remain stable in air or reducing atmosphere thermodynamically. Further investigation is needed to understand the SrO formation mechanism in real operation condition.

The second critical experimental observation is the impact of humidity on phase formation. It has been reported in several experimental observations that humidity increases the formation of secondary phases [67-69, 71, 85-88, 95, 100]; However, the current simulation shows typical humidity concentration in air (3 vol.%) may not alter the phase equilibria in LSM/YSZ system. It is suspected that it may be attributed to the fact that samples in experiments did not reach the equilibrium, i.e., the secondary phase formed in real samples is much less than the predicted concentration, and kinetics plays the main role in phase formations, especially in low temperatures. Additionally, it is also believed that the partial pressure of individual gas species is greatly affected by the humidity, which will change the gas-solid kinetics. In other words, humidity may enhance the perovskite deterioration kinetics and accelerate gas species diffusion into the perovskite. One of the most significant gas species, which may impact the perovskite degradation is Cr^{6+} species [85, 100]. To examine that, Figure 23 has been plotted to illustrate all the volatile Cr^{6+} gas species may evaporate from the Crofer 22H steel interconnect containing just main components (78% Fe and 22% Cr) at 900°C when (a) $P_{\text{O}_2} = 10^{-5}$ atm, (b) $P_{\text{O}_2} = 0.21$ atm and for LSM cathode containing 0.1% Cr at (c) $P_{\text{O}_2} = 10^{-5}$ atm, (d) $P_{\text{O}_2} = 0.21$ atm. Among all the species, CrO_3 and $\text{CrO}_2(\text{OH})_2$ seem to play the main role for Cr^{6+} poisoning, similarly reported by Sabarou et al. [91], which $\text{CrO}_2(\text{OH})_2$ activity significantly changes with humidity concentration, as previously claimed by Chen et al. [100]. CrO_3 partial pressure does not alter with humidity change, but $\text{CrO}_2(\text{OH})_2$ partial pressure increases noticeably as $P_{\text{H}_2\text{O}}$ increases and in high humidity concentration, $\text{CrO}_2(\text{OH})_2$ becomes the

dominant Cr^{6+} species ($P_{\text{H}_2\text{O}} > 0.1 \text{ atm}$). These diagrams could prove the fact that Cr^{6+} poisoning impact is greater in the presence of humidity in the atmosphere.

Figure 23. Cr^{6+} gas species partial pressure as a change of humidity at 900°C (a) 78%Fe, 22%, $P_{\text{O}_2} = 10^{-5} \text{ atm}$, (b) 78%Fe, 22%, $P_{\text{O}_2} = 0.21 \text{ atm}$, (c) LSM-20, 0.1%Cr, $P_{\text{O}_2} = 10^{-5} \text{ atm}$ and (d) LSM-20, 0.1%Cr, $P_{\text{O}_2} = 0.21 \text{ atm}$.

Comparing P_{CrO_3} and $P_{\text{CrO}_2(\text{OH})_2}$ from Figure 23-(a) and (b) with Figure 23-(c) and (d), respectively, shows that evaporation of CrO_3 and $\text{CrO}_2(\text{OH})_2$ from steel interconnect may lead to diffusion of a significant amount of Cr into the perovskite structure. From Figure 24 it could be concluded that at the highest partial pressure range of CrO_3 and $\text{CrO}_2(\text{OH})_2$, Cr^{3+} and Cr^{4+} , substitute in the B-site and Mn species concentrations lowered,

which could be correlated with the formation of Mn oxides on the LSM cathode. This effect could be more severe at the TPBs when P_{O_2} is lower (Figure 24-(c) and (d)).

Figure 24. B-site species concentration at 900°C in 3% humidified environment vs. (a) P_{CrO_3} at $P_{O_2} = 10^{-5} \text{ atm}$, (b) $P_{CrO_2(OH)_2}$ at $P_{O_2} = 10^{-5} \text{ atm}$, (c) P_{CrO_3} at $P_{O_2} = 0.21 \text{ atm}$, and (d) $P_{CrO_2(OH)_2}$ at $P_{O_2} = 0.21 \text{ atm}$.

The third and the most significant issue regarding the impact of the local microstructure on the formation of secondary phases. Figure 25 schematically represents the proposed mechanism for the impact of humidity on phase formation of LSM/YSZ system in the presence of Cr-containing humidified air. Figure 25-(a) illustrates the open circuit condition of a cell when no current is applied. With applying current Sr, Mn oxide

phases may form at the surface of LSM, which is as a result of Mn evaporation from LSM and condensation in the other form at the surface (Figure 25-(b)). Due to the Mn evaporation, local perovskite structure decomposes and releases Sr and La ions to react with ionic species of YSZ and Cr^{6+} gaseous species. As a result, secondary phases such as LZO, SZO $\text{Mn}(\text{Mn}, \text{Cr})_2\text{O}_4$ and $\text{Cr}_2\text{O}_3/\text{SrCrO}_4$ form at TPBs; and as it is explained humidity exists in the atmosphere, accelerates the secondary phase formation and perovskite degradation takes place faster due to the changes in phase stability and higher kinetics of reactions.

Figure 25. Schematic illustration of phase stability in presence and absence of humidified Cr-containing atmosphere

Overall, Current prediction presents thermodynamic results of LSM/YSZ in presence and absence of Cr^{6+} gaseous species in dry and humidified atmosphere. The other significant factors, such as kinetics of reactions, structure changes, etc. have been neglected, which could be a reason for discrepancies between the current and previous experimental results. On the other hand, it is worth noting that most of the experimental tests were conducted in the accelerated condition and may not provide the long-term tests results. Therefore, a different mechanism may control the reactions in extreme conditions. It is proposed that

typical humidity concentration in air (3% vol.) does not impact the phase stability in LSM/YSZ system, operated in typical operation condition for a long time (reaching equilibrium) unless in the presence of Cr^{6+} gas species.

5.6. Conclusion

A comprehensive investigation has been carried out to predict the phase stability for LSM/YSZ system in a broad range of temperature, oxygen partial pressure, and humidity level in the presence and absence of Cr-containing interconnect. Findings from the present work validate the effectiveness of the computational thermodynamic modeling in the prediction of interaction and performance stability of SOFC cathodes in the presence of contaminants.

The formation of various secondary phases including Mn oxides, LaZr_2O_7 , SrZrO_3 , spinel, and zirconia has been predicted in agreement with the previous experimental observations. Besides, the current predictions illustrate that the formation tendency of secondary phases in presence of humidity is more favorable, especially if the cell is exposed to the air containing Cr-gaseous species. It is proposed that humidity enhances the perovskite deterioration and accelerate Cr^{6+} diffusion into the perovskite, in the form of CrO_3 and $\text{CrO}_2(\text{OH})_2$ species. It proves the fact that Cr^{6+} poisoning impact is greater in the presence of humidity in the atmosphere. It was revealed that SrO does not form at any considered conditions in current work, while, La_2O_3 has been found to form at the surface and the TPBs of B-site deficient LSM. This work provides practical guidance on how to control operation condition of a SOFC, as humidity is an important factor for long-term degradation of Cr-containing cell. It is recommended to consider the secondary phase

stability during the SOFC cathode compositional optimization, especially for industrial SOFC applications.

Chapter 6 Weight Loss Mechanism of $(\text{La}_{0.8}\text{Sr}_{0.2})_{0.98}\text{MnO}_{3\pm\delta}$ during Thermal Cycles

6.1. Introduction

Thermo-mechanical property of alkaline earth (AE) metal doped lanthanum manganite, $\text{La}_{1-x}\text{AE}_x\text{MnO}_{3+\delta}$, is one of the most important reasons to be considered as the promising materials to be used as the cathode in solid oxide fuel cell (SOFC) [105]. However, it has been shown that the interface stability may become a problem in the long-term application and the thermomechanical property may be one of the most important failure mechanisms [106].

It is well known that the thermomechanical property and weight loss mechanism of perovskites are linked with each other. A study by Mori [107] showed that sintered $\text{La}_{1-x}\text{Sr}_x\text{MnO}_{3+\delta}$ perovskites with Sr content of $x \sim 0.4$ shrink during thermal cycling between 600 and 1100°C under an oxidizing atmosphere, which generates stress in the SOFC stack. This volume change is attributed to the change at the oxygen vacancy by absorbing and releasing oxygen in high temperatures [108]. In addition to the generated stress in the cathode, under current load cation vacancies in LSM could also cause the diffusion of cations from the interface to an outside environment. Due to increase in the number of TPB, this phenomenon might look helpful at first, but its continuation increases the interface resistance and deteriorates adhesion at the interface.

Mori et al. [107] have also reported a permanent change in sample dimensions with thermal cycle experiments. The A-site metal in lanthanum manganite and oxygen create a cubic closed pack structure, in which oxygen content is 3 and excessive oxygen is attributed

to cation vacancies rather than interstitial oxygen atoms. Mori [109, 110] argued that the release of oxygen at high temperature and formation of vacancies is due to charge compensation. Since ionic radius of Mn^{3+} (97 pm) and Mn^{2+} (81 pm) is larger than Mn^{4+} (67 pm), by reducing the Mn^{4+} to Mn^{3+} the crystal lattice expands with charge compensation. However, in case of AE doped LMO compound, the structure is more complex at high temperatures. Under oxidizing atmosphere at high temperatures, various perovskite compound are present in the structure that complicate the behavior of the material in that condition.

Despite the various investigation that shows the thermo-mechanical behavior of LSM at high temperatures the exact mechanism of this phenomena has not established yet and most of the researches are focused on the suppressing the effect by changing the composition of the compound [111, 112]. It has been showed [113] that replacing Mn in LSM structure by Mg, Cr, Co, Al and especially Ni could prevent the thermal cycling shrinkage. Changing the concentration of lanthanum and partially replacing it by another lanthanide could also enhance the volume stability in high temperatures cycles

It is well known that the weight loss is due to the absorption and release of oxygen from LSM. And the process is determined by the thermodynamics and kinetics combined effect. However, the detailed mechanism involved is still not clear. In the current work, we are trying to use the thermodynamic modeling and experimental investigation to understand the thermodynamics involved in the weight loss mechanism. It will pave the way to the comprehensive understanding of the thermomechanical property of perovskites.

At the same time, the thermodynamic database of the La-Sr-Mn-O system was developed by Grundy [44, 46, 114], which is mainly focused on the phase stability and

compatibility with yttria-stabilized zirconia (YSZ) for the SOFC application. However, no application has been done on the weight loss mechanism on the LSM. In the current investigation, we will carry out the preliminary experimental investigation and propose a new weight loss mechanism based on the thermodynamic analysis.

6.2. Experimental Setup

$(\text{La}_{0.8}\text{Sr}_{0.2})_{0.98}\text{MnO}_{3\pm\delta}$ (LSM-20) powder with granulated spherical structure was obtained from Inframat Advanced Material Company. The powder was synthesized in order to achieve desired stoichiometry and deficiency of the LSM structure. The LSM powdered then was pressed to a 10mm pellet and heat-treated in an air box furnace. Pelleted powder was heated up to 1200°C with the rate of 5°C/min and maintained at that temperature for 20 hours. The powder then was cooled down slowly with the same rate to room temperature. This powder was used as the base line for study the kinetic of the oxygen absorption and desorption behavior.

SDT Q600 from Texas Instrument was used to study the weight loss behavior of LSM powder. An alumina crucible was used as a container to heat up the powder. The empty cups were first used to calibrate the SDT machine at the beginning of each experiment and then almost 20 mg of LSM sample was poured into the crucible. An embedded microcontroller controls the heating profile and gas flow for the experiment. The results then were saved into the computer and analyzed with TI universal analysis software from TI instrument. All the experiments in the present work carried out in the air.

6.3. Results

6.3.1. Experimental Results

The weight loss behavior along with the thermo-mechanical properties is pretty complicated as it is a combination of thermodynamics and kinetics. In the current work, a preliminary experimental investigation on the weight loss behavior of LSM was carried out.

The as-received LSM powder was heated up to 1400°C and was maintained at 1400°C for 8 hours. The heated sample was then quickly cooled to room temperature very rapidly to keep the oxygen concentration close to the equilibrium condition at 1400°C. The heat-treated powder was heated to 1400°C with 10°C/min ramp. The powder was kept at 1400°C for 30 minutes and then that cooled down with the same rate, i.e., 10°C/min. The cycle was repeated for another three times to study the effect of temperature on the performance of the LSM powder. The results are shown in Figure 26. During the first cycle, close constant weight was observed during the heating up process, which is not shown here. As the sample was cooled down in a relative slow rate, i.e. 10°C/min. Starting from the second run, it shows very clearly that the weight is losing during the heating up process and keep dropping at 1400°C during the 30min holding time, when the sample was cooled down, the weight of the sample starts to increase again. Furthermore, with the more cycles, the more weight loss it shows. The maximum weight loss at the end of holding time at 1400°C in the fourth cycle is 1.2 wt.%. Only four cycles were chosen because of the limitation of the SDT Q660.

Even though the weight change behavior of LSM-20 powder is mainly due to the thermodynamic equilibrium especially at the slow heating rate, however, the diffusion

process of oxygen into and out of the LSM crystal is a kinetic process, which will also play an important role. As a consequence, the holding time, especially at 1400°C, could affect the weight loss behavior of the LSM powder. It shows that the sample hasn't reached the final equilibrium with the four cycles. Assuming of low enough holding time can be achieved, much more weight loss is expected.

Figure 26. Weight change behavior of the quenched LSM-20 powder in air atmosphere in various temperature cycles.

6.3.2. Simulation Results

It is well known that the weight change of LSM is due to the absorption and release of the oxygen from the LSM. It was believed that the weight loss is due to the oxygen site

vacancy concentration change. However, the accurate defect chemistry indicated a different mechanism on it. The model used in this work is with respect to the compound energy formalism based on CALculation of PHase Diagram (CALPHAD) approach proposed by Grundy [115], which has been carefully compared with the associate model proposed by Yokokawa et al. [116]. In the latter model, a non-stoichiometric perovskite was considered as a mixture of molecule-like associates. In the end, both models were compared with standard established classic defect chemistry model and the accuracy of the compound energy formalism was proved to be much more accurate and capture the defect chemistry inside LaMnO_3 .

The thermodynamic database of the La-Sr-Mn-O was developed based on the overall consideration of the phase stability, stoichiometry, and the detailed defect chemistry analysis at different conditions [44, 46, 114]. In the thermodynamic model, there are three different sites considered, i.e., A-site, B-site, and O site. Theoretically, La^{3+} ($\text{La}_A^\times$) will dominate the A site. With the doping of the Sr^{2+} , Sr'_A along with the antisite Mn^{3+} ($\text{Mn}_A^\times$), and vacancy (V_A''') will also occupy the A-site; Mn with different valence i.e., Mn^{2+} (Mn'_B), Mn^{3+} ($\text{Mn}_B^\times$), Mn^{4+} (Mn_B) will dominate the B-site, at the same time, vacancy (V_B''') in the B-site is also considered. In the O-site, and O^{2-} ($\text{O}_O^\times$) will dominate while the vacancy ($V_O^{\bullet\bullet}$) in the O site is also considered.

The breakthrough is with the correct thermodynamic model choice for LSM and the accurate Gibbs energy description, the quantitative Brouwer diagram at various conditions can be plotted out for the first time with the support from the CALPHAD approach with Thermo-Calc [117]. The quantitative Brouwer diagram indicated that the concentration of each species could be quantitatively plotted out. For example, the

quantitative Brouwer diagram of LSM in the air at different temperatures was plotted in Figure 27.

Figure 27. The quantitative Brouwer diagram with the description of all the species involved in LSM-20 in air at different temperature.

Specifically, the concentration of $V_O^{\bullet\bullet}$ was plotted in Figure 28. It shows the concentration of $V_O^{\bullet\bullet}$ does increase with temperature; however, it is less than 0.03% at 1400°C. The weight loss due to $V_O^{\bullet\bullet}$ increase was also plotted in Figure 28, which is 0.004% and much less than what we observed and is in contradiction with what people thought in the past. This observation rules out the possibility that the weight loss is mainly due to $V_O^{\bullet\bullet}$.

Figure 28. The quantitative Brouwer diagram on the concentration of $V_O^{..}$ at different temperature (left); the relative weight loss of LSM calculated based on $V_O^{..}$ concentration change (right).

However, at the same time, the thermodynamic calculation on the weight change of the LSM from room temperature to 1400 $^{\circ}\text{C}$ was shown in Figure 29. It is shown the maximum weight change of LSM-20 can be as large as 2.5wt.% assuming the thermodynamic equilibrium is reached at each temperature.

Figure 29. The weight change (left) and molar change (right) of LSM20 in the temperature range from room temperature to 1400 $^{\circ}\text{C}$ in air.

By plotting the molar change of the LSM-20, it is found that the molar change of LSM-20 can be as large as 8%. In another word, for every 1 mole LSM-20 at 1400°C, when the sample is cooled down to room temperature, LSM-20 will increase to 1.08mol.

Figure 30. The quantitative Brouwer diagram of LSM-20 for the concentration of V_A''' and V_B''' (left) and the antisite Mn_A^x in the temperature range from room temperature to 1400°C in air.

The detail defect chemistry analysis shows the concentration of cation vacancies, i.e., V_A''' and V_B''' are almost decreasing in pairs with the increase of temperature (Figure 30). It indicated the weight loss and molar change is due to the Schottky defects, i.e.,

At the same time, it can be observed, there is the concentration difference between the two cation vacancies, which is mainly due to the A site deficiency. It shows with the increase of temperature, the difference will drop, which is due to the formation of anti-site Mn ions (Mn_A^x). Further analysis of the combined approach with quantitative defect chemistry analysis and experimental investigations will yield insight into the problem.

6.4. Summary

With the combined approach of computational thermodynamics and experimental TGA analysis, we have investigated the weight loss mechanism for LSM-20. Instead of the

traditional belief that the weight change is due to the change of the vacancy in the third sublattice, we have proposed that the weight change is due to the molar change because the Schottky defect dominates during the heating and cooling process.

Chapter 7 Summary

The fundamental thermodynamic investigations of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_{3\pm\delta}$ (LSM), a cathode of solid oxide fuel cell (SOFC), have been carried out, utilizing the CALculation of PHase Diagram (CALPHAD) approach. The application of computational thermodynamics to the defect chemistry analysis, quantitative Brouwer diagrams, electronic conductivity, TPB stability, thermomechanical properties of the cathode, and the effect of gas impurities, like CO_2 as well as humidity, on the phase stability of cathode are comprehensively explained in detail. The quantitative Brouwer diagrams for LSM at 1000, 1100, and 1200°C are developed and the detailed analysis of the Mn^{3+} charge disproportionation behavior and the electronic conductivity in the temperature range of 1000-1200°C revealed a good agreement with the available experimental observations. The effects of temperature, CO_2 partial pressure, O_2 partial pressure, humidity level and the cathode composition on formation of secondary phases have been investigated and correlated with the available experimental results found in the literature. Formation of various Mn species, LaZr_2O_7 , SrZrO_3 , SrCO_3 , spinel, and Zr oxides has been predicted in good agreement with previous experimental efforts in presence and absence of CO_2 , humidity and Cr-containing atmosphere. The observed electrical conductivity drop, in case of the presence of CO_2 , is predicted to occur due to the formation of secondary phases at the LSM/YSZ interface, resulting in the blocking of the electron/ion transfer paths. It has been discussed that humidity enhances the perovskite deterioration and accelerate Cr^{6+} diffusion into the perovskite, in form of CrO_3 and $\text{CrO}_2(\text{OH})_2$ species. It proves the fact that Cr^{6+} poisoning impact is greater in the presence of humidity in atmosphere. It is recommended that unnecessary thermal cycles should be lessened in order to avoid

formation of stable secondary phases at lower temperature. Furthermore, a new volume/weight change mechanism for $(\text{La}_{0.8}\text{Sr}_{0.2})_{0.98}\text{MnO}_{3\pm\delta}$, explaining the impact of cation vacancies is proposed, with respect to the compound energy formalism model. Instead of the traditional belief that the weight change is due to the change of the vacancy in the third sublattice, it has been proposed that the weight change is due to the formation of Schottky defects, which dominate during the heating and cooling processes.

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APPENDICES

APPENDIX 1

Assessed La-Sr-Mn-O-Y-Zr-C Database

TEMP-LIM 298.15 6000.00 !
\$ELEMENT NAME REF. STATE ATOMIC MASS H0 S0 !
ELEMENT /- ELECTRON_GAS 0.0000E+00 0.0000E+00 0.0000E+00 !
ELEMENT VA VACUUM 0.0000E+00 0.0000E+00 0.0000E+00 !
ELEMENT LA DOUBLE_HCP(ABAC) 1.3891E+02 6665.112 56.9024 !
ELEMENT MN CBCC_A12 54.938 4996 32.008 !
ELEMENT SR SR_FCC_A1 8.7620E+01 6.5680E+03 5.5694E+01 !
ELEMENT Y HCP_A3 8.8906E+01 5.9664E+03 4.4434E+01 !
ELEMENT ZR HCP_A3 9.1224E+01 5.5663E+03 3.9181E+01 !
ELEMENT O 1/2_MOLE_O2(G) 1.5999E+01 4.3410E+03 1.0252E+02 !
ELEMENT C GRAPHITE 1.2011E+01 1.0540E+03 5.7400E+00!
ELEMENT H 1/2_MOLE_H2(GAS) 1.0079E+00 4.2340E+03 6.5285E+01!
ELEMENT S ORTHORHOMBIC_S 3.2066E+01 0.0000E+00 0.0000E+00!
ELEMENT AR 1_MOLE_AR1(G) 3.9948E+01 0.0000E+00 3.6982E+01!
\$
SPECIE LA+2 LA/+2 !
SPECIE LA+3 LA/+3 !
SPECIE LA1O1 LA1O1 !
SPECIE LA1O2 LA1O2 !
SPECIE LAO15 LA1O1.5 !
SPECIE LA2O1 LA2O1 !
SPECIE LA2O2 LA2O2 !
SPECIE LA2O3 LA2O3 !
SPECIE MN+2 MN/+2 !
SPECIE MN+3 MN/+3 !
SPECIE MN+4 MN/+4 !
SPECIE MNO MN1O1 !
SPECIE MNO2 MN1O2 !
SPECIE MN2O3 MN2O3 !
SPECIE MN3O4 MN3O4 !
SPECIE SR+2 SR/+2 !
SPECIE SR2 SR2 !
SPECIE SR2O SR2O1 !
SPECIE SRO SR1O1 !

SPECIE SRO2	SR1O2 !
SPECIE Y+3	Y/+3 !
SPECIE Y2O	Y2O1 !
SPECIE YO	Y1O1 !
SPECIE Y2O2	Y2O2 !
SPECIE YO2	Y1O2 !
SPECIE YO15	O1.5Y1 !
SPECIE Y2O3	O3Y2 !
SPECIE ZR+4	ZR1/+4 !
SPECIE ZR2	ZR2 !
SPECIE ZRO	ZR1O1 !
SPECIE ZRO2	ZR1O2 !
SPECIE LA2ZR2O7	LA2O7ZR2 !
SPECIE Y2ZR2O7	O7Y2ZR2 !
SPECIE O-2	O/-2 !
SPECIE O2	O2 !
SPECIE O3	O3 !
SPECIES C1H1	C1H1!
SPECIES C1H1O1	C1H1O1!
SPECIES C1H1O2	C1H1O2!
SPECIES C1H2	C1H2!
SPECIES C1H2O1	C1H2O1!
SPECIES C1H2O2	C1H2O2!
SPECIES C1H2O2_CIS	C1H2O2!
SPECIES C1H2O2_DIOXIRANE	C1H2O2!
SPECIES C1H2O2_TRANS	C1H2O2!
SPECIES C1H2S3	C1H2S3!
SPECIES C1H3	C1H3!
SPECIES C1H3O1_CH2OH	C1H3O1!
SPECIES C1H3O1_CH3O	C1H3O1!
SPECIES C1H4	C1H4!
SPECIES C1H4O1	C1H4O1!
SPECIES C1H4S1	C1H4S1!
SPECIES C1MN1O3	C1MN1O3!
SPECIES C1MN3	C1MN3!
SPECIES C1O1	C1O1!
SPECIES C1O1S1	C1O1S1!
SPECIES C1O2	C1O2!
SPECIES C1O3SR1	C1O3SR1!
SPECIES C1S1	C1S1!
SPECIES C1S2	C1S2!
SPECIES C1ZR1	C1ZR1!
SPECIES C2	C2!
SPECIES C2H1	C2H1!
SPECIES C2H2	C2H2!

SPECIES C2H2O1	C2H2O1!
SPECIES C2H3	C2H3!
SPECIES C2H4	C2H4!
SPECIES C2H4O1_ACETALDEHYDE	C2H4O1!
SPECIES C2H4O1_OXIRANE	C2H4O1!
SPECIES C2H4O2	C2H4O2!
SPECIES C2H4O2_ACETICACID	C2H4O2!
SPECIES C2H4O2_DIOXETANE	C2H4O2!
SPECIES C2H4O3_123TRIOXOLANE	C2H4O3!
SPECIES C2H4O3_124TRIOXOLANE	C2H4O3!
SPECIES C2H5	C2H5!
SPECIES C2H6	C2H6!
SPECIES C2H6O1	C2H6O1!
SPECIES C2H6O2	C2H6O2!
SPECIES C2MN5	C2MN5!
SPECIES C2O1	C2O1!
SPECIES C2SR1	C2SR1!
SPECIES C3	C3!
SPECIES C3H1	C3H1!
SPECIES C3H4_1	C3H4!
SPECIES C3H4_2	C3H4!
SPECIES C3H6O1	C3H6O1!
SPECIES C3H6_1	C3H6!
SPECIES C3H6_2	C3H6!
SPECIES C3H8	C3H8!
SPECIES C3MN7	C3MN7!
SPECIES C3O2	C3O2!
SPECIES C4	C4!
SPECIES C4H1	C4H1!
SPECIES C4H10_1	C4H10!
SPECIES C4H10_2	C4H10!
SPECIES C4H2_1	C4H2!
SPECIES C4H2_2	C4H2!
SPECIES C4H4_1	C4H4!
SPECIES C4H4_2	C4H4!
SPECIES C4H6_1	C4H6!
SPECIES C4H6_2	C4H6!
SPECIES C4H6_3	C4H6!
SPECIES C4H6_4	C4H6!
SPECIES C4H6_5	C4H6!
SPECIES C4H8_1	C4H8!
SPECIES C4H8_2	C4H8!
SPECIES C4H8_3	C4H8!
SPECIES C4H8_4	C4H8!
SPECIES C4H8_5	C4H8!

SPECIES C4H8_6	C4H8!
SPECIES C5	C5!
SPECIES C60	C60!
SPECIES C6H6	C6H6!
SPECIES C6H6O1	C6H6O1!
SPECIES C6MN23	C6MN23!
SPECIES H10O8S1	H10O8S1!
SPECIES H15O10.5S1	H15O10.5S1!
SPECIES H1MN1	H1MN1!
SPECIES H1MNO	H1MN1O1!
SPECIES H1MNO2	H1MN1O2!
SPECIES H1O1	H1O1!
SPECIES H1O1S1_HSO	H1O1S1!
SPECIES H1O1S1_SOH	H1O1S1!
SPECIES H1SRO	H1SR1O1!
SPECIES H1O2	H1O2!
SPECIES H1S1	H1S1!
SPECIES H1SR1	H1SR1!
SPECIES H1ZR1	H1ZR1!
SPECIES H2	H2!
SPECIES H2LA1	H2LA1!
SPECIES H2MNO2	H2MNO2!
SPECIES H2O1	H2O1!
SPECIES H2O1S1_H2SO	H2O1S1!
SPECIES H2O1S1_HSOH	H2O1S1!
SPECIES H2O2	H2O2!
SPECIES H2O2SR1	H2O2SR1!
SPECIES H2O4S1	H2O4S1!
SPECIES H2S1	H2S1!
SPECIES H2S2	H2S2!
SPECIES H2SR1	H2SR1!
SPECIES H2Y1	H2Y1!
SPECIES H2ZR1	H2ZR1!
SPECIES H3LA1O3	H3LA1O3!
SPECIES H3Y1	H3Y1!
SPECIES H4O5S1	H4O5S1!
SPECIES H6O6S1	H6O6S1!
SPECIES H8O7S1	H8O7S1!
SPECIES LA1MN1O3	LA1MN1O3!
SPECIES LA1S1	LA1S1!
SPECIES LA1S2	LA1S2!
SPECIES LA2S3	LA2S3!
SPECIES MN1O3SR1	MN1O3SR1!
SPECIES MN1O3Y1	MN1O3Y1!
SPECIES MN1O4S1	MN1O4S1!

SPECIES MN1O4SR2		MN1O4SR2!
SPECIES MN1S1		MN1S1!
SPECIES MN1S2		MN1S2!
SPECIES MN2O5Y1		MN2O5Y1!
SPECIES MN2O7		MN2O7!
SPECIES MN2O7SR3		MN2O7SR3!
SPECIES MN3O10SR4		MN3O10SR4!
SPECIES MN3O6SR1		MN3O6SR1!
SPECIES MN4O15SR7		MN4O15SR7!
SPECIES O1S1		O1S1!
SPECIES O1S2		O1S2!
SPECIES O2S1		O2S1!
SPECIES O3S1		O3S1!
SPECIES O3SR1ZR1		O3SR1ZR1!
SPECIES O4S1SR1		O4S1SR1!
SPECIES O8S2ZR1		O8S2ZR1!
SPECIES S1SR1		S1SR1!
SPECIES S1Y1		S1Y1!
SPECIES S1ZR1		S1ZR1!
SPECIES S2	S2!	
SPECIES S2ZR1		S2ZR1!
SPECIES S3	S3!	
SPECIES S3ZR2		S3ZR2!
SPECIES S4	S4!	
SPECIES S5	S5!	
SPECIES S6	S6!	
SPECIES S7	S7!	
SPECIES S8	S8!	

\$

DEFAULT_COM DEFINE_SYSTEM_ELEMENT VA /- !

TYPE-DEF % SEQ * !

TYPE-DEF Z SEQ * !

TYPE-DEF L GES AMEND_PHASE_DESCRIPTION IONIC_LIQ COMP_SET „

MN+2 : VA : !

TYPE_DEF B GES AMEND_PHASE_DESCRIPTION @ MAGNETIC -1 0.4 !

TYPE_DEF A GES AMEND_PHASE_DESCRIPTION @ MAGNETIC -3 0.28 !

\$

PHASE IONIC_LIQUID:Y ZL 2 1 1 !

CONST IONIC_LIQUID:Y : LA+3 MN+2 MN+3 SR+2 Y+3 ZR+4 : O-2 VA : !

PAR G(IONIC_LIQUID,LA+3:VA) 298.15

+GLALIQ; 3200 N !

PAR G(IONIC_LIQUID,LA+3:O-2) 298.15

+GLA2O3L; 6000 N !

PAR G(IONIC_LIQUID,MN+2:VA) 298.15

+GMNLIQ; 3000 N !

PAR G(IONIC_LIQUID,MN+2:O-2)	298.15
+2*GL11;	3000 N !
PAR G(IONIC_LIQUID,MN+3:VA)	298.15
+2*GMNLIQ+GL23-3*GL11;	3000 N !
PAR G(IONIC_LIQUID,MN+3:O-2)	298.15
+GL23;	6000 N !
PAR G(IONIC_LIQUID,SR+2:VA;0)	298.15
+GSRLIQ;	6000 N !
PAR G(IONIC_LIQUID,SR+2:O-2;0)	298.15
+2*GSROLIQ;	6000 N !
PAR G(IONIC_LIQUID,Y+3:VA)	298.15
+GYyliQ;	6000 N !
PAR G(IONIC_LIQUID,Y+3:O-2)	298.15 +2*GYyliQ+3*GHSEROO
-1824330+245.9*T;	6000 N !
PAR G(IONIC_LIQUID,ZR+4:VA)	298.15
+GZRLIQ;	6000 N !
PAR G(IONIC_LIQUID,ZR+4:O-2)	298.15
+2*GZRO2LIQ;	6000 N !
PAR L(IONIC_LIQUID,MN+2:O-2,VA;0)	298.15
+129519;	6000 N !
PAR L(IONIC_LIQUID,MN+2:O-2,VA;1)	298.15
-45459;	6000 N !
PAR L(IONIC_LIQUID,MN+2,MN+3:O-2;0)	298.15
-33859;	6000 N !
PAR L(IONIC_LIQUID,Y+3:O-2,VA;0)	298.15
+6900;	6000 N !
PAR L(IONIC_LIQUID,Y+3:O-2,VA;1)	298.15
-17000;	6000 N !
PAR L(IONIC_LIQUID,ZR+4:O-2,VA;0)	298.15
-26500;	6000 N !
PAR L(IONIC_LIQUID,ZR+4:O-2,VA;1)	298.15
+50000;	6000 N !
PAR L(IONIC_LIQUID,ZR+4:O-2,VA;2)	298.15
+72000;	6000 N !
PAR L(IONIC_LIQUID,LA+3,MN+2:O-2;0)	298.15
-119062;	6000 N !
PAR L(IONIC_LIQUID,LA+3,MN+3:O-2;0)	298.15
-119062;	6000 N !
PAR L(IONIC_LIQUID,LA+3,SR+2:O-2;0)	298.15
-8.891E+04;	6000 N !
PAR L(IONIC_LIQUID,LA+3,SR+2:O-2;1)	298.15
-7.368E+04;	6000 N !
PAR L(IONIC_LIQUID,LA+3,ZR+4:O-2;0)	298.15
-212088;	6000 N !
PAR L(IONIC_LIQUID,MN+2,SR+2:O-2;0)	298.15

-1.76300000E+05; 6000 N !
 PAR L(IONIC_LIQUID,MN+3,SR+2:O-2;0) 298.15
 -1.76300000E+05; 6000 N !
 PAR L(IONIC_LIQUID,MN+2,Y+3:VA;0) 298.15
 -26874.14+2.38277*T; 6000 N !
 PAR L(IONIC_LIQUID,MN+2,Y+3:VA;1) 298.15
 -12579.78; 6000 N !
 PAR L(IONIC_LIQUID,MN+2,ZR+4:VA;0) 298.15
 -45851.78+5.21718*T; 6000 N !
 PAR L(IONIC_LIQUID,MN+2,ZR+4:VA;1) 298.15
 -10658.06+9.26869*T; 6000 N !
 PAR L(IONIC_LIQUID,MN+2,ZR+4:VA;2) 298.15
 -11253.58; 6000 N !
 PAR L(IONIC_LIQUID,MN+2,ZR+4:O-2;0) 298.15
 -19432; 6000 N !
 PAR L(IONIC_LIQUID,MN+3,ZR+4:O-2;0) 298.15
 -19432; 6000 N !
 PAR L(IONIC_LIQUID,Y+3,ZR+4:VA;0) 298.15
 +24000; 6000 N !
 PAR L(IONIC_LIQUID,Y+3,ZR+4:VA;1) 298.15
 +3000; 6000 N !
 PAR L(IONIC_LIQUID,Y+3,ZR+4:O-2;0) 298.15
 +20100; 6000 N !
 PAR L(IONIC_LIQUID,Y+3,ZR+4:O-2;1) 298.15
 -13000; 6000 N !
 PAR L(IONIC_LIQUID,Y+3,ZR+4:O-2;2) 298.15
 -40000; 6000 N !
 \$
 PHASE LIQUID Z 1 1 !
 CONST LIQUID : LA MN SR Y ZR : !
 PAR G(LIQUID,LA) 298.15 +GLALIQ; 3200 N !
 PAR G(LIQUID,MN) 298.15 +GMNLIQ; 3000 N !
 PAR G(LIQUID,SR) 298.15 +GSRLIQ; 6000 N !
 PAR G(LIQUID,Y) 298.15 +GYYLIQ; 6000 N !
 PAR G(LIQUID,ZR) 298.15 +GZRLIQ; 6000 N !
 PAR L(LIQUID,MN,Y;0) 298.15 -26874.14+2.38277*T; 6000 N !
 PAR L(LIQUID,MN,Y;1) 298.15 -12579.78; 6000 N !
 PAR L(LIQUID,MN,ZR;0) 298.15 -45851.78+5.21718*T; 6000 N !
 PAR L(LIQUID,MN,ZR;1) 298.15 -10658.06+9.26869*T; 6000 N !
 PAR L(LIQUID,MN,ZR;2) 298.15 -11253.58; 6000 N !
 PAR L(LIQUID,Y,ZR;0) 298.15 +24000; 6000 N !
 PAR L(LIQUID,Y,ZR;1) 298.15 +3000; 6000 N !
 \$
 PHASE DHCP Z 2 1 0.5 !
 CONST DHCP : LA : VA% O : !

PAR G(DHCP,LA:VA) 298.15 +GHSERLA; 3200 N !
 PAR G(DHCP,LA:O) 298.15
 +GHSERLA+0.5*GHSEROO-285000+42.4*T; 3200 N !
 \$
 PHASE HCP_A3 Z 2 1 0.5 !
 CONST HCP_A3 : MN Y% ZR% : VA% O : !
 PAR G(HCP_A3,MN:VA) 298.15 +GMNHCP; 2000 N !
 PAR G(HCP_A3,MN:O) 298.15 +GMNHCP+0.5*GHSEROO; 6000 N !
 PAR G(HCP_A3,Y:VA) 298.15 +GHSERY; 3700 N !
 PAR G(HCP_A3,Y:O) 298.15 +GHSERY+0.5*GHSEROO
 -303600+37.5*T; 6000 N !
 PAR G(HCP_A3,ZR:VA) 298.15 +GHSERZR; 6000 N !
 PAR G(HCP_A3,ZR:O) 298.15 +GHSERZR+0.5*GHSEROO
 -280300+41*T; 6000 N !
 PAR L(HCP_A3,Y:O,VA;0) 298.15 +3500; 6000 N !
 PAR L(HCP_A3,ZR:O,VA;0) 298.15 -29100+15.5*T; 6000 N !
 PAR L(HCP_A3,ZR:O,VA;1) 298.15 -9150+3*T; 6000 N !
 PAR L(HCP_A3,MN,Y:VA;0) 298.15 +19000; 6000 N !
 PAR L(HCP_A3,MN,ZR:VA;0) 298.15 -8123.31; 6000 N !
 PAR L(HCP_A3,Y,ZR:VA;0) 298.15 +50000; 6000 N !
 \$
 PHASE BCC_A2 ZB 2 1 1.5 !
 CONST BCC_A2 : LA MN SR Y ZR : VA% O : !
 PAR G(BCC_A2,LA:VA) 298.15 +GLABCC; 3200 N !
 PAR G(BCC_A2,LA:O) 298.15
 +GLABCC+1.5*GHSEROO-855000+142.5*T; 3200 N !
 PAR G(BCC_A2,MN:VA) 298.15 +GMNBCC; 2000 N !
 PAR G(BCC_A2,MN:O) 298.15
 +GMNBCC+1.5*GHSEROO+50*T; 6000 N !
 PAR TC(BCC_A2,MN:VA) 298.15 -580; 2000 N !
 PAR BMAGN(BCC_A2,MN:VA) 298.15 -0.27; 2000 N !
 PAR G(BCC_A2,SR:VA;0) 298.15 +GSRBCC; 3000 N !
 PAR G(BCC_A2,SR:O;0) 298.15 +GSRBCC+GHSEROO; 3000 N !
 PAR G(BCC_A2,Y:VA) 298.15 +GYYBCC; 3700 N !
 PAR G(BCC_A2,Y:O) 298.15 +GYYBCC+1.5*GHSEROO
 -899200+123*T; 6000 N !
 PAR G(BCC_A2,ZR:VA) 298.15 +GZRBCC; 6000 N !
 PAR G(BCC_A2,ZR:O) 298.15 +GZRBCC+1.5*GHSEROO; 6000 N !
 PAR L(BCC_A2,Y:O,VA;0) 298.15 -5000; 3300 N !
 PAR L(BCC_A2,ZR:O,VA;0) 298.15 -1102000+155.4*T; 6000 N !
 PAR L(BCC_A2,ZR:O,VA;1) 298.15 -235000; 6000 N !
 PAR L(BCC_A2,MN,Y:VA;0) 298.15 +25000; 3300 N !
 PAR L(BCC_A2,MN,ZR:VA;0) 298.15 -54491.27+30.8108*T; 6000 N !
 PAR L(BCC_A2,MN,ZR:VA;1) 298.15 -6418.27+0.51346*T; 6000 N !
 PAR L(BCC_A2,Y,ZR:VA;0) 298.15 +40000; 6000 N !

PAR L(BCC_A2,Y,ZR:VA;1) 298.15 -9000; 6000 N !
 \$
 PHASE CBCC_A12 ZA 2 1 1 !
 CONST CBCC_A12 : MN : VA : !
 PAR G(CBCC_A12,MN:VA) 298.15 +GHSERMN; 2000 N !
 PAR TC(CBCC_A12,MN:VA) 298.15 -285; 2000 N !
 PAR BMAGN(CBCC_A12,MN:VA) 298.15 -0.66; 2000 N !
 \$
 PHASE FCC_A1 ZA 2 1 1 !
 CONST FCC_A1 : LA% MN% SR ZR : VA% O : !
 PAR G(FCC_A1,LA:VA) 298.15 +GLAFCC; 3200 N !
 PAR G(FCC_A1,LA:O) 298.15
 +GLAFCC+GHSEROO-570000+91.4*T; 3200 N !
 PAR G(FCC_A1,MN:VA) 298.15 +GMNFCC; 2000 N !
 PAR G(FCC_A1,MN:O) 298.15 +GMNFCC+GHSEROO; 2000 N !
 PAR TC(FCC_A1,MN:VA) 298.15 -1620; 2000 N !
 PAR BMAGN(FCC_A1,MN:VA) 298.15 -1.86; 2000 N !
 PAR G(FCC_A1,SR:VA;0) 298.15 +GHSERSR; 3000 N !
 PAR G(FCC_A1,SR:O;0) 298.15 +GHSERSR+GHSEROO; 3000 N !
 PAR G(FCC_A1,ZR:VA) 130.00 +GHSERZR+7600-0.9*T; 6000 N !
 PAR G(FCC_A1,ZR:O) 130.00
 +GHSERZR+7600-0.9*T+GHSEROO; 6000 N !
 PAR L(FCC_A1,MN,ZR:VA;0) 298.15 +5059.03-0.40472*T; 6000 N !
 PAR L(FCC_A1,MN,ZR:VA;1) 298.15 -26984.11+2.15873*T; 6000 N !
 \$
 PHASE CUB_A13 Z 2 1 1 !
 CONST CUB_A13 : MN : VA : !
 PAR G(CUB_A13,MN:VA) 298.15 +GMNCUB; 2000 N !
 \$
 PHASE MN12Y Z 2 12 1 !
 CONST MN12Y : MN : Y : !
 PAR G(MN12Y,MN:Y) 298.15 +GMN12Y; 2000 N !
 \$
 PHASE MN23Y6 Z 2 23 6 !
 CONST MN23Y6 : MN : Y : !
 PAR G(MN23Y6,MN:Y) 298.15 +GMN23Y6; 2000 N !
 \$
 PHASE MN2Y Z 2 2 1 !
 CONST MN2Y : MN : Y : !
 PAR G(MN2Y,MN:Y) 298.15 +GMN2Y; 2000 N !
 \$
 PHASE MN2ZR Z 2 2 1 !
 CONST MN2ZR : MN : ZR% VA : !
 PAR G(MN2ZR,MN:ZR) 298.15 +2*GHSERMN+GHSERZR
 -120013.95+36.9305*T; 6000 N !

PAR G(MN2ZR,MN:VA) 298.15 +2*GHSERMN+15000; 6000 N !
 PAR L(MN2ZR,MN:ZR,VA;0) 298.15 -2029.39+0.16235*T; 6000 N !
 \$
 PHASE LA2O3_A:I Z 3 2 3 1 !
 CONST LA2O3_A:I : LA LA+3% SR+2 Y+3 ZR+4 : O-2% VA : O-2 VA% : !
 PAR G(LA2O3_A,LA:VA:VA) 298.15 +2*GHSERLA+204124; 6000 N !
 PAR G(LA2O3_A,LA:O-2:O-2) 298.15
 +2*GHSERLA+4*GHSEROO+304124+15.87691*T; 6000 N !
 PAR G(LA2O3_A,LA:O-2:VA) 298.15
 +2*GHSERLA+3*GHSEROO+204124; 6000 N !
 PAR G(LA2O3_A,LA:VA:O-2) 298.15
 +2*GHSERLA+GHSEROO+304124+15.87691*T; 6000 N !
 PAR G(LA2O3_A,LA+3:O-2:VA) 298.15 +GLA2O3A; 6000 N !
 PAR G(LA2O3_A,LA+3:VA:VA) 298.15 +GLA2O3A-3*GHSEROO; 6000 N
 !
 PAR G(LA2O3_A,LA+3:VA:O-2) 298.15
 +GLA2O3A-2*GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(LA2O3_A,LA+3:O-2:O-2) 298.15
 +GLA2O3A+GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(LA2O3_A,SR+2:O-2:VA;0) 298.15
 +SR_ALPHA+GHSEROO+15.87691*T; 6000 N !
 PAR G(LA2O3_A,SR+2:VA:VA;0) 298.15
 +SR_ALPHA-2*GHSEROO+15.87691*T; 6000 N !
 PAR G(LA2O3_A,SR+2:O-2:O-2;0) 298.15
 +SR_ALPHA+GHSEROO+15.87691*T+GHSEROO+100000+15.87691*T;
 6000 N !
 PAR G(LA2O3_A,SR+2:VA:O-2;0) 298.15
 +SR_ALPHA-2*GHSEROO+15.87691*T+GHSEROO+100000+15.87691*T;
 6000 N !
 PAR G(LA2O3_A,Y+3:O-2:VA) 298.15 +2*GAAYO15; 6000 N !
 PAR G(LA2O3_A,Y+3:VA:VA) 298.15 +2*GAAYO15-3*GHSEROO; 6000 N
 !
 PAR G(LA2O3_A,Y+3:VA:O-2) 298.15
 +2*GAAYO15-2*GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(LA2O3_A,Y+3:O-2:O-2) 298.15
 +2*GAAYO15+GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(LA2O3_A,ZR+4:VA:VA) 298.15
 +2*GMAZRO2-4*GHSEROO-100000-15.87691*T; 6000 N !
 PAR G(LA2O3_A,ZR+4:O-2:O-2) 298.15 +2*GMAZRO2; 6000 N !
 PAR G(LA2O3_A,ZR+4:O-2:VA) 298.15
 +2*GMAZRO2-GHSEROO-100000-15.87691*T; 6000 N !
 PAR G(LA2O3_A,ZR+4:VA:O-2) 298.15 +2*GMAZRO2-3*GHSEROO; 6000
 N !
 PAR L(LA2O3_A,LA+3,SR+2:O-2:O-2;0) 298.15 +2.149E+05-7.81E+01*T; 6000 N !
 PAR L(LA2O3_A,LA+3,SR+2:O-2:VA;0) 298.15 +2.149E+05-7.81E+01*T; 6000 N !

PAR L(LA2O3_A,LA+3,SR+2:VA:O-2;0) 298.15 +2.149E+05-7.81E+01*T; 6000 N !
 PAR L(LA2O3_A,LA+3,SR+2:VA:VA;0) 298.15 +2.149E+05-7.81E+01*T; 6000 N !
 !
 PAR L(LA2O3_A,LA+3,Y+3:O-2:O-2;0) 298.15 +36269; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:O-2:VA;0) 298.15 +36269; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:VA:O-2;0) 298.15 +36269; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:VA:VA;0) 298.15 +36269; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:O-2:O-2;1) 298.15 +18981; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:O-2:VA;1) 298.15 +18981; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:VA:O-2;1) 298.15 +18981; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:VA:VA;1) 298.15 +18981; 6000 N !
 PAR L(LA2O3_A,LA+3,ZR+4:VA:VA;0) 298.15 -101793; 6000 N !
 PAR L(LA2O3_A,LA+3,ZR+4:O-2:O-2;0) 298.15 -101793; 6000 N !
 PAR L(LA2O3_A,LA+3,ZR+4:O-2:VA;0) 298.15 -101793; 6000 N !
 PAR L(LA2O3_A,LA+3,ZR+4:VA:O-2;0) 298.15 -101793; 6000 N !
 \$
 PHASE LA2O3_B:I Z 3 2 3 1 !
 CONST LA2O3_B:I : LA+3 Y+3 : O-2% VA : O-2 VA% : !
 PAR G(LA2O3_B,LA+3:O-2:VA) 298.15 +GLA2O3B; 6000 N !
 PAR G(LA2O3_B,LA+3:VA:VA) 298.15 +GLA2O3B-3*GHSEROO; 6000 N !
 !
 PAR G(LA2O3_B,LA+3:VA:O-2) 298.15
 +GLA2O3B-2*GHSEROO+15.87691*T+100000; 6000 N !
 PAR G(LA2O3_B,LA+3:O-2:O-2) 298.15
 +GLA2O3B+GHSEROO+15.87691*T+100000; 6000 N !
 PAR G(LA2O3_B,Y+3:O-2:VA) 298.15 +2*GBBYO15; 6000 N !
 PAR G(LA2O3_B,Y+3:VA:VA) 298.15 +2*GBBYO15-3*GHSEROO; 6000 N !
 !
 PAR G(LA2O3_B,Y+3:VA:O-2) 298.15
 +2*GBBYO15-2*GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(LA2O3_B,Y+3:O-2:O-2) 298.15
 +2*GBBYO15+GHSEROO+100000+15.87691*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:O-2:O-2;0) 298.15 -21475+26.2*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:O-2:VA;0) 298.15 -21475+26.2*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:VA:O-2;0) 298.15 -21475+26.2*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:VA:VA;0) 298.15 -21475+26.2*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:O-2:O-2;1) 298.15 -60190+31.5*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:O-2:VA;1) 298.15 -60190+31.5*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:VA:O-2;1) 298.15 -60190+31.5*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:VA:VA;1) 298.15 -60190+31.5*T; 6000 N !
 \$
 PHASE MNO:I Z 2 1 1 !
 CONST MNO:I : MN+2% MN+3 VA : O-2 : !
 PAR G(MNO,MN+2:O-2) 298.15 +GMNO; 6000 N !
 PAR G(MNO,MN+3:O-2) 298.15 +GMNO-21884-22.185*T; 6000 N !

PAR G(MNO,VA:O-2) 298.15 0; 6000 N !
 PAR L(MNO,MN+2,MN+3:O-2;0) 298.15 -42105; 6000 N !
 PAR L(MNO,MN+2,MN+3:O-2;1) 298.15 +46513; 6000 N !
 \$
 PHASE MN3O4_ALPHA:I Z 3 1 2 4 !
 CONST MN3O4_ALPHA:I : MN+2 : MN+3 : O-2 : !
 PAR G(MN3O4_ALPHA,MN+2:MN+3:O-2) 298.15 +GMN3O4; 6000 N !
 \$
 PHASE MN3O4_BETA:I Z 3 1 2 4 !
 CONST MN3O4_BETA:I : MN+2 : MN+3 : O-2 : !
 PAR G(MN3O4_BETA,MN+2:MN+3:O-2) 298.15 +GMN3O4B; 6000 N !
 \$
 PHASE MNO2:I Z 2 1 2 !
 CONST MNO2:I : MN+4 : O-2 : !
 PAR G(MNO2,MN+4:O-2) 298.15 +GMNO2; 6000 N !
 \$ SrO with La2O3 solubility
 PHASE SRO:I Z 2 1 1 !
 CONST SRO:I : LA+3 SR+2 VA : O-2 : !
 PAR G(SRO,SR+2:O-2;0) 298.15 +GSROSOL; 6000 N !
 PAR G(SRO,LA+3:O-2;0) 298.15 +0.5*GLA2O3A+1.137E+05; 6000 N !
 PAR G(SRO,VA:O-2;0) 298.15 0; 6000 N !
 \$
 PHASE SRO2:I Z 2 1 2 !
 CONST SRO2:I : SR : O : !
 PAR G(SRO2,SR:O;0) 298.15 +GSRO2SOL; 6000 N !
 \$
 PHASE Y2O3_CUB:I Z 3 2 3 1 !
 CONST Y2O3_CUB:I : LA+3 MN+3% Y Y+3% ZR+4 : O-2% VA : O-2 VA% : !
 \$ This is essentially an ordered fluorite structure
 \$ This is also Mn2O3
 PAR G(Y2O3_CUB,LA+3:O-2:VA) 298.15 +GLA2O3C; 6000 N !
 PAR G(Y2O3_CUB,LA+3:VA:VA) 298.15 +GLA2O3C-3*GHSEROO; 6000 N !
 !
 PAR G(Y2O3_CUB,LA+3:VA:O-2) 298.15
 +GLA2O3C-2*GHSEROO+15.87691*T+100000; 6000 N !
 PAR G(Y2O3_CUB,LA+3:O-2:O-2) 298.15
 +GLA2O3C+GHSEROO+15.87691*T+100000; 6000 N !
 PAR G(Y2O3_CUB,MN+3:O-2:VA) 298.15 +GMN2O3; 6000 N !
 PAR G(Y2O3_CUB,MN+3:VA:VA) 298.15 +GMN2O3-3*GHSEROO; 6000 N !
 !
 PAR G(Y2O3_CUB,MN+3:VA:O-2) 298.15 +GMN2O3-2*GHSEROO
 +15.87691*T+100000; 6000 N !
 PAR G(Y2O3_CUB,MN+3:O-2:O-2) 298.15 +GMN2O3+GHSEROO
 +15.87691*T+100000; 6000 N !
 PAR G(Y2O3_CUB,Y:VA:VA) 298.15 +2*GHSERY+245600; 6000 N !

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PAR G(Y2O3_CUB,Y:O-2:O-2)      298.15 +2*GHSERYYY+245600
      +4*GHSEROO+100000+15.87691*T;      6000 N !
PAR G(Y2O3_CUB,Y:O-2:VA)      298.15 +2*GHSERYYY+245600
      +3*GHSEROO;      6000 N !
PAR G(Y2O3_CUB,Y:VA:O-2)      298.15 +2*GHSERYYY+245600
      +GHSEROO+100000+15.87691*T;      6000 N !
PAR G(Y2O3_CUB,Y+3:O-2:VA)      298.15 +2*GCCYO15;      6000 N !
PAR G(Y2O3_CUB,Y+3:VA:VA)      298.15 +2*GCCYO15-3*GHSEROO; 6000 N
!
PAR G(Y2O3_CUB,Y+3:VA:O-2)      298.15 +2*GCCYO15-2*GHSEROO
      +15.87691*T+100000;      6000 N !
PAR G(Y2O3_CUB,Y+3:O-2:O-2)      298.15 +2*GCCYO15+GHSEROO
      +15.87691*T+100000;      6000 N !
PAR G(Y2O3_CUB,ZR+4:VA:VA)      298.15 +2*GMCZRO2-4*GHSEROO
      -100000-15.87691*T;      6000 N !
PAR G(Y2O3_CUB,ZR+4:O-2:O-2)      298.15 +2*GMCZRO2;      6000 N !
PAR G(Y2O3_CUB,ZR+4:O-2:VA)      298.15 +2*GMCZRO2-GHSEROO
      -100000-15.87691*T;      6000 N !
PAR G(Y2O3_CUB,ZR+4:VA:O-2)      298.15 +2*GMCZRO2-3*GHSEROO; 6000
N !
PAR L(Y2O3_CUB,LA+3,Y+3:O-2:O-2;0) 298.15 +31866;      6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:O-2:VA;0) 298.15 +31866;      6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:VA:O-2;0) 298.15 +31866;      6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:VA:VA;0) 298.15 +31866;      6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:O-2:O-2;1) 298.15 +29838;      6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:O-2:VA;1) 298.15 +29838;      6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:VA:O-2;1) 298.15 +29838;      6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:VA:VA;1) 298.15 +29838;      6000 N !
PAR L(Y2O3_CUB,MN+3,Y+3:VA:VA;0) 298.15 +100000;      6000 N !
PAR L(Y2O3_CUB,MN+3,Y+3:O-2:O-2;0) 298.15 +100000;      6000 N !
PAR L(Y2O3_CUB,MN+3,Y+3:O-2:VA;0) 298.15 +100000;      6000 N !
PAR L(Y2O3_CUB,MN+3,Y+3:VA:O-2;0) 298.15 +100000;      6000 N !
PAR L(Y2O3_CUB,MN+3,ZR+4:VA:VA;0) 298.15 +100000;      6000 N !
PAR L(Y2O3_CUB,MN+3,ZR+4:O-2:O-2;0) 298.15 +100000;      6000 N !
PAR L(Y2O3_CUB,MN+3,ZR+4:O-2:VA;0) 298.15 +100000;      6000 N !
PAR L(Y2O3_CUB,MN+3,ZR+4:VA:O-2;0) 298.15 +100000;      6000 N !
PAR L(Y2O3_CUB,Y+3,ZR+4:VA:VA;0) 298.15 -88700+13*T;      6000 N !
PAR L(Y2O3_CUB,Y+3,ZR+4:O-2:O-2;0) 298.15 -88700+13*T;      6000 N !
PAR L(Y2O3_CUB,Y+3,ZR+4:O-2:VA;0) 298.15 -88700+13*T;      6000 N !
PAR L(Y2O3_CUB,Y+3,ZR+4:VA:O-2;0) 298.15 -88700+13*T;      6000 N !
$
PHASE Y2O3_HEX:I Z 3 2 3 1 !
CONST Y2O3_HEX:I : LA LA+3% MN+3 SR+2 Y Y+3% ZR+4 : O-2% VA : O-2 VA%
: !
$ This is beta-Y2O3 (alias H-Y2O3)

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\$ This is also H-La2O3

PAR G(Y2O3_HEX,LA:VA:VA) 298.15 +2*GHSERLA+204124; 6000 N !
PAR G(Y2O3_HEX,LA:O-2:O-2) 298.15
+2*GHSERLA+4*GHSEROO+304124+15.87691*T; 6000 N !
PAR G(Y2O3_HEX,LA:O-2:VA) 298.15
+2*GHSERLA+3*GHSEROO+204124; 6000 N !
PAR G(Y2O3_HEX,LA:VA:O-2) 298.15
+2*GHSERLA+GHSEROO+304124+15.87691*T; 6000 N !
PAR G(Y2O3_HEX,LA+3:O-2:VA) 298.15 +GLA2O3H; 6000 N !
PAR G(Y2O3_HEX,LA+3:VA:VA) 298.15 +GLA2O3H-3*GHSEROO; 6000 N !
PAR G(Y2O3_HEX,LA+3:VA:O-2) 298.15
+GLA2O3H-2*GHSEROO+100000+15.87691*T; 6000 N !
PAR G(Y2O3_HEX,LA+3:O-2:O-2) 298.15
+GLA2O3H+GHSEROO+100000+15.87691*T; 6000 N !
PAR G(Y2O3_HEX,MN+3:O-2:VA) 298.15 +GMHNM2O3; 6000 N !
PAR G(Y2O3_HEX,MN+3:VA:VA) 298.15 +GMHNM2O3-3*GHSEROO; 6000 N !
PAR G(Y2O3_HEX,MN+3:VA:O-2) 298.15 +GMHNM2O3-2*GHSEROO
+15.87691*T+100000; 6000 N !
PAR G(Y2O3_HEX,MN+3:O-2:O-2) 298.15 +GMHNM2O3+GHSEROO
+15.87691*T+100000; 6000 N !
PAR G(Y2O3_HEX,SR+2:O-2:VA;0) 298.15
+SRH_ALPH+GHSEROO+15.87691*T; 6000 N !
PAR G(Y2O3_HEX,SR+2:VA:VA;0) 298.15
+SRH_ALPH-2*GHSEROO+15.87691*T; 6000 N !
PAR G(Y2O3_HEX,SR+2:O-2:O-2;0) 298.15
+SRH_ALPH+GHSEROO+15.87691*T+GHSEROO+100000+15.87691*T; 6000 N !
PAR G(Y2O3_HEX,SR+2:VA:O-2;0) 298.15
+SRH_ALPH-2*GHSEROO+15.87691*T+GHSEROO+100000+15.87691*T;
6000 N !
PAR G(Y2O3_HEX,Y:VA:VA) 298.15 +2*GHSERYY+245600; 6000 N !
PAR G(Y2O3_HEX,Y:O-2:O-2) 298.15 +2*GHSERYY+245600
+4*GHSEROO+100000+15.87691*T; 6000 N !
PAR G(Y2O3_HEX,Y:O-2:VA) 298.15 +2*GHSERYY+245600
+3*GHSEROO; 6000 N !
PAR G(Y2O3_HEX,Y:VA:O-2) 298.15 +2*GHSERYY+245600
+GHSEROO+100000+15.87691*T; 6000 N !
PAR G(Y2O3_HEX,Y+3:O-2:VA) 298.15 +2*GHHYO15; 6000 N !
PAR G(Y2O3_HEX,Y+3:VA:VA) 298.15 +2*GHHYO15-3*GHSEROO; 6000 N !
PAR G(Y2O3_HEX,Y+3:VA:O-2) 298.15 +2*GHHYO15-2*GHSEROO
+15.87691*T+100000; 6000 N !
PAR G(Y2O3_HEX,Y+3:O-2:O-2) 298.15 +2*GHHYO15+GHSEROO

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+15.87691*T+100000;                                6000 N !
PAR G(Y2O3_HEX,ZR+4:VA:VA)    298.15 +2*GMHZRO2-4*GHSEROO
-100000-15.87691*T;                                6000 N !
PAR G(Y2O3_HEX,ZR+4:O-2:O-2)  298.15 +2*GMHZRO2;          6000 N !
PAR G(Y2O3_HEX,ZR+4:O-2:VA)   298.15 +2*GMHZRO2-GHSEROO
-100000-15.87691*T;                                6000 N !
PAR G(Y2O3_HEX,ZR+4:VA:O-2)   298.15 +2*GMHZRO2-3*GHSEROO; 6000
N !
PAR L(Y2O3_HEX,LA+3,SR+2:O-2:O-2;0) 298.15 1.936E+05-7.81E+01*T; 6000 N !
PAR L(Y2O3_HEX,LA+3,SR+2:O-2:VA;0) 298.15 1.936E+05-7.81E+01*T; 6000 N !
PAR L(Y2O3_HEX,LA+3,SR+2:VA:O-2;0) 298.15 1.936E+05-7.81E+01*T; 6000 N !
PAR L(Y2O3_HEX,LA+3,SR+2:VA:VA;0) 298.15 1.936E+05-7.81E+01*T; 6000 N
!
PAR L(Y2O3_HEX,LA+3,Y+3:O-2:O-2;0) 298.15 +27920;          6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:O-2:VA;0) 298.15 +27920;          6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:VA:O-2;0) 298.15 +27920;          6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:VA:VA;0) 298.15 +27920;          6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:O-2:O-2;1) 298.15 +12879;          6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:O-2:VA;1) 298.15 +12879;          6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:VA:O-2;1) 298.15 +12879;          6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:VA:VA;1) 298.15 +12879;          6000 N !
PAR L(Y2O3_HEX,LA+3,ZR+4:VA:VA;0) 298.15 -144923;          6000 N !
PAR L(Y2O3_HEX,LA+3,ZR+4:O-2:O-2;0) 298.15 -144923;          6000 N !
PAR L(Y2O3_HEX,LA+3,ZR+4:O-2:VA;0) 298.15 -144923;          6000 N !
PAR L(Y2O3_HEX,LA+3,ZR+4:VA:O-2;0) 298.15 -144923;          6000 N !
PAR L(Y2O3_HEX,MN+3,Y+3:VA:VA;0) 298.15 +100000;          6000 N !
PAR L(Y2O3_HEX,MN+3,Y+3:O-2:O-2;0) 298.15 +100000;          6000 N !
PAR L(Y2O3_HEX,MN+3,Y+3:O-2:VA;0) 298.15 +100000;          6000 N !
PAR L(Y2O3_HEX,MN+3,Y+3:VA:O-2;0) 298.15 +100000;          6000 N !
$
PHASE ZRO2_MONO:I Z 2 1 2 !
CONST ZRO2_MONO:I : Y+3 ZR+4% : O-2% VA : !
PAR G(ZRO2_MONO,Y+3:O-2)    298.15 +GMMYO15+0.5*GHSEROO
+9.3511*T;                    6000 N !
PAR G(ZRO2_MONO,Y+3:VA)    298.15 +GMMYO15-1.5*GHSEROO
+9.3511*T;                    6000 N !
PAR G(ZRO2_MONO,ZR+4:O-2)  298.15 +GMMZRO2;          6000 N !
PAR G(ZRO2_MONO,ZR+4:VA)   298.15 +GMMZRO2-2*GHSEROO; 6000 N
!
$
PHASE ZRO2_TETR:I Z 2 1 2 !
CONST ZRO2_TETR:I : LA+3 MN+2 MN+3 Y+3 ZR+4% : O-2% VA : !
PAR G(ZRO2_TETR,LA+3:O-2)    298.15
+0.5*GMTLA2O3+0.5*GHSEROO+9.3511*T;          6000 N !
PAR G(ZRO2_TETR,LA+3:VA)    298.15

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+0.5*GMTLA2O3-1.5*GHSEROO+9.3511*T; 6000 N !
 PAR G(ZRO2_TETR,MN+2:O-2) 298.15 +GMTMNO+GHSEROO
 +11.5264*T; 6000 N !
 PAR G(ZRO2_TETR,MN+2:VA) 298.15 +GMTMNO-GHSEROO
 +11.5264*T; 6000 N !
 PAR G(ZRO2_TETR,MN+3:O-2) 298.15 +0.5*GMTMN2O3+0.5*GHSEROO
 +9.3511*T; 6000 N !
 PAR G(ZRO2_TETR,MN+3:VA) 298.15 +0.5*GMTMN2O3-1.5*GHSEROO
 +9.3511*T; 6000 N !
 PAR G(ZRO2_TETR,Y+3:O-2) 298.15 +GMTYO15+0.5*GHSEROO
 +9.3511*T; 6000 N !
 PAR G(ZRO2_TETR,Y+3:VA) 298.15 +GMTYO15-1.5*GHSEROO
 +9.3511*T; 6000 N !
 PAR G(ZRO2_TETR,ZR+4:O-2) 298.15 +GTTZRO2; 6000 N !
 PAR G(ZRO2_TETR,ZR+4:VA) 298.15 +GTTZRO2-2*GHSEROO; 6000 N !
 PAR L(ZRO2_TETR,LA+3,ZR+4:O-2;0) 298.15 -23609; 6000 N !
 PAR L(ZRO2_TETR,LA+3,ZR+4:VA;0) 298.15 -23609; 6000 N !
 PAR L(ZRO2_TETR,MN+2,ZR+4:O-2;0) 298.15 +20863; 6000 N !
 PAR L(ZRO2_TETR,MN+2,ZR+4:VA;0) 298.15 +20863; 6000 N !
 PAR L(ZRO2_TETR,MN+3,ZR+4:O-2;0) 298.15 +20863; 6000 N !
 PAR L(ZRO2_TETR,MN+3,ZR+4:VA;0) 298.15 +20863; 6000 N !
 PAR L(ZRO2_TETR,Y+3,ZR+4:O-2;0) 298.15 -48800+18.4*T; 6000 N !
 PAR L(ZRO2_TETR,Y+3,ZR+4:VA;0) 298.15 -48800+18.4*T; 6000 N !
 \$
 PHASE ZRO2_CUB:I Z 2 1 2 !
 CONST ZRO2_CUB:I : LA LA+3% MN+2 MN+3 SR+2 Y Y+3% ZR ZR+4% : O-2 VA
 : !
 \$ This is also X-La2O3
 PAR G(ZRO2_CUB,LA:O-2) 298.15
 +GHSERLA+2*GHSEROO+102062; 6000 N !
 PAR G(ZRO2_CUB,LA:VA) 298.15 +GHSERLA+102062; 6000 N !
 PAR G(ZRO2_CUB,LA+3:O-2) 298.15
 +0.5*GLA2O3X+0.5*GHSEROO+9.3511*T; 6000 N !
 PAR G(ZRO2_CUB,LA+3:VA) 298.15
 +0.5*GLA2O3X-1.5*GHSEROO+9.3511*T; 6000 N !
 PAR G(ZRO2_CUB,MN+2:O-2) 298.15 +GMFMNO+GHSEROO
 +11.5264*T; 6000 N !
 PAR G(ZRO2_CUB,MN+2:VA) 298.15 +GMFMNO-GHSEROO
 +11.5264*T; 6000 N !
 PAR G(ZRO2_CUB,MN+3:O-2) 298.15 +0.5*GMFMN2O3+0.5*GHSEROO
 +9.3511*T; 6000 N !
 PAR G(ZRO2_CUB,MN+3:VA) 298.15 +0.5*GMFMN2O3-1.5*GHSEROO
 +9.3511*T; 6000 N !
 PAR G(ZRO2_CUB,SR+2:O-2) 298.15
 +0.5*SRX_ALPH+GHSEROO+11.5264*T; 6000 N !

PAR G(ZRO2_CUB,SR+2:VA) 298.15
 +0.5*SRX_ALPH-GHSEROO+11.5264*T; 6000 N !
 PAR G(ZRO2_CUB,Y:O-2) 298.15 +GHSERY+2*GHSEROO
 +122800; 6000 N !
 PAR G(ZRO2_CUB,Y:VA) 298.15 +GHSERY+122800; 6000 N !
 PAR G(ZRO2_CUB,Y+3:O-2) 298.15 +GXXYO15+0.5*GHSEROO
 +9.3511*T; 6000 N !
 PAR G(ZRO2_CUB,Y+3:VA) 298.15 +GXXYO15-1.5*GHSEROO
 +9.3511*T; 6000 N !
 PAR G(ZRO2_CUB,ZR:O-2) 298.15 +100000+GHSERZR
 +2*GHSEROO; 6000 N !
 PAR G(ZRO2_CUB,ZR:VA) 298.15 +100000+GHSERZR; 6000 N !
 PAR G(ZRO2_CUB,ZR+4:O-2) 298.15 +GFFZRO2; 6000 N !
 PAR G(ZRO2_CUB,ZR+4:VA) 298.15 +GFFZRO2-2*GHSEROO; 6000 N !
 PAR L(ZRO2_CUB,ZR,ZR+4:O-2;0) 298.15 -66500-1.6*T; 6000 N !
 PAR L(ZRO2_CUB,ZR,ZR+4:VA;0) 298.15 -66500-1.6*T; 6000 N !
 PAR L(ZRO2_CUB,ZR,ZR+4:O-2;1) 298.15 -20000-42*T; 6000 N !
 PAR L(ZRO2_CUB,ZR,ZR+4:VA;1) 298.15 -20000-42*T; 6000 N !
 \$ To keep no MnOx solubility in X-La2O3
 PAR L(ZRO2_CUB,LA+3,MN+2:O-2;0) 298.15 +30000; 6000 N !
 PAR L(ZRO2_CUB,LA+3,MN+2:VA;0) 298.15 +30000; 6000 N !
 PAR L(ZRO2_CUB,LA+3,MN+3:O-2;0) 298.15 +30000; 6000 N !
 PAR L(ZRO2_CUB,LA+3,MN+3:VA;0) 298.15 +30000; 6000 N !
 PAR L(ZRO2_CUB,LA+3,SR+2:O-2;0) 298.15 +1.687E+05-7.81E+01*T; 6000 N !
 PAR L(ZRO2_CUB,LA+3,SR+2:VA;0) 298.15 +1.687E+05-7.81E+01*T; 6000 N !
 PAR L(ZRO2_CUB,LA+3,SR+2:O-2;1) 298.14 -2E+04; 6000 N !
 PAR L(ZRO2_CUB,LA+3,SR+2:VA;1) 298.14 -2E+04; 6000 N !
 PAR L(ZRO2_CUB,LA+3,Y+3:O-2;0) 298.15 +8527; 6000 N !
 PAR L(ZRO2_CUB,LA+3,Y+3:VA;0) 298.15 +8527; 6000 N !
 PAR L(ZRO2_CUB,LA+3,ZR+4:O-2;0) 298.15 +27621-32.2*T; 6000 N !
 PAR L(ZRO2_CUB,LA+3,ZR+4:VA;0) 298.15 +27621-32.2*T; 6000 N !
 PAR L(ZRO2_CUB,LA+3,ZR+4:O-2;1) 298.15 -17671; 6000 N !
 PAR L(ZRO2_CUB,LA+3,ZR+4:VA;1) 298.15 -17671; 6000 N !
 PAR L(ZRO2_CUB,MN+2,Y+3:O-2;0) 298.15 +30000; 6000 N !
 PAR L(ZRO2_CUB,MN+2,Y+3:VA;0) 298.15 +30000; 6000 N !
 PAR L(ZRO2_CUB,MN+3,Y+3:O-2;0) 298.15 +30000; 6000 N !
 PAR L(ZRO2_CUB,MN+3,Y+3:VA;0) 298.15 +30000; 6000 N !
 PAR L(ZRO2_CUB,MN+2,ZR+4:O-2;0) 298.15 +60656; 6000 N !
 PAR L(ZRO2_CUB,MN+2,ZR+4:VA;0) 298.15 +60656; 6000 N !
 PAR L(ZRO2_CUB,MN+2,ZR+4:O-2;1) 298.15 +64538; 6000 N !
 PAR L(ZRO2_CUB,MN+2,ZR+4:VA;1) 298.15 +64538; 6000 N !
 PAR L(ZRO2_CUB,MN+3,ZR+4:O-2;0) 298.15 +51416; 6000 N !
 PAR L(ZRO2_CUB,MN+3,ZR+4:VA;0) 298.15 +51416; 6000 N !
 PAR L(ZRO2_CUB,MN+3,ZR+4:O-2;1) 298.15 +43282; 6000 N !
 PAR L(ZRO2_CUB,MN+3,ZR+4:VA;1) 298.15 +43282; 6000 N !

PAR L(ZRO2_CUB,Y+3,ZR+4:O-2;0) 298.15 -84750+34.41*T; 6000 N !
 PAR L(ZRO2_CUB,Y+3,ZR+4:VA;0) 298.15 -84750+34.41*T; 6000 N !
 PAR L(ZRO2_CUB,Y+3,ZR+4:O-2;1) 298.15 +29880-7.69*T; 6000 N !
 PAR L(ZRO2_CUB,Y+3,ZR+4:VA;1) 298.15 +29880-7.69*T; 6000 N !
 PAR L(ZRO2_CUB,MN+2,Y+3,ZR+4:O-2;0) 298.15 -141939; 6000 N !
 PAR L(ZRO2_CUB,MN+2,Y+3,ZR+4:VA;0) 298.15 -141939; 6000 N !
 PAR L(ZRO2_CUB,MN+3,Y+3,ZR+4:O-2;0) 298.15 -141939; 6000 N !
 PAR L(ZRO2_CUB,MN+3,Y+3,ZR+4:VA;0) 298.15 -141939; 6000 N !
 \$
 PHASE L2MNO4:I Z 3 2 1 4 !
 CONST L2MNO4:I : LA+3 : MN+2 : O-2 : !
 PAR G(L2MNO4,LA+3:MN+2:O-2) 298.15 +GL2MNO4; 6000 N !
 \$
 PHASE BETA:I Z 2 2 3 !
 CONST BETA:I : LA+3 SR+2 : O-2 VA : !
 PAR G(BETA,LA+3:O-2;0) 298.15 +LA_BETA; 6000 N !
 PAR G(BETA,LA+3:VA;0) 298.15 +LA_BETA-3*GHSEROO; 6000 N !
 PAR G(BETA,SR+2:O-2;0) 298.15
 +SR_ALPHA+4.161E+05+GHSEROO+15.87691*T; 6000 N !
 PAR G(BETA,SR+2:VA;0) 298.15
 +SR_ALPHA+4.161E+05-2*GHSEROO+15.87691*T; 6000 N !
 PAR L(BETA,LA+3,SR+2:O-2;0) 298.15 -1.21E+05-2.378E+02*T; 6000 N !
 PAR L(BETA,LA+3,SR+2:VA;0) 298.15 -1.21E+05-2.378E+02*T; 6000 N !
 \$
 PHASE LA4SR3O9:I Z 3 4 3 9 !
 CONST LA4SR3O9:I : LA+3 : SR+2 : O-2 : !
 PAR G(LA4SR3O9,LA+3:SR+2:O-2;0) 298.15
 +2*GLA2O3A+3*GSROSOL+2.298E+05-1.3675E+02*T; 6000 N !
 \$
 PHASE LAYO3:I Z 3 1 1 3 !
 CONST LAYO3:I : LA+3 : Y+3 : O-2 : !
 PAR G(LAYO3,LA+3:Y+3:O-2) 298.15 +GLAYO3; 6000 N !
 \$ La2Zr2O7
 PHASE RLZO:I Z 3 2 2 7 !
 CONST RLZO:I : LA+3 : ZR+4 : O-2 : !
 PAR G(RLZO,LA+3:ZR+4:O-2) 298.15 +GLZOC; 6000 N !
 \$ C2
 PHASE C2:I Z 3 2 1 5 !
 CONST C2:I : LA+3 : ZR+4 : O-2 : !
 PAR G(C2,LA+3:ZR+4:O-2) 298.15 +GC2; 6000 N !
 \$
 PHASE SRMN3O6:I Z 5 1 2 3 1 3 !
 CONST SRMN3O6:I : SR+2 : MN+3 : O-2 : MN+3 MN+4 : O-2 VA : !
 PAR G(SRMN3O6,SR+2:MN+3:O-2:MN+4:O-2;0) 298.15 GSM4OZ; 6000 N !

PAR G(SRMN3O6,SR+2:MN+3:O-2:MN+4:VA;0) 298.15 GSM4OZ-3*GHSEROO;
 6000 N !
 PAR G(SRMN3O6,SR+2:MN+3:O-2:MN+3:O-2;0) 298.15
 +GSM3OZ+0.5*GHSEROO+11.23859*T; 6000 N !
 PAR G(SRMN3O6,SR+2:MN+3:O-2:MN+3:VA;0) 298.15
 +GSM3OZ-2.5*GHSEROO+11.23859*T; 6000 N !
 \$
 PHASE SR7MN4O15:I Z 3 7 4 15 !
 CONST SR7MN4O15:I : SR+2 : MN+4 : O-2 : !
 PAR G(SR7MN4O15,SR+2:MN+4:O-2;0) 298.15 +GS7M4; 6000 N !
 \$
 PHASE SR4MN3O10:I Z 3 4 3 10 !
 CONST SR4MN3O10:I : SR+2 : MN+4 : O-2 : !
 PAR G(SR4MN3O10,SR+2:MN+4:O-2;0) 298.15 +GSM4_RP3; 6000 N !
 \$
 PHASE SRMNO3_HEX:I Z 3 1 1 3 !
 CONST SRMNO3_HEX:I : SR+2 : MN+3 MN+4 : O-2 VA : !
 PAR G(SRMNO3_HEX,SR+2:MN+4:O-2;0) 298.15 GSM4_HEX; 6000 N !
 PAR G(SRMNO3_HEX,SR+2:MN+4:VA;0) 298.15 GSM4_HEX-3*GHSEROO;
 6000 N !
 PAR G(SRMNO3_HEX,SR+2:MN+3:O-2;0) 298.15
 +GSM3_HEX+0.5*GHSEROO+11.23859*T; 6000 N !
 PAR G(SRMNO3_HEX,SR+2:MN+3:VA;0) 298.15
 +GSM3_HEX-2.5*GHSEROO+11.23859*T; 6000 N !
 \$ SrZrO3
 PHASE SZO:I Z 3 1 1 3 !
 CONST SZO:I : SR+2 : ZR+4 : O-2 : !
 PAR G(SZO,SR+2:ZR+4:O-2;0) 298.15 +GSZOF; 6000 N !
 \$
 PHASE YMNO3H:I Z 3 1 1 3 !
 CONST YMNO3H:I : Y+3 : MN+3 : O-2 : !
 PAR G(YMNO3H,Y+3:MN+3:O-2) 298.15 +GYMNO3H; 6000 N !
 \$
 PHASE YMN2O5:I Z 4 1 1 1 5 !
 CONST YMN2O5:I : Y+3 : MN+3 : MN+4 : O-2 : !
 PAR G(YMN2O5,Y+3:MN+3:MN+4:O-2) 298.15 +GYMN2O5; 6000 N !
 \$
 PHASE ZR3Y4O12:I Z 3 3 4 12 !
 CONST ZR3Y4O12:I : ZR+4 : Y+3 : O-2 : !
 PAR G(ZR3Y4O12,ZR+4:Y+3:O-2) 298.15 +7*GZYO; 6000 N !
 \$
 PHASE PERV:I Z 3 1 1 3 !
 CONST PERV:I : LA+3 MN+3 SR+2 VA : MN+2 MN+3 MN+4 VA : O-2 VA : !
 PAR G(PERV,LA+3:MN+3:O-2;0) 298.15 GL3O; 6000 N !
 PAR G(PERV,LA+3:MN+3:VA;0) 298.15 GL3O-3*GHSEROO; 6000 N !

PAR G(PERV,LA+3:MN+4:O-2;0) 298.15
 0.66667*GL4O+0.5*GV4O-0.166667*GVVV-0.5*GHSEROO+5.76318*T; 6000
 N!
 PAR G(PERV,LA+3:MN+4:VA;0) 298.15
 0.66667*GL4O+0.5*GV4O-0.166667*GVVV-3.5*GHSEROO+5.76318*T; 6000
 N!
 PAR G(PERV,LA+3:MN+2:O-2;0) 298.15 GL2O+0.5*GHSEROO+11.2386*T; 6000
 N!
 PAR G(PERV,LA+3:MN+2:VA;0) 298.15 GL2O-2.5*GHSEROO+11.2386*T; 6000
 N!
 PAR G(PERV,LA+3:VA:O-2;0) 298.15
 2*GL4O-1.5*GV4O+0.5*GVVV+1.5*GHSEROO+1.41263*T; 6000 N!
 PAR G(PERV,LA+3:VA:VA;0) 298.15
 2*GL4O+0.5*GVVV-1.5*GV4O-1.5*GHSEROO+1.41263*T; 6000 N!
 PAR G(PERV,MN+3:MN+3:O-2;0) 298.15 GL3O+ANTI; 6000 N!
 PAR G(PERV,MN+3:MN+3:VA;0) 298.15 GL3O-3*GHSEROO+ANTI; 6000 N!
 !
 PAR G(PERV,MN+3:MN+4:O-2;0) 298.15 0.66667*GL4O+0.5*GV4O
 -0.166667*GVVV-0.5*GHSEROO+5.76318*T+ANTI; 6000 N!
 PAR G(PERV,MN+3:MN+4:VA;0) 298.15 0.66667*GL4O+0.5*GV4O
 -0.166667*GVVV-3.5*GHSEROO+5.76318*T+ANTI; 6000 N!
 PAR G(PERV,MN+3:MN+2:O-2;0) 298.15
 GL2O+0.5*GHSEROO+11.2386*T+ANTI; 6000 N!
 PAR G(PERV,MN+3:MN+2:VA;0) 298.15
 GL2O-2.5*GHSEROO+11.2386*T+ANTI; 6000 N!
 PAR G(PERV,MN+3:VA:O-2;0) 298.15
 2*GL4O-1.5*GV4O+0.5*GVVV+1.5*GHSEROO+1.41263*T+ANTI; 6000 N!
 !
 PAR G(PERV,MN+3:VA:VA;0) 298.15
 2*GL4O+0.5*GVVV-1.5*GV4O-1.5*GHSEROO+1.41263*T+ANTI; 6000 N!
 !
 PAR G(PERV,VA:MN+3:O-2;0) 298.15
 GL3O+1.5*GV4O+0.5*GVVV-2*GL4O+1.5*GHSEROO-1.41263*T; 6000 N!
 !
 PAR G(PERV,VA:MN+3:VA;0) 298.15
 GL3O+1.5*GV4O+0.5*GVVV-2*GL4O-1.5*GHSEROO-1.41263*T; 6000 N!
 !
 PAR G(PERV,VA:MN+4:O-2;0) 298.15
 2*GV4O+0.33333*GVVV-1.33333*GL4O+GHSEROO+4.35056*T; 6000 N!
 PAR G(PERV,VA:MN+4:VA;0) 298.15
 2*GV4O+0.3333*GVVV-1.333*GL4O-2*GHSEROO+4.35057*T; 6000 N!
 PAR G(PERV,VA:MN+2:O-2;0) 298.15
 GL2O+1.5*GV4O+0.5*GVVV-2*GL4O+2*GHSEROO+9.82596*T; 6000 N!
 !
 PAR G(PERV,VA:MN+2:VA;0) 298.15

GL2O+1.5*GV4O+0.5*GVVV-2*GL4O-GHSEROO#+9.82596*T; 6000 N !
 PAR G(PERV,VA:VA:O-2;0) 298.15 GVVV+3*GHSEROO; 6000 N !
 PAR G(PERV,VA:VA:VA;0) 298.15 GVVV; 6000 N !
 PAR G(PERV,SR+2:MN+2:O-2;0) 298.15
 GS3O+GL2O-GL3O+GHSEROO+22.47717*T; 6000 N !
 PAR G(PERV,SR+2:MN+3:O-2;0) 298.15
 GS3O+0.5*GHSEROO+11.23859*T; 6000 N !
 PAR G(PERV,SR+2:MN+4:O-2;0) 298.15 GS4O; 6000 N !
 PAR G(PERV,SR+2:VA:O-2;0) 298.15
 GS3O-GL3O+2*GL4O-1.5*GV4O+0.5*GVVV+2*GHSEROO+12.62121*T;
 6000 N !
 PAR G(PERV,SR+2:MN+2:VA;0) 298.15
 GS3O+GL2O-GL3O-2*GHSEROO+22.47717*T; 6000 N !
 PAR G(PERV,SR+2:MN+3:VA;0) 298.15 GS3O-2.5*GHSEROO+11.23859*T; 6000
 N !
 PAR G(PERV,SR+2:MN+4:VA;0) 298.15 GS4O-3*GHSEROO; 6000 N !
 PAR G(PERV,SR+2:VA:VA;0) 298.15
 GS3O+2*GL4O-1.5*GV4O+0.5*GVVV-GL3O-GHSEROO+12.62121*T; 6000
 N !
 PAR L(PERV,LA+3,SR+2:MN+4:O-2;1) 298.15 -117000; 6000 N !
 PAR L(PERV,LA+3,SR+2:MN+2:O-2;1) 298.15 -136000; 6000 N !
 PAR L(PERV,LA+3,SR+2:MN+4:VA;1) 298.15 -117000; 6000 N !
 PAR L(PERV,LA+3,SR+2:MN+2:VA;1) 298.15 -136000; 6000 N !
 \$
 PHASE LS2MNO4:I Z 4 1 1 1 4 !
 CONST LS2MNO4:I : SR+2 : LA+3 SR+2 : MN+3 MN+4 : O-2 : !
 PAR G(LS2MNO4,SR+2:SR+2:MN+3:O-2;0) 298.15
 2*GSROSOL+0.5*GMN2O3+0.5*GHSEROO; 6000 N !
 PAR G(LS2MNO4,SR+2:SR+2:MN+4:O-2;0) 298.15 GS4O_RP1; 6000 N !
 PAR G(LS2MNO4,SR+2:LA+3:MN+3:O-2;0) 298.15 GL3O_RP1; 6000 N !
 PAR G(LS2MNO4,SR+2:LA+3:MN+4:O-2;0) 298.15
 GL3O_RP1+GS4O_RP1-2*GSROSOL-0.5*GMN2O3-0.5*GHSEROO; 6000
 N !
 \$
 PHASE LS3MN2O7:I Z 4 1 2 2 7 !
 CONST LS3MN2O7:I : SR+2 : LA+3 SR+2 : MN+3 MN+4 : O-2 : !
 PAR G(LS3MN2O7,SR+2:SR+2:MN+3:O-2;0) 298.15
 3*GSROSOL+GMN2O3+GHSEROO ; 6000 N !
 PAR G(LS3MN2O7,SR+2:SR+2:MN+4:O-2;0) 298.15 GS4O_RP2; 6000 N !
 PAR G(LS3MN2O7,SR+2:LA+3:MN+3:O-2;0) 298.15 GL3O_RP2; 6000 N !
 PAR G(LS3MN2O7,SR+2:LA+3:MN+4:O-2;0) 298.15
 GL3O_RP2+GS4O_RP2-3*GSROSOL-GMN2O3-GHSEROO; 6000 N !

\$Phases from ssub5

PHASE C1H2O2_L % 1 1.0 !
CONSTITUENT C1H2O2_L :C1H2O2 : !

PARAMETER G(C1H2O2_L,C1H2O2;0) 298.15 +F4559T#; 6000 N REF3949 !

PHASE C1H2S3_L % 1 1.0 !
CONSTITUENT C1H2S3_L :C1H2S3 : !

PARAMETER G(C1H2S3_L,C1H2S3;0) 298.15 +F4561T#; 6000 N REF3953 !

PHASE C1H4O1_L % 1 1.0 !
CONSTITUENT C1H4O1_L :C1H4O1 : !

PARAMETER G(C1H4O1_L,C1H4O1;0) 298.15 +F4605T#; 6000 N REF3974 !

PHASE C1H4S1_L % 1 1.0 !
CONSTITUENT C1H4S1_L :C1H4S1 : !

PARAMETER G(C1H4S1_L,C1H4S1;0) 298.15 +F4612T#; 6000 N REF3979 !

PHASE C1MN1O3_S % 1 1.0 !
CONSTITUENT C1MN1O3_S :C1MN1O3 : !

PARAMETER G(C1MN1O3_S,C1MN1O3;0) 298.15 +F4712T#; 6000 N REF4040 !

PHASE C1MN3_S % 1 1.0 !
CONSTITUENT C1MN3_S :C1MN3 : !

PARAMETER G(C1MN3_S,C1MN3;0) 298.15 +F4714T#; 6000 N REF4043 !

PHASE C1MN3_S2 % 1 1.0 !
CONSTITUENT C1MN3_S2 :C1MN3 : !

PARAMETER G(C1MN3_S2,C1MN3;0) 298.15 +F4714T#+14936.9
-11.4022137*T; 6000 N REF4043 !

PHASE C1O3SR1_L % 1 1.0 !

CONSTITUENT C1O3SR1_L :C1O3SR1 : !

 PARAMETER G(C1O3SR1_L,C1O3SR1;0) 298.15 +F4827T#+56700-
 36.5771381*T;
 6000 N REF4121 !

 PHASE C1O3SR1_S % 1 1.0 !
 CONSTITUENT C1O3SR1_S :C1O3SR1 : !

 PARAMETER G(C1O3SR1_S,C1O3SR1;0) 298.15 +F4827T#; 6000 N REF4121 !

 PHASE C1O3SR1_S2 % 1 1.0 !
 CONSTITUENT C1O3SR1_S2 :C1O3SR1 : !

 PARAMETER G(C1O3SR1_S2,C1O3SR1;0) 298.15 +F4827T#+16700-
 13.9398998*T;
 6000 N REF4121 !

 PHASE C1S2_L % 1 1.0 !
 CONSTITUENT C1S2_L :C1S2 : !

 PARAMETER G(C1S2_L,C1S2;0) 298.15 +F4869T#; 6000 N REF4155 !

 PHASE C1ZR1_L % 1 1.0 !
 CONSTITUENT C1ZR1_L :C1ZR1 : !

 PARAMETER G(C1ZR1_L,C1ZR1;0) 298.15 +F4932T#+79496-20.8925099*T;
 6000 N REF4214 !

 PHASE C1ZR1_S % 1 1.0 !
 CONSTITUENT C1ZR1_S :C1ZR1 : !

 PARAMETER G(C1ZR1_S,C1ZR1;0) 298.15 +F4932T#; 6000 N REF4214 !

 PHASE C2H4O2_L % 1 1.0 !
 CONSTITUENT C2H4O2_L :C2H4O2 : !

 PARAMETER G(C2H4O2_L,C2H4O2;0) 298.15 +F5341T#; 6000 N REF4412 !

PHASE C2H6O1_L % 1 1.0 !
CONSTITUENT C2H6O1_L :C2H6O1 : !

PARAMETER G(C2H6O1_L,C2H6O1;0) 298.15 +F5381T#; 6000 N REF4436 !

PHASE C2H6O2_L % 1 1.0 !
CONSTITUENT C2H6O2_L :C2H6O2 : !

PARAMETER G(C2H6O2_L,C2H6O2;0) 298.15 +F5387T#; 6000 N REF4447 !

PHASE C2MN5_S % 1 1.0 !
CONSTITUENT C2MN5_S :C2MN5 : !

PARAMETER G(C2MN5_S,C2MN5;0) 298.15 +F5443T#; 6000 N REF4480 !

PHASE C2SR1_S % 1 1.0 !
CONSTITUENT C2SR1_S :C2SR1 : !

PARAMETER G(C2SR1_S,C2SR1;0) 298.15 +F5502T#; 6000 N REF4518 !

PHASE C3MN7_S % 1 1.0 !
CONSTITUENT C3MN7_S :C3MN7 : !

PARAMETER G(C3MN7_S,C3MN7;0) 298.15 +F5569T#; 6000 N REF4578 !

PHASE C60_S % 1 1.0 !
CONSTITUENT C60_S :C60 : !

PARAMETER G(C60_S,C60;0) 298.15 +F5722T#; 6000 N REF4708 !

PHASE C6H6_L % 1 1.0 !
CONSTITUENT C6H6_L :C6H6 : !

PARAMETER G(C6H6_L,C6H6;0) 298.15 +F5746T#; 6000 N REF4746 !

PHASE C6MN23_L % 1 1.0 !
CONSTITUENT C6MN23_L :C6MN23 : !

PARAMETER G(C6MN23_L,C6MN23;0) 298.15 +F5752T#+340000
-223.243598*T; 6000 N REF4752 !

PHASE C6MN23_S % 1 1.0 !
CONSTITUENT C6MN23_S :C6MN23 : !

PARAMETER G(C6MN23_S,C6MN23;0) 298.15 +F5752T#; 6000 N REF4752 !

PHASE DIAMOND % 1 1.0 !
CONSTITUENT DIAMOND :C : !

PARAMETER G(DIAMOND,C;0) 298.15 +F3986T#; 6000 N REF3620 !

PHASE GRAPHITE % 1 1.0 !
CONSTITUENT GRAPHITE :C : !

PARAMETER G(GRAPHITE,C;0) 298.15 +F3970T#; 6000 N REF3609 !

PHASE GRAPHITE_L % 1 1.0 !
CONSTITUENT GRAPHITE_L :C : !

PARAMETER G(GRAPHITE_L,C;0) 298.15 +F3970T#+117369
-24.6299289*T; 6000 N REF3609 !

PHASE H10O8S1_L % 1 1.0 !
CONSTITUENT H10O8S1_L :H10O8S1 : !

PARAMETER G(H10O8S1_L,H10O8S1;0) 298.15 +F11513T#; 6000 N REF9624
!

PHASE H15O10_5S1_L % 1 1.0 !
CONSTITUENT H15O10_5S1_L :H15O10.5S1 : !

PARAMETER G(H15O10_5S1_L,H15O10.5S1;0) 298.15 +F11516T#; 6000 N
REF9628 !

PHASE H1MNO2_S % 1 1.0 !

CONSTITUENT H1MNO2_S :H1MNO2 : !
 PARAMETER G(H1MNO2_S,H1MNO2;0) 298.15 +F11644T#; 6000 N REF9704
 !
 PHASE H1ZR1_S % 1 1.0 !
 CONSTITUENT H1ZR1_S :H1ZR1 : !
 PARAMETER G(H1ZR1_S,H1ZR1;0) 298.15 +F11793T#; 6000 N REF9803 !
 PHASE H2LA1_S % 1 1.0 !
 CONSTITUENT H2LA1_S :H2LA1 : !
 PARAMETER G(H2LA1_S,H2LA1;0) 298.15 +F11813T#; 6000 N REF9820 !
 PHASE H2MNO2_S % 1 1.0 !
 CONSTITUENT H2MNO2_S :H2MNO2 : !
 PARAMETER G(H2MNO2_S,H2MNO2;0) 298.15 +F11833T#; 6000 N REF9843
 !
 PHASE H2O1_L % 1 1.0 !
 CONSTITUENT H2O1_L :H2O1 : !
 PARAMETER G(H2O1_L,H2O1;0) 298.15 +F11290T#; 6000 N REF9502 !
 PHASE H2O2SR1_L % 1 1.0 !
 CONSTITUENT H2O2SR1_L :H2O2SR1 : !
 PARAMETER G(H2O2SR1_L,H2O2SR1;0) 298.15 +F11868T#+23000
 -28.4653465*T; 6000 N REF9871 !
 PHASE H2O2SR1_S % 1 1.0 !
 CONSTITUENT H2O2SR1_S :H2O2SR1 : !
 PARAMETER G(H2O2SR1_S,H2O2SR1;0) 298.15 +F11868T#; 6000 N REF9871
 !

PHASE H2O2_L % 1 1.0 !
CONSTITUENT H2O2_L :H2O2 : !

PARAMETER G(H2O2_L,H2O2;0) 298.15 +F11318T#; 6000 N REF9517 !

PHASE H2O4S1_L % 1 1.0 !
CONSTITUENT H2O4S1_L :H2O4S1 : !

PARAMETER G(H2O4S1_L,H2O4S1;0) 298.15 +F11503T#; 6000 N REF9611 !

PHASE H2S1_L % 1 1.0 !
CONSTITUENT H2S1_L :H2S1 : !

PARAMETER G(H2S1_L,H2S1;0) 298.15 +F11472T#; 6000 N REF9593 !

PHASE H2S2_L % 1 1.0 !
CONSTITUENT H2S2_L :H2S2 : !

PARAMETER G(H2S2_L,H2S2;0) 298.15 +F11476T#; 6000 N REF9598 !

PHASE H2SR1_L % 1 1.0 !
CONSTITUENT H2SR1_L :H2SR1 : !

PARAMETER G(H2SR1_L,H2SR1;0) 298.15 +F11914T#+30200
-23.7677104*T; 6000 N REF9920 !

PHASE H2SR1_S % 1 1.0 !
CONSTITUENT H2SR1_S :H2SR1 : !

PARAMETER G(H2SR1_S,H2SR1;0) 298.15 +F11914T#; 6000 N REF9920 !

PHASE H2SR1_S2 % 1 1.0 !
CONSTITUENT H2SR1_S2 :H2SR1 : !

PARAMETER G(H2SR1_S2,H2SR1;0) 298.15 +F11914T#+7200-6.38297872*T;
6000 N REF9920 !

PHASE H2Y1_S % 1 1.0 !

CONSTITUENT H2Y1_S :H2Y1 : !
 PARAMETER G(H2Y1_S,H2Y1;0) 298.15 +F11932T#; 6000 N REF9933 !

 PHASE H2ZR1_S % 1 1.0 !
 CONSTITUENT H2ZR1_S :H2ZR1 : !
 PARAMETER G(H2ZR1_S,H2ZR1;0) 298.15 +F11934T#; 6000 N REF9936 !

 PHASE H3LA1O3_S % 1 1.0 !
 CONSTITUENT H3LA1O3_S :H3LA1O3 : !
 PARAMETER G(H3LA1O3_S,H3LA1O3;0) 298.15 +F11941T#; 6000 N REF9940 !

 PHASE H3Y1_S % 1 1.0 !
 CONSTITUENT H3Y1_S :H3Y1 : !
 PARAMETER G(H3Y1_S,H3Y1;0) 298.15 +F11961T#; 6000 N REF9966 !

 PHASE H4O5S1_L % 1 1.0 !
 CONSTITUENT H4O5S1_L :H4O5S1 : !
 PARAMETER G(H4O5S1_L,H4O5S1;0) 298.15 +F11508T#; 6000 N REF9616 !

 PHASE H6O6S1_L % 1 1.0 !
 CONSTITUENT H6O6S1_L :H6O6S1 : !
 PARAMETER G(H6O6S1_L,H6O6S1;0) 298.15 +F11511T#; 6000 N REF9620 !

 PHASE H8O7S1_L % 1 1.0 !
 CONSTITUENT H8O7S1_L :H8O7S1 : !
 PARAMETER G(H8O7S1_L,H8O7S1;0) 298.15 +F11986T#; 6000 N REF10001 !

 PHASE LA1MN1O3_S % 1 1.0 !
 CONSTITUENT LA1MN1O3_S :LA1MN1O3 : !

PARAMETER G(LA1MN1O3_S,LA1MN1O3;0) 298.15 +F13015T#; 6000 N
REF10935 !

PHASE LA1MN1O3_S2 % 1 1.0 !
CONSTITUENT LA1MN1O3_S2 :LA1MN1O3 : !

PARAMETER G(LA1MN1O3_S2,LA1MN1O3;0) 298.15 +F13015T#+4000-
5.92592593*T;
6000 N REF10935 !

PHASE LA1S1_S % 1 1.0 !
CONSTITUENT LA1S1_S :LA1S1 : !

PARAMETER G(LA1S1_S,LA1S1;0) 298.15 +F13040T#; 6000 N REF10954 !

PHASE LA1S2_S % 1 1.0 !
CONSTITUENT LA1S2_S :LA1S2 : !

PARAMETER G(LA1S2_S,LA1S2;0) 298.15 +F13042T#; 6000 N REF10957 !

PHASE LA2S3_S % 1 1.0 !
CONSTITUENT LA2S3_S :LA2S3 : !

PARAMETER G(LA2S3_S,LA2S3;0) 298.15 +F13072T#; 6000 N REF10993 !

PHASE MN1O4S1_S % 1 1.0 !
CONSTITUENT MN1O4S1_S :MN1O4S1 : !

PARAMETER G(MN1O4S1_S,MN1O4S1;0) 298.15 +F13451T#; 6000 N
REF11314 !

PHASE MN1O4SR2_S % 1 1.0 !
CONSTITUENT MN1O4SR2_S :MN1O4SR2 : !

PARAMETER G(MN1O4SR2_S,MN1O4SR2;0) 298.15 +F13445T#; 6000 N
REF11304 !

PHASE MN1S1_L % 1 1.0 !
CONSTITUENT MN1S1_L :MN1S1 : !

PARAMETER G(MN1S1_L,MN1S1;0) 298.15 +F13459T#+26108
-14.4803106*T; 6000 N REF11328 !

PHASE MN1S1_S % 1 1.0 !
CONSTITUENT MN1S1_S :MN1S1 : !

PARAMETER G(MN1S1_S,MN1S1;0) 298.15 +F13459T#; 6000 N REF11328 !

PHASE MN1S2_S % 1 1.0 !
CONSTITUENT MN1S2_S :MN1S2 : !

PARAMETER G(MN1S2_S,MN1S2;0) 298.15 +F13466T#; 6000 N REF11335 !

PHASE MN2O7_L % 1 1.0 !
CONSTITUENT MN2O7_L :MN2O7 : !

PARAMETER G(MN2O7_L,MN2O7;0) 298.15 +F13496T#; 6000 N REF11379
!

PHASE MN_L % 1 1.0 !
CONSTITUENT MN_L :MN : !

PARAMETER G(MN_L,MN;0) 298.15 +F13407T#+19236.4
-13.7426497*T; 6000 N REF11270 !

PHASE O3S1_L % 1 1.0 !
CONSTITUENT O3S1_L :O3S1 : !

PARAMETER G(O3S1_L,O3S1;0) 298.15 +F15125T#; 6000 N REF12616 !

PHASE O4S1SR1_L % 1 1.0 !

CONSTITUENT O4S1SR1_L :O4S1SR1 : !
 PARAMETER G(O4S1SR1_L,O4S1SR1;0) 298.15 +F15267T#+46000
 -26.1419432*T; 6000 N REF12733 !
 PHASE O4S1SR1_S % 1 1.0 !
 CONSTITUENT O4S1SR1_S :O4S1SR1 : !
 PARAMETER G(O4S1SR1_S,O4S1SR1;0) 298.15 +F15267T#; 6000 N REF12733
 !
 PHASE O4S1SR1_S2 % 1 1.0 !
 CONSTITUENT O4S1SR1_S2 :O4S1SR1 : !
 PARAMETER G(O4S1SR1_S2,O4S1SR1;0) 298.15 +F15267T#+10000
 -6.99300699*T; 6000 N REF12733 !
 PHASE O8S2ZR1_S % 1 1.0 !
 CONSTITUENT O8S2ZR1_S :O8S2ZR1 : !
 PARAMETER G(O8S2ZR1_S,O8S2ZR1;0) 298.15 +F15431T#; 6000 N REF12895
 !
 PHASE S1SR1_L % 1 1.0 !
 CONSTITUENT S1SR1_L :S1SR1 : !
 PARAMETER G(S1SR1_L,S1SR1;0) 298.15 +F16101T#+63000-25.2*T;
 6000 N REF13418 !
 PHASE S1SR1_S % 1 1.0 !
 CONSTITUENT S1SR1_S :S1SR1 : !
 PARAMETER G(S1SR1_S,S1SR1;0) 298.15 +F16101T#; 6000 N REF13418 !
 PHASE S1Y1_S % 1 1.0 !
 CONSTITUENT S1Y1_S :S1Y1 : !
 PARAMETER G(S1Y1_S,S1Y1;0) 298.15 +F16149T#; 6000 N REF13470 !

PHASE S2ZR1_L % 1 1.0 !
CONSTITUENT S2ZR1_L :S2ZR1 : !

PARAMETER G(S2ZR1_L,S2ZR1;0) 298.15 +F16209T#+45000
-24.6845859*T; 6000 N REF13526 !

PHASE S2ZR1_S % 1 1.0 !
CONSTITUENT S2ZR1_S :S2ZR1 : !

PARAMETER G(S2ZR1_S,S2ZR1;0) 298.15 +F16209T#; 6000 N REF13526 !

PHASE S3ZR2_S % 1 1.0 !
CONSTITUENT S3ZR2_S :S3ZR2 : !

PARAMETER G(S3ZR2_S,S3ZR2;0) 298.15 +F16238T#; 6000 N REF13553 !

PHASE S_L % 1 1.0 !
CONSTITUENT S_L :S : !

PARAMETER G(S_L,S;0) 298.15 +F15998T#+2122-5.52092641*T;
6000 N REF13353 !

PHASE S_S % 1 1.0 !
CONSTITUENT S_S :S : !

PARAMETER G(S_S,S;0) 298.15 +F15998T#; 6000 N REF13353 !

PHASE S_S2 % 1 1.0 !
CONSTITUENT S_S2 :S : !

PARAMETER G(S_S2,S;0) 298.15 +F15998T#+401-1.08878632*T;
6000 N REF13353 !

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PHASE GAS:G % 1 1.0 !

CONSTITUENT GAS:G :C,C1H1,C1H1O1,C1H1O2,C1H2,C1H2O1,C1H2O2_CIS,
 C1H2O2_DIOXIRANE,C1H2O2_TRANS,C1H3,C1H3O1_CH2OH,C1H3O1_CH3O,C
 1H4,C1H4O1,
 C1H4S1,C1O1,C1O1S1,C1O2,C1S1,C1S2,C2,C2H1,C2H2,C2H2O1,C2H3,C2H4,
 C2H4O1_ACETALDEHYDE,C2H4O1_OXIRANE,C2H4O2_ACETICACID,C2H4O2_
 DIOXETANE,
 C2H4O3_123TRIOXOLANE,C2H4O3_124TRIOXOLANE,C2H5,C2H6,C2H6O1,C2H
 6O2,C2O1,
 C3,C3H1,C3H4_1,C3H4_2,C3H6O1,C3H6_1,C3H6_2,C3H8,C3O2,C4,C4H1,C4H10_1,
 C4H10_2,C4H2_1,C4H2_2,C4H4_1,C4H4_2,C4H6_1,C4H6_2,C4H6_3,C4H6_4,C4H6
 _5,
 C4H8_1,C4H8_2,C4H8_3,C4H8_4,C4H8_5,C4H8_6,C5,C6O,C6H6,C6H6O1,H,H1MN1
 ,
 H1MNO,H1O1,H1O1S1_HSO,H1O1S1_SOH,H1SRO,H1O2,H1S1,H1SR1,H1ZR1,H2,
 H2O1,
 H2O1S1_H2SO,H2O1S1_HSOH,H2O2,H2O2SR1,H2O4S1,H2S1,H2S2,LA,LA1O1,LA
 1S1,
 LA2O1,LA2O2,MN,MNO,MNO2,MN1S1,O1S1,O1S2,SRO,YO,Y2O,ZRO,O2S1,
 YO2,Y2O2,ZRO2,O2,O3,O3S1,S,S1SR1,S1Y1,S1ZR1,S2,S2ZR1,S3,S4,S5,S6,S7,S8,S
 R,
 SR2,Y,ZR,ZR2,AR : !

PARAMETER G(GAS,C;0) 6000 N REF3612 !	298.15 +F3974T#+R#*T*LN(1E-05*P);
PARAMETER G(GAS,O2;0) 6000 N REF12142 !	298.15 +F14375T#+R#*T*LN(1E-05*P);
PARAMETER G(GAS,C1H1;0) 6000 N REF3902 !	298.15 +F4469T#+R#*T*LN(1E-05*P);
PARAMETER G(GAS,C1H1O1;0) 6000 N REF3923 !	298.15 +F4509T#+R#*T*LN(1E-05*P);
PARAMETER G(GAS,C1H1O2;0) 6000 N REF3926 !	298.15 +F4514T#+R#*T*LN(1E-05*P);
PARAMETER G(GAS,C1H2;0) 6000 N REF3931 !	298.15 +F4525T#+R#*T*LN(1E-05*P);
PARAMETER G(GAS,C1H2O1;0) 6000 N REF3938 !	298.15 +F4538T#+R#*T*LN(1E-05*P);

PARAMETER G(GAS,C1H2O2_CIS;0) 298.15 +F4543T#+R#*T*LN(1E-05*P);
 6000 N REF3941 !
 PARAMETER G(GAS,C1H2O2_DIOXIRANE;0) 298.15 +F4548T#+R#*T*LN(1E-05*P);
 6000 N REF3943 !
 PARAMETER G(GAS,C1H2O2_TRANS;0) 298.15 +F4554T#+R#*T*LN(1E-05*P);
 6000 N REF3947 !
 PARAMETER G(GAS,C1H3;0) 298.15 +F4563T#+R#*T*LN(1E-05*P);
 6000 N REF3955 !
 PARAMETER G(GAS,C1H3O1_CH2OH;0) 298.15 +F4574T#+R#*T*LN(1E-05*P);
 6000 N REF3960 !
 PARAMETER G(GAS,C1H3O1_CH3O;0) 298.15 +F4580T#+R#*T*LN(1E-05*P);
 6000 N REF3962 !
 PARAMETER G(GAS,C1H4;0) 298.15 +F4591T#+R#*T*LN(1E-05*P);
 6000 N REF3966 !
 PARAMETER G(GAS,C1H4O1;0) 298.15 +F4599T#+R#*T*LN(1E-05*P);
 6000 N REF3971 !
 PARAMETER G(GAS,C1H4S1;0) 298.15 +F4607T#+R#*T*LN(1E-05*P);
 6000 N REF3977 !
 PARAMETER G(GAS,C1O1;0) 298.15 +F4794T#+R#*T*LN(1E-05*P);
 6000 N REF4098 !
 PARAMETER G(GAS,C1O1S1;0) 298.15 +F4799T#+R#*T*LN(1E-05*P);
 6000 N REF4102 !
 PARAMETER G(GAS,C1O2;0) 298.15 +F4815T#+R#*T*LN(1E-05*P);
 6000 N REF4111 !
 PARAMETER G(GAS,C1S1;0) 298.15 +F4859T#+R#*T*LN(1E-05*P);
 6000 N REF4149 !
 PARAMETER G(GAS,C1S2;0) 298.15 +F4864T#+R#*T*LN(1E-05*P);
 6000 N REF4152 !
 PARAMETER G(GAS,C2;0) 298.15 +F4954T#+R#*T*LN(1E-05*P);
 6000 N REF4224 !
 PARAMETER G(GAS,C2H1;0) 298.15 +F5282T#+R#*T*LN(1E-05*P);
 6000 N REF4380 !
 PARAMETER G(GAS,C2H2;0) 298.15 +F5293T#+R#*T*LN(1E-05*P);
 6000 N REF4385 !
 PARAMETER G(GAS,C2H2O1;0) 298.15 +F5299T#+R#*T*LN(1E-05*P);
 6000 N REF4388 !
 PARAMETER G(GAS,C2H3;0) 298.15 +F5305T#+R#*T*LN(1E-05*P);
 6000 N REF4393 !
 PARAMETER G(GAS,C2H4;0) 298.15 +F5311T#+R#*T*LN(1E-05*P);
 6000 N REF4396 !

PARAMETER G(GAS,C2H4O1_ACETALDEHYDE;0) 298.15
 +F5317T#+R#*T*LN(1E-05*P);
 6000 N REF4399 !
 PARAMETER G(GAS,C2H4O1_OXIRANE;0) 298.15 +F5323T#+R#*T*LN(1E-
 05*P);
 6000 N REF4401 !
 PARAMETER G(GAS,C2H4O2_ACETICACID;0) 298.15 +F5330T#+R#*T*LN(1E-
 05*P);
 6000 N REF4405 !
 PARAMETER G(GAS,C2H4O2_DIOXETANE;0) 298.15 +F5334T#+R#*T*LN(1E-
 05*P);
 6000 N REF4407 !
 PARAMETER G(GAS,C2H4O3_123TRIOXOLANE;0) 298.15
 +F5343T#+R#*T*LN(1E-05*P);
 6000 N REF4416 !
 PARAMETER G(GAS,C2H4O3_124TRIOXOLANE;0) 298.15
 +F5350T#+R#*T*LN(1E-05*P);
 6000 N REF4420 !
 PARAMETER G(GAS,C2H5;0) 298.15 +F5357T#+R#*T*LN(1E-05*P);
 6000 N REF4425 !
 PARAMETER G(GAS,C2H6;0) 298.15 +F5369T#+R#*T*LN(1E-05*P);
 6000 N REF4430 !
 PARAMETER G(GAS,C2H6O1;0) 298.15 +F5375T#+R#*T*LN(1E-05*P);
 6000 N REF4433 !
 PARAMETER G(GAS,C2H6O2;0) 298.15 +F5385T#+R#*T*LN(1E-05*P);
 6000 N REF4444 !
 PARAMETER G(GAS,C2O1;0) 298.15 +F5466T#+R#*T*LN(1E-05*P);
 6000 N REF4495 !
 PARAMETER G(GAS,C3;0) 298.15 +F5510T#+R#*T*LN(1E-05*P);
 6000 N REF4528 !
 PARAMETER G(GAS,C3H1;0) 298.15 +F5527T#+R#*T*LN(1E-05*P);
 6000 N REF4543 !
 PARAMETER G(GAS,C3H4_1;0) 298.15 +F5539T#+R#*T*LN(1E-05*P);
 6000 N REF4554 !
 PARAMETER G(GAS,C3H4_2;0) 298.15 +F5542T#+R#*T*LN(1E-05*P);
 6000 N REF4558 !
 PARAMETER G(GAS,C3H6O1;0) 298.15 +F5554T#+R#*T*LN(1E-05*P);
 6000 N REF4568 !
 PARAMETER G(GAS,C3H6_1;0) 298.15 +F5545T#+R#*T*LN(1E-05*P);
 6000 N REF4562 !
 PARAMETER G(GAS,C3H6_2;0) 298.15 +F5550T#+R#*T*LN(1E-05*P);
 6000 N REF4564 !
 PARAMETER G(GAS,C3H8;0) 298.15 +F5557T#+R#*T*LN(1E-05*P);
 6000 N REF4572 !
 PARAMETER G(GAS,C3O2;0) 298.15 +F5577T#+R#*T*LN(1E-05*P);

6000 N REF4588 !	
PARAMETER G(GAS,C4;0)	298.15 +F5587T#+R#*T*LN(1E-05*P);
6000 N REF4595 !	
PARAMETER G(GAS,C4H1;0)	298.15 +F5592T#+R#*T*LN(1E-05*P);
6000 N REF4597 !	
PARAMETER G(GAS,C4H10_1;0)	298.15 +F5597T#+R#*T*LN(1E-05*P);
6000 N REF4601 !	
PARAMETER G(GAS,C4H10_2;0)	298.15 +F5602T#+R#*T*LN(1E-05*P);
6000 N REF4605 !	
PARAMETER G(GAS,C4H2_1;0)	298.15 +F5607T#+R#*T*LN(1E-05*P);
6000 N REF4611 !	
PARAMETER G(GAS,C4H2_2;0)	298.15 +F5610T#+R#*T*LN(1E-05*P);
6000 N REF4613 !	
PARAMETER G(GAS,C4H4_1;0)	298.15 +F5614T#+R#*T*LN(1E-05*P);
6000 N REF4615 !	
PARAMETER G(GAS,C4H4_2;0)	298.15 +F5619T#+R#*T*LN(1E-05*P);
6000 N REF4619 !	
PARAMETER G(GAS,C4H6_1;0)	298.15 +F5623T#+R#*T*LN(1E-05*P);
6000 N REF4623 !	
PARAMETER G(GAS,C4H6_2;0)	298.15 +F5626T#+R#*T*LN(1E-05*P);
6000 N REF4627 !	
PARAMETER G(GAS,C4H6_3;0)	298.15 +F5630T#+R#*T*LN(1E-05*P);
6000 N REF4631 !	
PARAMETER G(GAS,C4H6_4;0)	298.15 +F5633T#+R#*T*LN(1E-05*P);
6000 N REF4635 !	
PARAMETER G(GAS,C4H6_5;0)	298.15 +F5636T#+R#*T*LN(1E-05*P);
6000 N REF4639 !	
PARAMETER G(GAS,C4H8_1;0)	298.15 +F5641T#+R#*T*LN(1E-05*P);
6000 N REF4642 !	
PARAMETER G(GAS,C4H8_2;0)	298.15 +F5647T#+R#*T*LN(1E-05*P);
6000 N REF4644 !	
PARAMETER G(GAS,C4H8_3;0)	298.15 +F5653T#+R#*T*LN(1E-05*P);
6000 N REF4646 !	
PARAMETER G(GAS,C4H8_4;0)	298.15 +F5659T#+R#*T*LN(1E-05*P);
6000 N REF4648 !	
PARAMETER G(GAS,C4H8_5;0)	298.15 +F5664T#+R#*T*LN(1E-05*P);
6000 N REF4650 !	
PARAMETER G(GAS,C4H8_6;0)	298.15 +F5670T#+R#*T*LN(1E-05*P);
6000 N REF4652 !	
PARAMETER G(GAS,C5;0)	298.15 +F5696T#+R#*T*LN(1E-05*P);
6000 N REF4673 !	
PARAMETER G(GAS,C60;0)	298.15 +F5719T#+R#*T*LN(1E-05*P);
6000 N REF4694 !	
PARAMETER G(GAS,C6H6;0)	298.15 +F5740T#+R#*T*LN(1E-05*P);
6000 N REF4742 !	

PARAMETER G(GAS,C6H6O1;0)	298.15 +F5748T#+R#*T*LN(1E-05*P);
6000 N REF4748 !	
PARAMETER G(GAS,H;0)	298.15 +F11215T#+R#*T*LN(1E-05*P);
6000 N REF9468 !	
PARAMETER G(GAS,H1MN1;0)	298.15 +F11630T#+R#*T*LN(1E-05*P);
6000 N REF9698 !	
PARAMETER G(GAS,H1MNO;0)	298.15 +F11635T#+R#*T*LN(1E-05*P);
6000 N REF9700 !	
PARAMETER G(GAS,H1O1;0)	298.15 +F11257T#+R#*T*LN(1E-05*P);
6000 N REF9492 !	
PARAMETER G(GAS,H1O1S1_HSO;0)	298.15 +F11478T#+R#*T*LN(1E-
05*P);	
6000 N REF9600 !	
PARAMETER G(GAS,H1O1S1_SOH;0)	298.15 +F11483T#+R#*T*LN(1E-
05*P);	
6000 N REF9602 !	
PARAMETER G(GAS,H1SRO;0)	298.15 +F11704T#+R#*T*LN(1E-05*P);
6000 N REF9742 !	
PARAMETER G(GAS,H1O2;0)	298.15 +F11280T#+R#*T*LN(1E-05*P);
6000 N REF9498 !	
PARAMETER G(GAS,H1S1;0)	298.15 +F11456T#+R#*T*LN(1E-05*P);
6000 N REF9586 !	
PARAMETER G(GAS,H1SR1;0)	298.15 +F11767T#+R#*T*LN(1E-05*P);
6000 N REF9782 !	
PARAMETER G(GAS,H1ZR1;0)	298.15 +F11795T#+R#*T*LN(1E-05*P);
6000 N REF9805 !	
PARAMETER G(GAS,H2;0)	298.15 +F11227T#+R#*T*LN(1E-05*P);
6000 N REF9480 !	
PARAMETER G(GAS,H2O1;0)	298.15 +F11295T#+R#*T*LN(1E-05*P);
6000 N REF9506 !	
PARAMETER G(GAS,H2O1S1_H2SO;0)	298.15 +F11488T#+R#*T*LN(1E-
05*P);	
6000 N REF9604 !	
PARAMETER G(GAS,H2O1S1_HSOH;0)	298.15 +F11493T#+R#*T*LN(1E-
05*P);	
6000 N REF9606 !	
PARAMETER G(GAS,H2O2;0)	298.15 +F11314T#+R#*T*LN(1E-05*P);
6000 N REF9514 !	
PARAMETER G(GAS,H2O2SR1;0)	298.15 +F11871T#+R#*T*LN(1E-05*P);
6000 N REF9873 !	
PARAMETER G(GAS,H2O4S1;0)	298.15 +F11498T#+R#*T*LN(1E-05*P);
6000 N REF9608 !	
PARAMETER G(GAS,H2S1;0)	298.15 +F11467T#+R#*T*LN(1E-05*P);
6000 N REF9590 !	
PARAMETER G(GAS,H2S2;0)	298.15 +F11474T#+R#*T*LN(1E-05*P);

6000 N REF9595 !	
PARAMETER G(GAS,LA;0)	298.15 +F12997T#+R#*T*LN(1E-05*P);
6000 N REF10925 !	
PARAMETER G(GAS,LA1O1;0)	298.15 +F13020T#+R#*T*LN(1E-05*P);
6000 N REF10942 !	
PARAMETER G(GAS,LA1S1;0)	298.15 +F13037T#+R#*T*LN(1E-05*P);
6000 N REF10950 !	
PARAMETER G(GAS,LA2O1;0)	298.15 +F13057T#+R#*T*LN(1E-05*P);
6000 N REF10978 !	
PARAMETER G(GAS,LA2O2;0)	298.15 +F13061T#+R#*T*LN(1E-05*P);
6000 N REF10982 !	
PARAMETER G(GAS,MN;0)	298.15 +F13413T#+R#*T*LN(1E-05*P);
6000 N REF11273 !	
PARAMETER G(GAS,MNO;0)	298.15 +F13428T#+R#*T*LN(1E-05*P);
6000 N REF11287 !	
PARAMETER G(GAS,MNO2;0)	298.15 +F13435T#+R#*T*LN(1E-05*P);
6000 N REF11294 !	
PARAMETER G(GAS,MN1S1;0)	298.15 +F13461T#+R#*T*LN(1E-05*P);
6000 N REF11332 !	
PARAMETER G(GAS,O1S1;0)	298.15 +F14527T#+R#*T*LN(1E-05*P);
6000 N REF12217 !	
PARAMETER G(GAS,O1S2;0)	298.15 +F14532T#+R#*T*LN(1E-05*P);
6000 N REF12220 !	
PARAMETER G(GAS,SRO;0)	298.15 +F14596T#+R#*T*LN(1E-05*P);
6000 N REF12252 !	
PARAMETER G(GAS,YO;0)	298.15 +F14718T#+R#*T*LN(1E-05*P);
6000 N REF12317 !	
PARAMETER G(GAS,Y2O;0)	298.15 +F14734T#+R#*T*LN(1E-05*P);
6000 N REF12323 !	
PARAMETER G(GAS,ZRO;0)	298.15 +F14754T#+R#*T*LN(1E-05*P);
6000 N REF12334 !	
PARAMETER G(GAS,O2S1;0)	298.15 +F14849T#+R#*T*LN(1E-05*P);
6000 N REF12407 !	
PARAMETER G(GAS,YO2;0)	298.15 +F15054T#+R#*T*LN(1E-05*P);
6000 N REF12557 !	
PARAMETER G(GAS,Y2O2;0)	298.15 +F15060T#+R#*T*LN(1E-05*P);
6000 N REF12559 !	
PARAMETER G(GAS,ZRO2;0)	298.15 +F15071T#+R#*T*LN(1E-05*P);
6000 N REF12568 !	
PARAMETER G(GAS,O3;0)	298.15 +F14415T#+R#*T*LN(1E-05*P);
6000 N REF12151 !	
PARAMETER G(GAS,O3S1;0)	298.15 +F15120T#+R#*T*LN(1E-05*P);
6000 N REF12612 !	
PARAMETER G(GAS,S;0)	298.15 +F16008T#+R#*T*LN(1E-05*P);
6000 N REF13357 !	

PARAMETER G(GAS,S1SR1;0)	298.15 +F16104T#+R#*T*LN(1E-05*P);
6000 N REF13421 !	
PARAMETER G(GAS,S1Y1;0)	298.15 +F16146T#+R#*T*LN(1E-05*P);
6000 N REF13456 !	
PARAMETER G(GAS,S1ZR1;0)	298.15 +F16162T#+R#*T*LN(1E-05*P);
6000 N REF13484 !	
PARAMETER G(GAS,S2;0)	298.15 +F16023T#+R#*T*LN(1E-05*P);
6000 N REF13366 !	
PARAMETER G(GAS,S2ZR1;0)	298.15 +F16212T#+R#*T*LN(1E-05*P);
6000 N REF13529 !	
PARAMETER G(GAS,S3;0)	298.15 +F16033T#+R#*T*LN(1E-05*P);
6000 N REF13372 !	
PARAMETER G(GAS,S4;0)	298.15 +F16042T#+R#*T*LN(1E-05*P);
6000 N REF13378 !	
PARAMETER G(GAS,S5;0)	298.15 +F16046T#+R#*T*LN(1E-05*P);
6000 N REF13381 !	
PARAMETER G(GAS,S6;0)	298.15 +F16051T#+R#*T*LN(1E-05*P);
6000 N REF13384 !	
PARAMETER G(GAS,S7;0)	298.15 +F16056T#+R#*T*LN(1E-05*P);
6000 N REF13387 !	
PARAMETER G(GAS,S8;0)	298.15 +F16060T#+R#*T*LN(1E-05*P);
6000 N REF13390 !	
PARAMETER G(GAS,SR;0)	298.15 +F16551T#+R#*T*LN(1E-05*P);
6000 N REF13855 !	
PARAMETER G(GAS,SR2;0)	298.15 +F16566T#+R#*T*LN(1E-05*P);
6000 N REF13861 !	
PARAMETER G(GAS,Y;0)	298.15 +F16895T#+R#*T*LN(1E-05*P);
6000 N REF14072 !	
PARAMETER G(GAS,ZR;0)	298.15 +F16956T#+R#*T*LN(1E-05*P);
6000 N REF14106 !	
PARAMETER G(GAS,ZR2;0)	298.15 +F16975T#+R#*T*LN(1E-05*P);
6000 N REF14114 !	
PARAMETER G(GAS,AR;0)	298.15 +F877T#+R#*T*LN(1E-05*P);
6.00000E+03 N !	

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FUNCTION GHSERLA

298.15 -7968.403+120.284604*T-26.34*T*LN(T)-.001295165*T**2;
550 Y -3381.413+59.06113*T-17.1659411*T*LN(T)-.008371705*T**2
+6.8932E-07*T**3-399448*T**(-1);
2000 Y -15608.882+181.390071*T-34.3088*T*LN(T);

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4000 N !
FUNCTION GLABCC
298.15 -3952.161+88.072353*T-21.7919*T*LN(T)-0.004045175*T**2
      -5.25865E-07*T**3;
800 Y +321682.673-3565.08252*T+513.440708*T*LN(T)-0.387295093*T**2
      +4.9547989E-05*T**3-36581228*T**(-1);
1134 Y -16377.894+218.492988*T-39.5388*T*LN(T);
1193 Y -136609.91+1123.34397*T-163.413074*T*LN(T)+0.053968535*T**2
      -4.056395E-06*T**3+21167204*T**(-1);
2000 Y -8205.988+174.836315*T-34.3088*T*LN(T);
4000 N !
FUNCTION GLAFCC
298.15 -6109.797+89.878761*T-21.7919*T*LN(T)
      -0.004045175*T**2-5.25865E-07*T**3;
1134 Y -124598.976+955.878375*T-139.346741*T*LN(T)+0.042032405*T**2
      -3.066199E-06*T**3+20994153*T**(-1);
2000 Y -12599.386+178.54399*T-34.3088*T*LN(T);
4000 N !
FUNCTION GLALIQ
298.15 +5332.653+18.23012*T-11.0188191*T*LN(T)-0.020171603*T**2
      +2.93775E-06*T**3-133541*T**(-1);
1134 Y -3942.004+171.018431*T-34.3088*T*LN(T);
4000 N !
$
FUNCTION GHSERSR
298.15 -7532.367+107.183879*T-23.905*T*LN(T)
      -4.61225E-3*T**2-1.67477E-07*T**3-2055*T**(-1);
820 Y -13380.102+153.196104*T-30.0905432*T*LN(T)
      -3.251266E-3*T**2+1.84189E-07*T**3+850134*T**(-1);
3000 N !
FUNCTION GSRBCC
298.15 -6779.234+116.583654*T-25.6708365*T*LN(T)
      -3.126762E-3*T**2+2.2965E-7*T**3+27649*T**(-1);
820 Y -6970.594+122.067301*T-26.57*T*LN(T)
      -1.9493E-3*T**2-1.7895E-8*T**3+16495*T**(-1);
1050 Y +8168.357+0.423037*T-9.7788593*T*LN(T)
      -9.539908E-3*T**2+5.20221E-7*T**3-2414794*T**(-1);
3000 N !
FUNCTION GSRLIQ
298.15 +2194.997-10.118994*T-5.0668978*T*LN(T)
      -3.1840595E-2*T**2+4.981237E-06*T**3-265559*T**(-1);
1050 Y -10855.29+213.406219*T-39.463*T*LN(T);
3000 N !
$
FUNCTION GHSERMN 298.15 -8115.28+130.059*T-23.4582*T*LN(T)

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-0.00734768*T**2+69827*T**(-1);
1519.00 Y -28733.41+312.2648*T-48*T*LN(T)+1.656847E+30*T**(-9);
2000.00 N !
FUNCTION GMNCUB 298.15 -5800.4+135.995*T-24.8785*T*LN(T)
-0.00583359*T**2+70269*T**(-1);
1519.00 Y +442.65-0.9715*T+GHSERMN+2.310723E+30*T**(-9);
2000.00 N !
FUNCTION GMNFCC 298.15 -3439.3+131.884*T-24.5177*T*LN(T)
-0.006*T**2+69600*T**(-1);
1519.00 Y +2663.31-2.5984*T+GHSERMN+2.205113E+30*T**(-9);
2000.00 N !
FUNCTION GMNBCC 298.15 -3235.3+127.85*T-23.7*T*LN(T)
-0.00744271*T**2+60000*T**(-1);
1519.00 Y +5544.58-4.5605*T+GHSERMN-3.91695E+29*T**(-9);
2000.00 N !
FUNCTION GMNHCP 298.15 -4439.3+133.007*T-24.5177*T*LN(T)
-0.006*T**2+69600*T**(-1);
1519.00 Y +1663.31-1.4754*T+GHSERMN+2.205113E+30*T**(-9);
2000.00 N !
FUNCTION GMNLIQ 298.15 +17859.91-12.6208*T+GHSERMN-4.41929E-
21*T**7;
1519.00 Y -9993.9+299.036*T-48*T*LN(T);
2000.00 N !
$
FUNCTION GHSERY 100.00 -8011.09379+128.572856*T-25.6656992*T*LN(T)
-0.00175716414*T**2-4.17561786E-07*T**3+26911.509*T**(-1);
1000.00 Y -7179.74574+114.497104*T-23.4941827*T*LN(T)
-0.0038211802*T**2-8.2534534E-08*T**3;
1795.15 Y -67480.7761+382.124727*T-56.9527111*T*LN(T)
+0.00231774379*T**2-7.22513088E-08*T**3+18077162.6*T**(-1);
3700.00 N !
FUNCTION GYYBCC 100.00 -833.658863+123.667346*T-25.5832578*T*LN(T)
-0.00237175965*T**2+9.10372497E-09*T**3+27340.0687*T**(-1);
1000.00 Y -1297.79829+134.528352*T-27.3038477*T*LN(T)
-5.41757644E-04*T**2-3.05012175E-07*T**3;
1795.15 Y +15389.4975+0.981325399*T-8.88296647*T*LN(T)
-0.00904576576*T**2+4.02944768E-07*T**3-2542575.96*T**(-1);
3700.00 N !
FUNCTION GYYLIQ 100.00 +2098.50738+119.41873*T-24.6467508*T*LN(T)
-0.00347023463*T**2-8.12981167E-07*T**3+23713.7332*T**(-1);
1000.00 Y +7386.44846+19.4520171*T-9.0681627*T*LN(T)
-0.0189533369*T**2+1.7595327E-06*T**3;
1795.15 Y -12976.5957+257.400783*T-43.0952*T*LN(T);
3700.00 N !
$

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FUNCTION GHSERZR 130.00 -7827.595+125.64905*T-24.1618*T*LN(T)
-0.00437791*T**2+34971*T**(-1);
2128.00 Y -26085.921+262.724183*T-42.144*T*LN(T)-1.342896E+31*T**(-9);
6000.00 N !
FUNCTION GZRBCC 130.00 -525.539+124.9457*T-25.607406*T*LN(T)
-3.40084E-04*T**2-9.729E-09*T**3+25233*T**(-1)-7.6143E-11*T**4;
2128.00 Y -4620.034+1.55998*T+GHSERZR+1.4103476E+32*T**(-9);
6000.00 N !
FUNCTION GZRLIQ 130.00 +18147.69-9.080812*T+GHSERZR+1.6275E-22*T**7;
2128.00 Y -8281.26+253.812609*T-42.144*T*LN(T);
6000.00 N !
$
FUNCTION GHSEROO 298.15 -3480.87-25.503038*T-11.136*T*LN(T)
-0.005098888*T**2+6.61846E-07*T**3-38365*T**(-1);
1000.00 Y -6568.763+12.65988*T-16.8138*T*LN(T)
-5.95798E-04*T**2+6.781E-09*T**3+262905*T**(-1);
3300.00 Y -13986.728+31.259625*T-18.9536*T*LN(T)
-4.25243E-04*T**2+1.0721E-08*T**3+4383200*T**(-1);
6000.00 N !
$
FUNCTION GMN12Y 298.15 +12*GHSERMN+GHSEYYY-142346.62+58.97073*T;
6000.00 N !
FUNCTION GMN23Y6 298.15 +23*GHSERMN+6*GHSEYYY-
334013.88+27.83478*T;
6000.00 N !
FUNCTION GMN2Y 298.15 +2*GHSERMN+GHSEYYY-41092.59+3.42435*T;
6000.00 N !
$
FUNCTION GLA2O3A 298.15
-1835600+674.72*T-118*T*LN(T)-0.008*T**2+620000*T**(-1); 6000 N !
FUNCTION GLA2O3B 298.15 +GLA2O3A+6388+0.508*T; 6000 N !
FUNCTION GLA2O3C 298.15 +GLA2O3A+10586+5.938*T; 6000 N !
FUNCTION GLA2O3H 298.15
-1789600+654.83*T-118*T*LN(T)-0.008*T**2+620000*T**(-1); 6000 N !
FUNCTION GLA2O3X 298.15
-1724440+626.61*T-118*T*LN(T)-0.008*T**2+620000*T**(-1); 6000 N !
FUNCTION GLA2O3L
298.15 -1807513+1282.48*T-200*T*LN(T); 6000 N !

FUNCTION GMTLA2O3 298.15 +GLA2O3A+30000; 6000 N !
$
FUNCTION GSROSOL 298.15 -607870+268.9*T-47.56*T*LN(T)
-3.07E-03*T**2+190000*T**(-1); 6000 N !
FUNCTION GSRO2SOL 298.15 +GSROSOL+GHSEROO-43740+70*T; 6000 N !
FUNCTION GSROLIQ 298.15 -566346+449.0*T-73.1*T*LN(T); 6000 N !

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\$
 FUNCTION GMNO 298.15 -4.02478000E+05+2.59356E+02*T-
 4.6835E+01*T*LN(T)
 -3.8500E-03*T**2+2.12922E+05*T**(-1); 6000 N !
 FUNCTION GMNO2 298.15 -5.45091000E+05+3.95379E+02*T-
 6.5277E+01*T*LN(T)
 -7.803E-03*T**2+6.64955E+05*T**(-1); 6000 N !
 FUNCTION GMN2O3 298.15 -9.98618000E+05+5.88619E+02*T-
 1.01956E+02*T*LN(T)
 -1.8844E-02*T**2+5.89055E+05*T**(-1); 6000 N !
 FUNCTION GMN3O4 298.15 -1.43703700E+06+8.89568E+02*T-
 1.54748E+02*T*LN(T)
 -1.7408E-02*T**2+9.86139E+05*T**(-1); 6000 N !
 FUNCTION GMN3O4B 298.15 -1.41618900E+06+8.75120E+02*T-
 1.54748E+02*T*LN(T)
 -1.7408E-02*T**2+9.86139E+05*T**(-1); 6000 N !
 FUNCTION GL11 298.15 +GMNO+4.3947E+04-2.0628E+01*T; 6000 N !
 FUNCTION GL23 298.15
 +2*GMNO+GHSEROO-6.4953E+04+4.3144E+01*T; 6000 N !
 FUNCTION GMTMNO 298.15 +GMNO+40000; 6000 N !
 FUNCTION GMFMNO 298.15 +GMNO+20000; 6000 N !
 FUNCTION GMTMN2O3 298.15 +GMN2O3+100000; 6000 N !
 FUNCTION GMFMN2O3 298.15 +GMN2O3+60000; 6000 N !
 FUNCTION GMHMN2O3 298.15 +GMN2O3+60000; 6000 N !
 \$
 FUNCTION GCCYO15 298.15 -990900+381.86*T-62.85*T*LN(T)
 -0.0025*T**2+1172000*T**(-1)-59000000*T**(-2); 6000 N !
 FUNCTION GAAYO15 298.15 +GCCYO15+10584-3.3*T; 6000 N !
 FUNCTION GBBYO15 298.15 +GCCYO15+5654-2.034*T; 6000 N !
 FUNCTION GHHYO15 298.15 +GCCYO15+12500-4.808*T; 6000 N !
 FUNCTION GXXYO15 298.15 +GCCYO15+20000-8.1*T; 6000 N !
 FUNCTION GMMYO15 298.15 +GCCYO15+32700+20*T; 6000 N !
 FUNCTION GMTYO15 298.15 +GCCYO15+15000; 6000 N !
 \$
 FUNCTION GMMZRO2 298.15 -1125300+416.9*T-68.4*T*LN(T)
 -0.00335*T**2+586000*T**(-1); 6000 N !
 FUNCTION GTTZRO2 298.15 +GMMZRO2+6000-4.326*T; 6000 N !
 FUNCTION GFFZRO2 298.15 +GMMZRO2+13500-7.159*T; 6000 N !
 FUNCTION GZRO2LIQ 298.15 -1077400+561.1*T-90*T*LN(T); 6000 N !
 FUNCTION GMAZRO2 298.15 +GMMZRO2+50000; 6000 N !
 FUNCTION GMCZRO2 298.15 +GFFZRO2+45000; 6000 N !
 FUNCTION GMHZRO2 298.15 +GFFZRO2+45000; 6000 N !
 \$
 \$ Ternary compounds
 \$ LaMnO3: (La+3, Mn+3, Va)(Mn+2, Mn+3, Mn+4, Va)(O-2, Va)3

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FUNCTION GL3O    298.15
0.5*GLA2O3A+0.5*GMN2O3-63367+51.77*T-7.19*T*LOG(T)+232934*T**(-1);
6000 N !
FUNCTION GL2O    298.15 0.5*GLA2O3A+GMNO+27672;          6000 N !
FUNCTION GL4O    298.15 0.5*GLA2O3A+0.75*GMNO2-91857+20.31*T; 6000 N
!
FUNCTION GV4O    298.15 0.333333*GLA2O3A+GMNO2-53760;      6000 N !
FUNCTION GVVV    298.15 +6*GL2O+4*GL4O+3*GV4O-12*GL3O-254212; 6000
N !
FUNCTION ANTI    298.15 +547422;                          6000 N !
$(La+3)2(Mn+2)(O-2)4
FUNCTION GL2MNO4 298.15 +GLA2O3A+GMNO+47276-28.61*T;      6000 N
!
$ Functions from the La-Sr-O system
FUNCTION SR_ALPHA 298.15 +2*GSROSOL+2.5E+04;              6000 N !
FUNCTION SRH_ALPHA 298.15 +2*GSROSOL+2.5E+04;             6000 N !
FUNCTION SRX_ALPHA 298.15 +2*GSROSOL+2.5E+04;             6000 N !
FUNCTION LA_BETA  298.15 +GLA2O3A+2.158E+04;              6000 N !
$ LaYO3
FUNCTION GLAYO3   298.15 +0.5*GLA2O3A+GCCYO15-8517-0.75*T; 6000
N !
$ La2Zr2O7 (old and new:GLZOC)
FUNCTION GL2Z2O7  298.15 +GLA2O3X+2*GFFZRO2-271791+51.9*T; 6000
N !
FUNCTION GLZOC    298.15 +GLA2O3X+2*GFFZRO2-271791+51.9*T+30000;
6000 N !
$ C2
FUNCTION GC2      298.15 +GLA2O3X+GFFZRO2-94433+2.5*T;      6000 N !
$ Functions from the Sr - Mn - O system
$ HEX Phase
FUNCTION GSM4_HEX 298.15 +GSROSOL+GMNO2-1.11300000E+05;     6000
N !
FUNCTION GSM3_HEX 298.15 +GSROSOL+0.5*GMN2O3
-7.73000000E+03-1.70000000E+01*T;          6000 N !
FUNCTION GSM4OZ   298.15 +GMN2O3+GSM4_HEX-8.79100000E+03;   6000
N !
FUNCTION GSM3OZ   298.15 +GMN2O3+GSM3_HEX-2.19200000E+04;   6000
N !
FUNCTION GS4O_RP1 298.15 +2*GSROSOL+GMNO2-1.32830000E+05;   6000
N !
FUNCTION GL3O_RP1 298.15 +GSROSOL+0.5*GLA2O3A+0.5*GMN2O3-68300;
6000 N !
$ Sr7Mn4O15
FUNCTION GS7M4    298.15 +7*GSROSOL+4*GMNO2-6.12450000E+05+50*T;
6000 N !

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\$ RP2
 FUNCTION GS4O_RP2 298.15 +3*GSROSOL+2*GMNO2-8.99100000E+04-90*T;
 6000 N !
 FUNCTION GL3O_RP2 298.15 +GSROSOL+GLA2O3A+GMN2O3-137400;
 6000 N !
 \$ RP3
 FUNCTION GSM4_RP3 298.15 +4*GSROSOL+3*GMNO2-3.78500000E+05; 6000
 N !
 \$
 FUNCTION GS3O 298.15 GSROSOL+0.5*GMN2O3
 -7.73000000E+03-1.44550000E+04-1.70000000E+01*T; 6000 N !
 FUNCTION GS4O 298.15
 GSROSOL+GMNO2-1.11300000E+05+2.26500000E+04-7.69000000E+00*T; 6000
 N !
 \$
 \$ SrZrO3
 FUNCTION GSZOF 298.15 -1822143.95+719.115283*T-121.25232*T*LN(T)
 -0.00610864*T**2+1080727.2*T**(-1); 6000 N !
 \$ h-YMnO3
 FUNCTION GYMNO3H 298.15 -1515274+618*T-105.4*T*LN(T)
 -0.017*T**2+669185*T**(-1); 6000 N !
 \$ YMn2O5
 FUNCTION GYMNO3H 298.15
 +GYMNO3H+0.5*GMN2O3+0.5*GHSEROO-100383+62.2*T; 6000 N !
 \$ 1/7 Y3Zr4O12
 FUNCTION GZYO 298.15
 +0.4286*GFFZRO2+0.5714*GCCYO15-15900+1*T; 6000 N !
 \$
 FUNCTION RTLNP 298.15 +8.31451*T*LN(1E-05*P); 6000 N !
 \$ La(g)
 FUNCTION F12026T
 298.15 +422273.955-30.3347881*T-22.06299*T*LN(T)-0.005444405*T**2
 +4.71447833E-07*T**3+102710.1*T**(-1);
 600 Y +426628.905-85.4786162*T-13.83676*T*LN(T)-0.011938995*T**2
 +1.33826017E-06*T**3-312130.2*T**(-1);
 1300 Y +404460.17+114.016725*T-42.00406*T*LN(T)+0.0037094435*T**2
 -2.70261E-07*T**3+2891891*T**(-1);
 3200 Y +497751.747-246.085237*T+2.791973*T*LN(T)-0.006002155*T**2
 +1.30043383E-07*T**3-34158815*T**(-1);
 8200 Y -92343.0441+773.338363*T-111.0188*T*LN(T)+0.0037862445*T**2
 -2.82257667E-08*T**3+5.418475E+08*T**(-1);
 10000 N !
 \$ LaO(g)
 FUNCTION F12049T
 298.15 -131496.968-24.5469483*T-31.53764*T*LN(T)-0.0051956*T**2

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+7.60442333E-07*T**3+103677.85*T**(-1);
900 Y -133112.849+7.93847638*T-36.65559*T*LN(T)+2.4937065E-04*T**2
-2.05688333E-07*T**3+108868.35*T**(-1);
2500 Y -137735.323-23.9414477*T-31.58251*T*LN(T)-0.003177688*T**2
+6.84986667E-08*T**3+5676870*T**(-1);
5400 Y -39118.6731-213.786313*T-10.21743*T*LN(T)-0.005021225*T**2
+9.162985E-08*T**3-74562000*T**(-1);
10000 N !
$ La2O(g)
FUNCTION F12085T
298.15 -69316.3279+46.9195461*T-51.12563*T*LN(T)-0.005701935*T**2
+8.637425E-07*T**3+212452.95*T**(-1);
1000 Y -73167.5826+93.9280358*T-58.13034*T*LN(T)-1.332372E-05*T**2
+4.41584333E-10*T**3+616730*T**(-1);
6000 N !
$ La2O2(g)
FUNCTION F12089T
298.15 -642532.065+54.8487791*T-51.72813*T*LN(T)-0.028452875*T**2
+4.99643833E-06*T**3+271002.95*T**(-1);
700 Y -657497.385+256.452173*T-82.32033*T*LN(T)-1.8245965E-04*T**2
+6.891315E-09*T**3+1664162*T**(-1);
5100 Y -672122.137+293.83814*T-86.72291*T*LN(T)+4.319301E-04*T**2
-9.75906E-09*T**3+11187120*T**(-1);
6000 N !
$ Sr(g) :
FUNCTION F14450T
298.15 +154227.522-24.1431703*T-20.98549*T*LN(T)
+1.951298E-04*T**2-3.09095833E-08*T**3+4675.2365*T**(-1);
1800 Y +111247.483+242.365806*T-56.52776*T*LN(T)
+0.0133862*T**2-9.57800833E-07*T**3+9843260*T**(-1);
3300 Y +770872.513-2114.76782*T+233.253*T*LN(T)
-0.04337796*T**2+1.134592E-06*T**3-2.7250735E+08*T**(-1);
4900 Y -196742.694+263.327068*T-44.45892*T*LN(T)
-0.008078665*T**2+2.96671167E-07*T**3+3.57637E+08*T**(-1);
6200 Y -949056.902+1952.13337*T-239.3059*T*LN(T)
+0.01421437*T**2-1.79062E-07*T**3+8.9842E+08*T**(-1);
9600 Y +34305.7758+474.957384*T-77.25547*T*LN(T)
+0.00232914*T**2-1.54504333E-08*T**3-2.2245325E+08*T**(-1);
10000 N !
$ Sr2(g) :
FUNCTION F14465T
298.15 +295010.66+61.845039*T-54.13634*T*LN(T)
+0.040485225*T**2-9.264165E-06*T**3-70453.75*T**(-1);
500 Y +307156.188-147.411671*T-20.95926*T*LN(T)
+1.012636E-04*T**2-8.03856667E-09*T**3-905190.5*T**(-1);

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3000 N !

\$ SrO(g) :

FUNCTION F12810T

298.15 -25476.9742+3.04351985*T-34.37623*T*LN(T)
-0.0026980695*T**2+3.78874167E-07*T**3+120146.05*T**(-1);

900 Y -44602.142+205.651627*T-63.83687*T*LN(T)
+0.017645965*T**2-2.284235E-06*T**3+2463047*T**(-1);

1800 Y +243278.077-1500.21201*T+161.9497*T*LN(T)
-0.0612273*T**2+2.896125E-06*T**3-66468000*T**(-1);

2900 Y -571113.316+1685.71589*T-234.6556*T*LN(T)
+0.024571595*T**2-5.82819833E-07*T**3+2.468897E+08*T**(-1);

4500 Y -14433.8514+256.066959*T-66.76292*T*LN(T)
+0.002226246*T**2-2.98498E-08*T**3-97083400*T**(-1);

8800 Y +52967.3441+134.904343*T-53.17021*T*LN(T)
+0.001008387*T**2-9.46948833E-09*T**3-1.6008755E+08*T**(-1);

10000 N !

\$ Mn(g)

FUNCTION F12439T 298.15 +276164.054-34.4987547*T-20.786*T*LN(T);

1575.00 Y +275547.585-29.2480566*T-21.52064*T*LN(T)
+3.819474E-04*T**2-3.66030333E-08*T**3+95180.95*T**(-1);

2100.00 Y +274521.741-16.3844926*T-23.35302*T*LN(T)
+0.0013469965*T**2-1.18903067E-07*T**3;

2400.00 N !

\$ MnO(g)

FUNCTION F12454T 298.15 +151356.092-24.1662496*T-31.02229*T*LN(T)
-0.005519525*T**2+8.47063667E-07*T**3+97921.9*T**(-1);

900.00 Y +146503.882+29.4389965*T-38.90434*T*LN(T)
+4.8722855E-04*T**2-5.46958333E-08*T**3+687003.5*T**(-1);

4100.00 Y +163891.797+1.24225715*T-35.94693*T*LN(T)
+6.220655E-04*T**2-7.949125E-08*T**3-12461235*T**(-1);

6000.00 N !

\$ MnO2(g)

FUNCTION F12461T 298.15 +9095.11807-9.18675027*T-36.92694*T*LN(T)
-0.01944391*T**2+3.43552E-06*T**3+201368.45*T**(-1);

700.00 Y -4061.05468+167.414546*T-63.68895*T*LN(T)
+0.004964408*T**2-7.80481667E-07*T**3+1423101*T**(-1);

2000.00 Y +74138.9718-312.782575*T+1.646534*T*LN(T)
-0.01801756*T**2+7.59669E-07*T**3-16355180*T**(-1);

3900.00 Y -269662.307+860.503282*T-143.1466*T*LN(T)
+0.008591745*T**2-1.67854167E-07*T**3+1.388169E+08*T**(-1);

6000.00 N !

\$ Y(g):

FUNCTION F14722T 298.15 +413926.156+43.942359*T-34.19791*T*LN(T)
+0.0122297*T**2-2.14534333E-06*T**3+97071.5*T**(-1);

700.00 Y +417505.307-13.2762864*T-25.29082*T*LN(T)

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+0.002768476*T**2-3.169895E-07*T**3-157006.6*T**(-1);
2000.00 Y +439627.78-100.082079*T-14.64876*T*LN(T)
+0.001182233*T**2-3.39037833E-07*T**3-7693105*T**(-1);
3300.00 Y +656873.926-957.210194*T+92.15071*T*LN(T)
-0.022050485*T**2+6.04918167E-07*T**3-90137500*T**(-1);
5500.00 Y -81672.0087+877.446829*T-122.4532*T*LN(T)
+0.005666115*T**2-6.61492667E-08*T**3+3.865857E+08*T**(-1);
10000.00 N !
$ Y2O(g):
FUNCTION F12945T 298.15 -18834.6011+47.2728187*T-49.14357*T*LN(T)
-0.007582635*T**2+1.2067E-06*T**3+211591.55*T**(-1);
900.00 Y -23590.8983+106.946886*T-58.08361*T*LN(T)
-2.2921245E-05*T**2+7.790445E-10*T**3+695520*T**(-1);
6000.00 N !
$ YO(g):
FUNCTION F12929T 298.15 -55980.1334-24.7804591*T-30.58571*T*LN(T)
-0.005797885*T**2+9.044075E-07*T**3+92955.75*T**(-1);
900.00 Y -62402.7508+43.7949244*T-40.60318*T*LN(T)
+0.0014897095*T**2-1.41268333E-07*T**3+896318.5*T**(-1);
3100.00 Y +22970.3078-236.507016*T-6.632106*T*LN(T)
-0.004295709*T**2+3.30261667E-08*T**3-38281150*T**(-1);
5900.00 Y +78439.9263-450.3653*T+19.37683*T*LN(T)
-0.00859432*T**2+1.53217517E-07*T**3-45013010*T**(-1);
9600.00 Y -949291.433+1103.17067*T-151.1803*T*LN(T)
+0.004000447*T**2-2.13031E-08*T**3+1.118062E+09*T**(-1);
10000.00 N !
$ Y2O2(g):
FUNCTION F13270T 298.15 -575737.712+51.4042333*T-49.55549*T*LN(T)
-0.030210885*T**2+5.27799667E-06*T**3+255509.3*T**(-1);
700.00 Y -591679.029+265.724012*T-82.06371*T*LN(T)
-2.6169375E-04*T**2+1.0952625E-08*T**3+1742125.5*T**(-1);
4500.00 Y -594803.763+277.512452*T-83.52789*T*LN(T)
+4.9195245E-05*T**2-1.17628333E-09*T**3+3139224*T**(-1);
6000.00 N !
$ YO2(g):
FUNCTION F13266T 298.15 -453353.172+38.0172466*T-44.87379*T*LN(T)
-0.011836705*T**2+2.00650833E-06*T**3+281931.45*T**(-1);
800.00 Y -459941.788+124.969156*T-58.0167*T*LN(T)
-3.724498E-05*T**2+1.29613517E-09*T**3+910973.5*T**(-1);
6000.00 N !
$ Gas Zr
FUNCTION GZRGAS 298.15 +586876.841+74.4171195*T-38.69111*T*LN(T)
+0.01152846*T**2-1.693255E-06*T**3+270638.8*T**(-1);
700.00 Y +595990.293-26.0530509*T-24.06106*T*LN(T)
+0.001743641*T**2-5.94312333E-07*T**3-748947.5*T**(-1);

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1300.00 Y +593841.673-46.0204551*T-20.46361*T*LN(T)
-0.002961084*T**2+1.08391433E-07*T**3+526352.5*T**(-1);
2700.00 Y +630745.052-161.965371*T-6.647343*T*LN(T)
-0.0046738955*T**2+1.06833583E-07*T**3-15872340*T**(-1);
6600.00 Y +504260.272+131.813821*T-40.68801*T*LN(T)
-6.38357E-04*T**2+1.79125333E-08*T**3+71496950*T**(-1);
10000.00 N !
$ Gas Zr2 (ssub)
FUNCTION F15702T 298.15 +892794.963-14.4120751*T-37.13672*T*LN(T)
-3.2039655E-04*T**2-4.30605167E-09*T**3+85422.15*T**(-1);
3600.00 Y +874148.858+9.34917918*T-39.33356*T*LN(T)
-0.001019669*T**2+6.09799667E-08*T**3+14065805*T**(-1);
6000.00 N !
$ Gas ZrO (ssub)
FUNCTION F12964T 298.15 +84650.2479-322.816859*T+21.98592*T*LN(T)
-0.10713165*T**2+2.81704E-05*T**3-333363.35*T**(-1);
500.00 Y +42648.3264+404.464721*T-93.37933*T*LN(T)
+0.03332466*T**2-3.80849833E-06*T**3+2526299*T**(-1);
1100.00 Y +84838.707+11.527709*T-37.46259*T*LN(T)
+9.16682E-05*T**2-7.005105E-08*T**3-3491878*T**(-1);
4100.00 Y +106867.647-98.6658671*T-23.49987*T*LN(T)
-0.00315689*T**2+5.93994E-08*T**3-6661880*T**(-1);
9600.00 Y +255442.536-262.961955*T-6.281221*T*LN(T)
-0.0038787795*T**2+6.18786667E-08*T**3-2.2466925E+08*T**(-1);
10000.00 N !
$ Gas ZrO2 (ssub)
FUNCTION F13281T 298.15 -332610.845+3.22325893*T-38.10718*T*LN(T)
-0.01852473*T**2+3.29626E-06*T**3+218721.05*T**(-1);
700.00 Y -342836.09+140.579945*T-58.93983*T*LN(T)
+6.65405E-04*T**2-8.11812167E-08*T**3+1173742*T**(-1);
2600.00 Y -272800.105-96.5265444*T-30.24766*T*LN(T)
-0.0038011495*T**2-1.83201667E-11*T**3-28436635*T**(-1);
4900.00 Y -36436.1523-803.246487*T+54.45089*T*LN(T)
-0.017172935*T**2+3.92562833E-07*T**3-1.509956E+08*T**(-1);
6000.00 N !
$ O(g) :
FUNCTION F7397T 298.15 +243206.529-42897.0876*T**(-1)-20.7513421*T
-21.0155542*T*LN(T)+1.26870532E-04*T**2-1.23131285E-08*T**3;
2950.00 Y +252301.473-3973170.33*T**(-1)-51.974853*T
-17.2118798*T*LN(T)-5.41356254E-04*T**2+7.64520703E-09*T**3;
6000.00 N !
$ O3(g) :
FUNCTION F7683T 298.15 +133772.042-11328.9959*T**(-1)-84.8602165*T
-19.8314069*T*LN(T)-0.0392015696*T**2+7.90727187E-06*T**3;
600.00 Y +120765.524+997137.156*T**(-1)+120.113376*T

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-51.8410152*T*LN(T)-0.00353983136*T**2+3.20640143E-07*T**3;
 1500.00 Y +115412.196+1878139.02*T**(-1)+164.679664*T
 -58.069736*T*LN(T)-2.84399032E-04*T**2+5.95650279E-10*T**3;
 6000.00 N !

\$Functions from ssub5

FUNCTION F3974T 298.15 +710430.933-17.7062919*T-20.97529*T*LN(T)
 +1.998237E-04*T**2-3.34617167E-08*T**3+1680.6515*T**(-1); 3400 Y
 +698015.711+2.57175186*T-23.05071*T*LN(T)-6.04604E-05*T**2
 +6.74291667E-10*T**3+8558245*T**(-1); 10000 Y
 +736197.571-32.7975309*T-19.44529*T*LN(T)-1.5396035E-04*T**2
 -6.15402167E-11*T**3-56188350*T**(-1); 20000 N !

FUNCTION F4469T 298.15 +589091.036+6.37586112*T-28.31773*T*LN(T)
 +2.3216165E-04*T**2-7.36439667E-07*T**3-27186.245*T**(-1); 900 Y
 +591708.657-35.2925324*T-21.90158*T*LN(T)-.00592793*T**2
 +2.9876E-07*T**3-172733.6*T**(-1); 2800 Y
 +579194.621+42.13831*T-32.13932*T*LN(T)-.002507963*T**2
 +9.59279833E-08*T**3+2285342*T**(-1); 6400 Y
 +409696.643+452.714152*T-79.92745*T*LN(T)+.003347292*T**2
 -3.63044167E-08*T**3+1.115888E+08*T**(-1); 12000 Y
 +800166.03-30.0457765*T-28.18561*T*LN(T)+2.7641345E-04*T**2
 -1.923675E-09*T**3-4.4613505E+08*T**(-1); 20000 N !

FUNCTION F4509T 298.15 +34663.1187-68.3993353*T-21.87253*T*LN(T)
 -.018848125*T**2+1.978875E-06*T**3-112550.6*T**(-1); 1100 Y
 +10875.4517+145.536698*T-52.16378*T*LN(T)-.001376625*T**2
 +4.73872167E-08*T**3+3443852*T**(-1); 3600 Y
 +3695.68232+174.659191*T-55.81562*T*LN(T)-5.33191E-04*T**2
 +1.07304333E-08*T**3+6222210*T**(-1); 6000 N !

FUNCTION F4514T 298.15 -224579.294-49.1626181*T-27.13519*T*LN(T)
 -.03548659*T**2+5.02649167E-06*T**3+89572.2*T**(-1); 700 Y
 -239557.575+145.651699*T-56.49751*T*LN(T)-.00960395*T**2
 +6.83389333E-07*T**3+1534296*T**(-1); 1900 Y
 -268690.124+327.648549*T-80.82941*T*LN(T)-3.4153865E-04*T**2
 +9.43135333E-09*T**3+8273490*T**(-1); 6000 N !

FUNCTION F4525T 298.15 +381898.015-5.8112289*T-27.63198*T*LN(T)
 -.007897355*T**2-3.87669333E-08*T**3-62547*T**(-1); 900 Y
 +378165.881+8.88081456*T-29.13698*T*LN(T)-.00988883*T**2
 +6.15529E-07*T**3+710779*T**(-1); 2200 Y
 +340850.246+220.65528*T-57.01662*T*LN(T)-4.862414E-04*T**2
 +1.48344217E-08*T**3+10277000*T**(-1); 6000 N !

FUNCTION F4538T 298.15 -113219.01-136.968085*T-9.266226*T*LN(T)
 -.039279425*T**2+4.39612833E-06*T**3-223966.05*T**(-1); 900 Y

$-140078.823+144.485426*T-50.12368*T*LN(T)-.01134191*T**2$
 $+7.60462333E-07*T**3+3113545*T**(-1); 2000 Y$
 $-178622.186+374.929455*T-80.70841*T*LN(T)-3.54568E-04*T**2$
 $+9.67480833E-09*T**3+12424215*T**(-1); 6000 N !$
 FUNCTION F4543T 298.15 -388781.001-103.90421*T-16.81765*T*LN(T)
 $-.05671885*T**2+7.970165E-06*T**3+48801.55*T**(-1); 700 Y$
 $-409999.916+178.628265*T-59.57362*T*LN(T)-.0180534*T**2$
 $+1.33848133E-06*T**3+2039066.5*T**(-1); 1700 Y$
 $-459640.338+500.116138*T-102.7958*T*LN(T)-8.65375E-04*T**2$
 $+2.308845E-08*T**3+13013465*T**(-1); 6000 N !$
 FUNCTION F4548T 298.15 +29599.1942-208.348585*T+1.9*T*LN(T)
 $-.0857775*T**2+1.53734017E-05*T**3-125650*T**(-1); 500 Y$
 $+13784.1438+63.3004634*T-41.129*T*LN(T)-.0338256*T**2+3.6233E-06*T**3$
 $+962100*T**(-1); 900 Y$
 $-5210.22569+265.701863*T-70.581*T*LN(T)-.01342365*T**2$
 $+9.55723333E-07*T**3+3267820*T**(-1); 1700 Y$
 $-40799.5929+496.66709*T-101.611*T*LN(T)-.0012286*T**2+4.446E-08*T**3$
 $+11026610*T**(-1); 4000 N !$
 FUNCTION F4554T 298.15 -372453.966-100.891302*T-17.32496*T*LN(T)
 $-.05637795*T**2+7.91681333E-06*T**3+42419.085*T**(-1); 700 Y$
 $-393558.584+180.039941*T-59.83597*T*LN(T)-.01795244*T**2$
 $+1.330329E-06*T**3+2022398*T**(-1); 1700 Y$
 $-442917.663+499.668746*T-102.8073*T*LN(T)-8.671225E-04*T**2$
 $+2.304695E-08*T**3+12935575*T**(-1); 6000 N !$
 FUNCTION F4563T 298.15 +137013.412-8.99457393*T-25.84363*T*LN(T)
 $-.021245325*T**2+1.58670483E-06*T**3-33266.495*T**(-1); 1600 Y$
 $+84303.6035+343.362209*T-73.42088*T*LN(T)-.0017754415*T**2$
 $+6.12003E-08*T**3+11112475*T**(-1); 4400 Y$
 $+64161.9832+414.726089*T-82.17617*T*LN(T)-1.024296E-04*T**2$
 $+2.10901667E-09*T**3+19781775*T**(-1); 6000 N !$
 FUNCTION F4574T 298.15 -31298.3817-55.7322048*T-24.61425*T*LN(T)
 $-.04353285*T**2+5.34829833E-06*T**3+55658.25*T**(-1); 700 Y$
 $-43832.867+109.01195*T-49.49554*T*LN(T)-.02127646*T**2$
 $+1.55219067E-06*T**3+1252337.5*T**(-1); 1700 Y$
 $-103097.337+489.690506*T-100.6003*T*LN(T)-.0011952165*T**2$
 $+3.56136E-08*T**3+14443730*T**(-1); 5300 Y$
 $-120483.247+545.193751*T-107.3055*T*LN(T)-7.377055E-05*T**2$
 $+1.335003E-09*T**3+22773150*T**(-1); 6000 N !$
 FUNCTION F4580T 298.15 +10647.9115-220.041163*T+2.897875*T*LN(T)
 $-.0631791*T**2+7.98735833E-06*T**3-294680.9*T**(-1); 700 Y$
 $-8352.38175+27.9795444*T-34.49142*T*LN(T)-.03027099*T**2$
 $+2.51015167E-06*T**3+1523708*T**(-1); 1400 Y$
 $-65111.0776+451.440995*T-92.64558*T*LN(T)-.003388665*T**2$
 $+1.41701483E-07*T**3+12047630*T**(-1); 3500 Y$
 $-92729.9649+564.732519*T-106.8476*T*LN(T)-1.4186865E-04*T**2$

+3.13837167E-09*T**3+22203380*T**(-1); 6000 N !
 FUNCTION F4591T 298.15 -77295.563-147.095197*T-2.234656*T*LN(T)
 -.048463265*T**2+4.33754333E-06*T**3-305431.45*T**(-1); 1000 Y
 -110499.85+168.104152*T-47.22933*T*LN(T)-.021108925*T**2
 +1.1779525E-06*T**3+4316954*T**(-1); 2000 Y
 -181918.388+576.950971*T-101.1311*T*LN(T)-.002684469*T**2
 -2.361885E-08*T**3+22404635*T**(-1); 6000 N !
 FUNCTION F4599T 298.15 -205205.838-196.101493*T-1.169187*T*LN(T)
 -.06931275*T**2+8.62977667E-06*T**3-275306.2*T**(-1); 700 Y
 -225205.951+67.2670437*T-40.94166*T*LN(T)-.033860495*T**2
 +2.6413E-06*T**3+1622706*T**(-1); 1500 Y
 -296381.314+570.842619*T-109.5301*T*LN(T)-.0039814965*T**2
 +1.5649925E-07*T**3+15683740*T**(-1); 3700 Y
 -332630.415+711.963927*T-127.0897*T*LN(T)-1.98456E-04*T**2
 +4.28468667E-09*T**3+29832830*T**(-1); 6000 N !
 FUNCTION F4607T 298.15 -31736.4469-89.1033474*T-15.16373*T*LN(T)
 -.063031*T**2+8.16689E-06*T**3-82700.35*T**(-1); 700 Y
 -46383.122+111.337204*T-45.70366*T*LN(T)-.033846515*T**2
 +2.77622667E-06*T**3+1272194*T**(-1); 1500 Y
 -108832.18+573.167289*T-109.0654*T*LN(T)-.0047151195*T**2
 +2.206415E-07*T**3+13048610*T**(-1); 3000 N !
 FUNCTION F4794T 298.15 -118162.143-23.1824004*T-25.84624*T*LN(T)
 -.003281553*T**2-1.63612533E-07*T**3-55604.1*T**(-1); 800 Y
 -122211.036+7.61017665*T-29.9366*T*LN(T)-.0027053115*T**2
 +1.75559167E-07*T**3+541480.5*T**(-1); 2200 Y
 -131274.213+62.1198833*T-37.17593*T*LN(T)-1.020237E-04*T**2
 -6.44914833E-10*T**3+2724014*T**(-1); 6000 N !
 FUNCTION F4799T 298.15 -155898.194+38.3213499*T-38.72307*T*LN(T)
 -.014479075*T**2+1.74655E-06*T**3+217410.4*T**(-1); 1000 Y
 -171053.04+186.600669*T-60.03812*T*LN(T)-7.119685E-04*T**2
 +1.860925E-08*T**3+2292921*T**(-1); 4300 Y
 -180299.2+219.213216*T-64.04515*T*LN(T)+7.092145E-05*T**2
 -1.00343517E-08*T**3+6457110*T**(-1); 6000 N !
 FUNCTION F4815T 298.15 -404733.623-4.69677711*T-29.32959*T*LN(T)
 -.01996358*T**2+2.45837833E-06*T**3+124430.9*T**(-1); 900 Y
 -421187.23+168.064895*T-54.43846*T*LN(T)-.002556694*T**2
 +1.34184133E-07*T**3+2179368*T**(-1); 2700 Y
 -462626.164+339.502796*T-76.00339*T*LN(T)+.0026074805*T**2
 -1.06680183E-07*T**3+17540465*T**(-1); 7600 Y
 +322101.769-1097.44815*T+85.62125*T*LN(T)-.01226122*T**2
 +1.50875083E-07*T**3-7.00947E+08*T**(-1); 10000 N !
 FUNCTION F4859T 298.15 +272140.472-48.4187493*T-23.3441*T*LN(T)
 -.01107766*T**2+1.68426167E-06*T**3-32940.83*T**(-1); 800 Y
 +264409.117+43.3441104*T-36.96841*T*LN(T)-1.4749435E-04*T**2
 -4.47593333E-09*T**3+806237.5*T**(-1); 3700 Y

$+195465.035+281.919465*T-66.19102*T*LN(T)+.005436525*T**2$
 $-2.06924833E-07*T**3+31805505*T**(-1); 6000 N !$
 FUNCTION F4864T 298.15 +101622.94+54.9268214*T-42.16114*T*LN(T)
 $-.014747895*T**2+2.07496667E-06*T**3+194649.25*T**(-1); 900 Y$
 $+89045.1937+192.156083*T-62.25744*T*LN(T)-5.65491E-07*T**2$
 $-2.34309833E-08*T**3+1714276.5*T**(-1); 3700 Y$
 $+92590.9311+229.395211*T-67.6485*T*LN(T)+.002282751*T**2$
 $-1.47672533E-07*T**3-7203595*T**(-1); 6000 N !$
 FUNCTION F4954T 298.15 +803005.137+419.915369*T-97.48141*T*LN(T)
 $+0.08202995*T**2-1.97357E-05*T**3+690749.5*T**(-1); 500 Y$
 $+826732.964-2.78397075*T-30.08349*T*LN(T)-.002621389*T**2$
 $+8.30959667E-08*T**3-868501*T**(-1); 4300 Y$
 $+850321.493-26.7776267*T-27.96957*T*LN(T)-.0019408995*T**2$
 $+3.222655E-08*T**3-22380050*T**(-1); 12000 Y$
 $+409662.376+520.53814*T-86.66656*T*LN(T)+.0015642485*T**2$
 $-7.28093667E-09*T**3+6.04612E+08*T**(-1); 20000 N !$
 FUNCTION F5282T 298.15 +555907.867+57.0634842*T-39.08261*T*LN(T)
 $-.00569665*T**2-4.27085667E-07*T**3+135750.65*T**(-1); 1000 Y$
 $+560368.69-14.5499453*T-28.12154*T*LN(T)-.015627865*T**2$
 $+1.1143725E-06*T**3-38275.195*T**(-1); 2100 Y$
 $+500130.672+354.303072*T-77.12859*T*LN(T)+.001864081*T**2$
 $-4.41159667E-08*T**3+13617155*T**(-1); 6400 Y$
 $+548031.854+234.921123*T-63.15948*T*LN(T)+6.031155E-05*T**2$
 $-8.38662167E-10*T**3-17395655*T**(-1); 10000 N !$
 FUNCTION F5293T 298.15 +210657.364+102.660059*T-43.33318*T*LN(T)
 $-.015969725*T**2+1.09745783E-06*T**3+366936*T**(-1); 1700 Y$
 $+162805.829+400.859267*T-83.17592*T*LN(T)-8.50672E-04*T**2$
 $-8.40052167E-09*T**3+11371695*T**(-1); 4700 Y$
 $+284779.332+156.173741*T-55.55581*T*LN(T)-.003209261*T**2$
 $+1.402618E-08*T**3-81696300*T**(-1); 9200 Y$
 $+643212.249-464.67941*T+13.72962*T*LN(T)-.009112535*T**2$
 $+1.07541683E-07*T**3-4.2679415E+08*T**(-1); 10000 N !$
 FUNCTION F5299T 298.15 +154201.38+12.5688014*T-33.93*T*LN(T)
 $-.0509885*T**2+8.81055833E-06*T**3+241035*T**(-1); 500 Y$
 $+145311.134+167.937778*T-58.623*T*LN(T)-.0205257*T**2$
 $+1.76653333E-06*T**3+840645*T**(-1); 1200 Y$
 $+119932.693+377.102222*T-87.801*T*LN(T)-.0054466*T**2$
 $+2.84168333E-07*T**3+5014060*T**(-1); 2600 Y$
 $+93863.2024+508.137727*T-104.726*T*LN(T)-5.387E-04*T**2$
 $+1.68116667E-08*T**3+12610965*T**(-1); 3800 N !$
 FUNCTION F5305T 298.15 +253597.563-148.811942*T-7.989506*T*LN(T)
 $-.0560301*T**2+7.22032833E-06*T**3-86107.5*T**(-1); 700 Y$
 $+237578.897+66.4331994*T-40.61565*T*LN(T)-.026213335*T**2$
 $+2.05575833E-06*T**3+1400582*T**(-1); 1500 Y$
 $+180976.129+465.400317*T-94.92649*T*LN(T)-.0026392345*T**2$

$+1.00493533E-07*T^{**3}+12635730*T^{*(-1)}$; 3900 Y
 $+155481.051+562.46419*T-106.9625*T*LN(T)-1.2237275E-04*T^{**2}$
 $+2.58523833E-09*T^{**3}+22815630*T^{*(-1)}$; 6000 N !
 FUNCTION F5311T 298.15 +47209.5269-186.336653*T+1.510335*T*LN(T)
 $-.0796424*T^{**2}+1.11523633E-05*T^{**3}-126378.45*T^{*(-1)}$; 600 Y
 $+30955.0457+58.8547956*T-36.41994*T*LN(T)-.040167385*T^{**2}$
 $+3.41469333E-06*T^{**3}+1183016*T^{*(-1)}$; 1300 Y
 $-31590.202+549.033592*T-104.2592*T*LN(T)-.007018595*T^{**2}$
 $+3.29534167E-07*T^{**3}+12115675*T^{*(-1)}$; 3000 Y
 $-77650.6893+755.842185*T-130.5377*T*LN(T)-3.066123E-04*T^{**2}$
 $+7.24598833E-09*T^{**3}+27459580*T^{*(-1)}$; 6000 N !
 FUNCTION F5317T 298.15 -173989.405-156.99242*T-9.305309*T*LN(T)
 $-.08173745*T^{**2}+1.02731833E-05*T^{**3}-121696.15*T^{*(-1)}$; 700 Y
 $-197927.136+155.523133*T-56.42274*T*LN(T)-.040210435*T^{**2}$
 $+3.34282833E-06*T^{**3}+2170644*T^{*(-1)}$; 1400 Y
 $-274280.51+724.192005*T-134.4989*T*LN(T)-.004176673*T^{**2}$
 $+1.71613167E-07*T^{**3}+16359150*T^{*(-1)}$; 3600 Y
 $-316924.333+892.309086*T-155.4574*T*LN(T)+4.1221575E-04*T^{**2}$
 $-1.63666333E-08*T^{**3}+32783160*T^{*(-1)}$; 4000 N !
 FUNCTION F5323T 298.15 -52587.4389-367.766736*T+29.42306*T*LN(T)
 $-.137048*T^{**2}+2.3549E-05*T^{**3}-324160*T^{*(-1)}$; 500 Y
 $-76085.3585+34.7597657*T-34.304*T*LN(T)-.060357*T^{**2}$
 $+6.25980167E-06*T^{**3}+1297050*T^{*(-1)}$; 900 Y
 $-104329.9+338.34938*T-78.541*T*LN(T)-.02944585*T^{**2}$
 $+2.19053167E-06*T^{**3}+4688375*T^{*(-1)}$; 1500 Y
 $-164106.057+757.400795*T-135.495*T*LN(T)-.0051316*T^{**2}$
 $+2.26323333E-07*T^{**3}+16533735*T^{*(-1)}$; 3100 Y
 $-197141.811+902.107269*T-153.807*T*LN(T)-6.159E-04*T^{**2}$
 $+1.78383333E-08*T^{**3}+27759575*T^{*(-1)}$; 4000 N !
 FUNCTION F5330T 298.15 -443770.401-168.903162*T-8.022861*T*LN(T)
 $-.10740745*T^{**2}+1.413715E-05*T^{**3}+49334.8*T^{*(-1)}$; 700 Y
 $-479189.377+285.05528*T-76.23373*T*LN(T)-.048655465*T^{**2}$
 $+4.55710833E-06*T^{**3}+3510111*T^{*(-1)}$; 1500 N !
 FUNCTION F5334T 298.15 +8621.94322-384.629098*T+31.208*T*LN(T)
 $-.1601795*T^{**2}+2.74755333E-05*T^{**3}-313025*T^{*(-1)}$; 500 Y
 $-15763.4055+36.5705507*T-35.576*T*LN(T)-.079073*T^{**2}$
 $+9.04395833E-06*T^{**3}+1352495*T^{*(-1)}$; 800 Y
 $-44961.4649+381.012139*T-86.565*T*LN(T)-.039451*T^{**2}$
 $+3.26033833E-06*T^{**3}+4489500*T^{*(-1)}$; 1300 Y
 $-101873.985+828.994926*T-148.57*T*LN(T)-.00926205*T^{**2}+4.8636E-07*T^{**3}$
 $+14328215*T^{*(-1)}$; 2500 Y
 $-145162.193+1047.94919*T-176.8774*T*LN(T)-9.897E-04*T^{**2}$
 $+3.14933333E-08*T^{**3}+26837355*T^{*(-1)}$; 4000 N !
 FUNCTION F5343T 298.15 -110016.264-269.84409*T+9.078*T*LN(T)
 $-.1689285*T^{**2}+3.00849667E-05*T^{**3}-104210*T^{*(-1)}$; 500 Y

-137759.296+212.911373*T-67.573*T*LN(T)-.0750225*T**2
 +8.56395667E-06*T**3+1774235*T**(-1); 800 Y
 -167528.954+560.705951*T-118.974*T*LN(T)-.03550545*T**2
 +2.85085167E-06*T**3+5010055*T**(-1); 1400 Y
 -228407.378+1017.82394*T-181.782*T*LN(T)-.0064669*T**2
 +3.10746667E-07*T**3+16155935*T**(-1); 2800 Y
 -264379.384+1186.6594*T-203.3669*T*LN(T)-6.9185E-04*T**2
 +2.07466667E-08*T**3+27465860*T**(-1); 3800 N !
 FUNCTION F5350T 298.15 -213863.964-386.53547*T+29.724*T*LN(T)
 -.183427*T**2+3.207855E-05*T**3-280095*T**(-1); 500 Y
 -242918.696+115.241998*T-49.834*T*LN(T)-.086823*T**2+1.012866E-05*T**3
 +1704720*T**(-1); 800 Y
 -276566.651+513.323611*T-108.793*T*LN(T)-.0408541*T**2
 +3.39678667E-06*T**3+5307685*T**(-1); 1300 Y
 -333853.749+967.614253*T-171.745*T*LN(T)-.0099489*T**2
 +5.34976667E-07*T**3+15125605*T**(-1); 2400 Y
 -378502.295+1197.47539*T-201.544*T*LN(T)-.00104675*T**2
 +3.36483333E-08*T**3+27781530*T**(-1); 4000 N !
 FUNCTION F5357T 298.15 +103695.78-248.192017*T+6.535456*T*LN(T)
 -.0876786*T**2+1.08003583E-05*T**3-293497.1*T**(-1); 700 Y
 +80275.9858+60.5182301*T-40.0912*T*LN(T)-.046084495*T**2
 +3.772465E-06*T**3+1925892*T**(-1); 1400 Y
 -4338.1575+691.320485*T-126.6998*T*LN(T)-.00614309*T**2
 +2.665555E-07*T**3+17610670*T**(-1); 3300 Y
 -50997.0146+888.071661*T-151.4679*T*LN(T)-2.7785525E-04*T**2
 +6.34659667E-09*T**3+34266230*T**(-1); 6000 N !
 FUNCTION F5369T 298.15 -90150.09-192.644467*T+2.384174*T*LN(T)
 -.0962022*T**2+1.15030917E-05*T**3-161159.75*T**(-1); 700 Y
 -114140.24+121.641652*T-45.03662*T*LN(T)-.05415545*T**2
 +4.43007333E-06*T**3+2130084*T**(-1); 1400 Y
 -212082.164+853.908038*T-145.619*T*LN(T)-.007637925*T**2
 +3.37957333E-07*T**3+20220470*T**(-1); 3200 Y
 -268113.331+1093.5554*T-175.8524*T*LN(T)-3.4791075E-04*T**2
 +8.02933833E-09*T**3+39919465*T**(-1); 6000 N !
 FUNCTION F5375T 298.15 -243272.597-221.374773*T+.7796648*T*LN(T)
 -.12058845*T**2+1.72144833E-05*T**3-164276.9*T**(-1); 600 Y
 -269097.38+168.629562*T-59.56378*T*LN(T)-.05772375*T**2
 +4.884735E-06*T**3+1912790*T**(-1); 1300 Y
 -358292.955+867.098816*T-156.2194*T*LN(T)-.010522415*T**2
 +4.92514167E-07*T**3+17521960*T**(-1); 3000 Y
 -427579.406+1177.35994*T-195.6293*T*LN(T)-4.820784E-04*T**2
 +1.14137917E-08*T**3+40682500*T**(-1); 6000 N !
 FUNCTION F5385T 298.15 -416598.432+134.357846*T-60.84898*T*LN(T)
 -.0824635*T**2+9.70528667E-06*T**3+345719.2*T**(-1); 1000 N !
 FUNCTION F5466T 298.15 +277813.193+28.9798334*T-37.78569*T*LN(T)

$-.01453685*T^{**2}+1.57701533E-06*T^{**3}+112606.3*T^{**(-1)}$; 1000 Y
 $+264063.563+160.518573*T-56.6296*T*LN(T)-.0026141425*T^{**2}$
 $+9.85593667E-08*T^{**3}+2048364*T^{**(-1)}$; 3500 Y
 $+234215.001+257.69025*T-68.43674*T*LN(T)-4.895632E-04*T^{**2}$
 $+2.485785E-08*T^{**3}+16450450*T^{**(-1)}$; 6000 N !
 FUNCTION F5510T 298.15 +829826.554-14.7696351*T-32.21563*T*LN(T)
 $-.014548565*T^{**2}+1.77806833E-06*T^{**3}-100277.6*T^{**(-1)}$; 1000 Y
 $+809388.444+179.25291*T-59.93982*T*LN(T)+.0025413955*T^{**2}$
 $-2.54139667E-07*T^{**3}+2769455*T^{**(-1)}$; 2800 Y
 $+959399.017-367.175865*T+7.286391*T*LN(T)-.010483215*T^{**2}$
 $+2.00694833E-07*T^{**3}-58720050*T^{**(-1)}$; 5100 Y
 $+645204.419+237.848566*T-60.73106*T*LN(T)-.0047721765*T^{**2}$
 $+1.3846755E-07*T^{**3}+1.945987E+08*T^{**(-1)}$; 8000 Y
 $-79243.2062+1580.27099*T-211.8741*T*LN(T)+.009202285*T^{**2}$
 $-1.030498E-07*T^{**3}+8.44019E+08*T^{**(-1)}$; 10000 N !
 FUNCTION F5527T 298.15 +613954.728+55.2249448*T-41.546*T*LN(T)
 $-.03016625*T^{**2}+4.92478333E-06*T^{**3}+184525*T^{**(-1)}$; 500 Y
 $+608835.447+142.14087*T-55.285*T*LN(T)-.01377825*T^{**2}$
 $+1.25349667E-06*T^{**3}+541765*T^{**(-1)}$; 1100 Y
 $+596532.167+252.757204*T-70.937*T*LN(T)-.0048276505*T^{**2}$
 $+2.80586667E-07*T^{**3}+2371295*T^{**(-1)}$; 2200 Y
 $+578080.168+354.305523*T-84.237*T*LN(T)-5.236E-04*T^{**2}+1.732E-08*T^{**3}$
 $+7230080*T^{**(-1)}$; 4000 N !
 FUNCTION F5539T 298.15 +181410.617-122.851573*T-10.20607*T*LN(T)
 $-.09533745*T^{**2}+1.50758583E-05*T^{**3}$; 600 Y
 $+166868.714+123.51993*T-49.16033*T*LN(T)-.048685235*T^{**2}$
 $+4.554395E-06*T^{**3}+1025661.5*T^{**(-1)}$; 1350 N !
 FUNCTION F5542T 298.15 +173490.978-86.0624782*T-17.22925*T*LN(T)
 $-.0839689*T^{**2}+1.23994933E-05*T^{**3}$; 600 Y
 $+164149.935+76.784887*T-43.11068*T*LN(T)-.05198975*T^{**2}$
 $+4.980055E-06*T^{**3}+635844.5*T^{**(-1)}$; 1350 N !
 FUNCTION F5554T 298.15 -230878.388-155.527401*T-10.67908*T*LN(T)
 $-.1200629*T^{**2}+1.5123685E-05*T^{**3}+38056.18*T^{**(-1)}$; 600 Y
 $-239483.66-23.861997*T-31.11135*T*LN(T)-.09829625*T^{**2}$
 $+1.0728685E-05*T^{**3}+723035.5*T^{**(-1)}$; 1000 N !
 FUNCTION F5545T 298.15 +47561.7797-249.248396*T+11.66591*T*LN(T)
 $-.1167726*T^{**2}+7.967175E-06*T^{**3}-110552.1*T^{**(-1)}$; 500 Y
 $+6255.96595+329.947357*T-75.60937*T*LN(T)-.049720245*T^{**2}$
 $+3.64736667E-06*T^{**3}+3227275.5*T^{**(-1)}$; 2100 Y
 $-24416.4858+744.596724*T-135.1962*T*LN(T)-.016624375*T^{**2}$
 $+7.0133E-07*T^{**3}$; 4000 N !
 FUNCTION F5550T 298.15 +14789.4507-271.642378*T+11.34939*T*LN(T)
 $-.13386645*T^{**2}+2.00341833E-05*T^{**3}-272154.55*T^{**(-1)}$; 600 Y
 $-5877.08746+63.1182105*T-41.1683*T*LN(T)-.07381185*T^{**2}$
 $+7.01085E-06*T^{**3}+1272695.5*T^{**(-1)}$; 1350 N !

FUNCTION F5557T 298.15 -109364.396-321.907815*T+21.52618*T*LN(T)
 -.1721779*T**2+2.66239E-05*T**3-291993*T**(-1); 600 Y
 -136284.127+126.13378*T-49.09882*T*LN(T)-.08908635*T**2
 +8.15831167E-06*T**3+1652173.5*T**(-1); 1000 Y
 -139266.757+270.053278*T-72.22463*T*LN(T)-.0649997*T**2
 +4.53440333E-06*T**3; 1473.10 Y
 +257891.373-1948.43811*T+217.2249*T*LN(T)-.15124325*T**2
 +8.672805E-06*T**3-96828650*T**(-1); 2200 Y
 +99792.4667-390.62824*T+2.18137*T*LN(T)-.0596624*T**2
 +2.314065E-06*T**3-1.0470605E+08*T**(-1); 2800 Y
 +4552037.53-17003.1518*T+2055.691*T*LN(T)-.47848015*T**2
 +1.82760667E-05*T**3-1.903921E+09*T**(-1); 3400 Y
 -224887.496+1106.77062*T-188.6147*T*LN(T)-.01046*T**2; 4000 N !
 FUNCTION F5577T 298.15 -118237.391+100.762627*T-53.19108*T*LN(T)
 -.030805495*T**2+3.59023833E-06*T**3+332492.95*T**(-1); 1000 Y
 -150856.91+416.603392*T-98.47748*T*LN(T)-.0022049665*T**2
 +1.09623667E-07*T**3+4818702*T**(-1); 3300 Y
 -164679.617+482.276431*T-106.8785*T*LN(T)+2.986764E-05*T**2
 +4.29362E-10*T**3+9089650*T**(-1); 6000 N !
 FUNCTION F5587T 298.15 +1015583.43+114.927796*T-53.39543*T*LN(T)
 -.01399763*T**2+8.26027167E-07*T**3+181008.25*T**(-1); 2500 Y
 +937071.116+522.054721*T-106.1735*T*LN(T)+.0016641645*T**2
 -4.03015E-08*T**3+21906740*T**(-1); 7000 Y
 +974994.003+406.652032*T-92.4518*T*LN(T)-2.6888155E-04*T**2
 +7.07303167E-09*T**3+7587140*T**(-1); 10000 N !
 FUNCTION F5592T 298.15 +751541.722+252.532282*T-73.01*T*LN(T)
 -.0216856*T**2+2.96625833E-06*T**3+733430*T**(-1); 800 Y
 +739011.333+395.36198*T-94.137*T*LN(T)-.00478225*T**2+2.37405E-07*T**3
 +2194465*T**(-1); 3200 Y
 +712634.362+524.463672*T-110.728*T*LN(T)-2.049E-04*T**2+5.39E-09*T**3
 +10118465*T**(-1); 4000 N !
 FUNCTION F5597T 298.15 -137766.886-262.245087*T+8.962001*T*LN(T)
 -.1969312*T**2+2.74147E-05*T**3-206440*T**(-1); 600 Y
 -178579.034+346.123228*T-84.951*T*LN(T)-.10048435*T**2
 +8.73554E-06*T**3+3128305*T**(-1); 1300 Y
 -258789.548+1055.24805*T-184.924*T*LN(T)-.04513245*T**2
 +2.99413E-06*T**3+15193975*T**(-1); 1500 N !
 FUNCTION F5602T 298.15 -146155.003-277.516061*T+14.289*T*LN(T)
 -.2069239*T**2+2.98628333E-05*T**3-154585*T**(-1); 600 Y
 -195079.37+449.056779*T-97.801*T*LN(T)-.09222675*T**2
 +7.70571667E-06*T**3+3862255*T**(-1); 1500 N !
 FUNCTION F5607T 298.15 +457808.944-44.7518867*T-21.76299*T*LN(T)
 -.11261945*T**2+2.86132667E-05*T**3; 500 Y
 +443516.683+275.781658*T-75.16975*T*LN(T)-.02513559*T**2
 +2.115835E-06*T**3+708872*T**(-1); 1000 N !

FUNCTION F5610T 298.15 +473135.073-401.772245*T+38.1181*T*LN(T)
 -.21418665*T**2+6.02402333E-05*T**3-719254.5*T**(-1); 500 Y
 +443504.881+275.881177*T-75.18027*T*LN(T)-.02512842*T**2
 +2.11473333E-06*T**3+709293*T**(-1); 1000 N !
 FUNCTION F5614T 298.15 +370172.153-109.109385*T-11.397*T*LN(T)
 -.1111325*T**2+1.61656983E-05*T**3+358940*T**(-1); 700 Y
 +325301.98+486.389913*T-101.491*T*LN(T)-.0296325*T**2
 +2.12065333E-06*T**3+4595505*T**(-1); 1900 Y
 +243710.536+1013.16655*T-172.226*T*LN(T)-.00194705*T**2
 +6.80733333E-08*T**3+22628525*T**(-1); 4000 N !
 FUNCTION F5619T 298.15 +288051.702-62.1217039*T-23.51726*T*LN(T)
 -.10484665*T**2+1.70475E-05*T**3+166261.7*T**(-1); 600 Y
 +271269.255+222.99465*T-68.63141*T*LN(T)-.05050485*T**2
 +4.70099667E-06*T**3+1349256.5*T**(-1); 1350 N !
 FUNCTION F5623T 298.15 +148974.923-154.988667*T-9.679935*T*LN(T)
 -.13252255*T**2+1.875805E-05*T**3-64604.3*T**(-1); 700 Y
 +143586.528-18.9490501*T-32.19739*T*LN(T)-.0996706*T**2
 +1.0683635E-05*T**3; 1350 N !
 FUNCTION F5626T 298.15 +121653.925-773.246123*T+98.0989*T*LN(T)
 -.3288666*T**2+8.00427167E-05*T**3-1078152*T**(-1); 500 Y
 +69670.1413+288.910378*T-76.01784*T*LN(T)-.06784355*T**2
 +6.41405167E-06*T**3+1865350.5*T**(-1); 1350 N !
 FUNCTION F5630T 298.15 +171954.749-626.535566*T+70.21254*T*LN(T)
 -.27331145*T**2+6.370085E-05*T**3-1007086.5*T**(-1); 500 Y
 +134813.21+143.300138*T-56.40032*T*LN(T)-.0793759*T**2
 +7.720665E-06*T**3+1073901*T**(-1); 1350 N !
 FUNCTION F5633T 298.15 +137810.196-224.576236*T+2.364458*T*LN(T)
 -.14050145*T**2+2.03154833E-05*T**3-328490*T**(-1); 600 Y
 +121325.209+49.3857422*T-40.8135*T*LN(T)-.0897223*T**2
 +9.02328333E-06*T**3+865653*T**(-1); 1350 N !
 FUNCTION F5636T 298.15 +151050.533-349.7586*T+27.653*T*LN(T)
 -.17688495*T**2+2.748815E-05*T**3-55550*T**(-1); 600 Y
 +103768.902+358.874068*T-81.845*T*LN(T)-.0637295*T**2
 +5.44480167E-06*T**3+3783270*T**(-1); 1400 Y
 -17659.4864+1268.26244*T-206.872*T*LN(T)-.0052678*T**2
 +2.01658333E-07*T**3+26324075*T**(-1); 4000 N !
 FUNCTION F5641T 298.15 -8210.219-329.421377*T+18.37912*T*LN(T)
 -.1889842*T**2+2.93304167E-05*T**3-306315.8*T**(-1); 600 Y
 -42178.1931+215.960694*T-67.05554*T*LN(T)-.09210105*T**2
 +8.450665E-06*T**3+2263202*T**(-1); 1200 Y
 -130121.873+993.754763*T-176.8323*T*LN(T)-.030438405*T**2
 +1.87789167E-06*T**3+15637365*T**(-1); 2000 Y
 -216193.539+1506.20974*T-244.7327*T*LN(T)-.006487595*T**2
 +2.86020333E-07*T**3+36241530*T**(-1); 3000 N !
 FUNCTION F5647T 298.15 -18945.8335-283.556707*T+11.98474*T*LN(T)

$-1.17460525 \cdot T^{**2} + 2.51491167E-05 \cdot T^{**3} - 397894.75 \cdot T^{**(-1)}$; 600 Y
 $-44950.4819 + 130.117298 \cdot T - 52.691 \cdot T \cdot \text{LN}(T) - .1022542 \cdot T^{**2}$
 $+ 9.79442167E-06 \cdot T^{**3} + 1585811.5 \cdot T^{**(-1)}$; 1100 Y
 $-116824.16 + 814.53923 \cdot T - 150.4492 \cdot T \cdot \text{LN}(T) - .042630065 \cdot T^{**2}$
 $+ 2.91602167E-06 \cdot T^{**3} + 11581820 \cdot T^{**(-1)}$; 1750 Y
 $-219547.969 + 1479.9903 \cdot T - 239.7939 \cdot T \cdot \text{LN}(T) - .00777792 \cdot T^{**2}$
 $+ 3.4526E-07 \cdot T^{**3} + 33938005 \cdot T^{**(-1)}$; 3000 N !
 FUNCTION F5653T 298.15 -11391.893-395.309325*T+29.39824*T*LN(T)
 $- .1936934 \cdot T^{**2} + 2.94108167E-05 \cdot T^{**3} - 432631.6 \cdot T^{**(-1)}$; 600 Y
 $-43481.5748 + 120.364328 \cdot T - 51.38171 \cdot T \cdot \text{LN}(T) - .1021776 \cdot T^{**2}$
 $+ 9.74020833E-06 \cdot T^{**3} + 1988277.5 \cdot T^{**(-1)}$; 1100 Y
 $-128709.639 + 909.729836 \cdot T - 163.6294 \cdot T \cdot \text{LN}(T) - .035726125 \cdot T^{**2}$
 $+ 2.273825E-06 \cdot T^{**3} + 14245785 \cdot T^{**(-1)}$; 2000 Y
 $-233778.194 + 1541.4989 \cdot T - 247.4912 \cdot T \cdot \text{LN}(T) - .005688125 \cdot T^{**2}$
 $+ 2.41366833E-07 \cdot T^{**3} + 39223410 \cdot T^{**(-1)}$; 3000 N !
 FUNCTION F5659T 298.15 +30711.3286-548.35032*T+61.29298*T*LN(T)
 $- .2385237 \cdot T^{**2} + 3.930995E-05 \cdot T^{**3} - 470526.3 \cdot T^{**(-1)}$; 600 Y
 $-14782.0589 + 192.903424 \cdot T - 55.11038 \cdot T \cdot \text{LN}(T) - .1046635 \cdot T^{**2}$
 $+ 1.01558083E-05 \cdot T^{**3} + 2903410 \cdot T^{**(-1)}$; 1100 Y
 $-75595.0552 + 789.682221 \cdot T - 140.7766 \cdot T \cdot \text{LN}(T) - .05058985 \cdot T^{**2}$
 $+ 3.71002667E-06 \cdot T^{**3} + 11071240 \cdot T^{**(-1)}$; 1500 N !
 FUNCTION F5664T 298.15 -28097.5305-228.033699*T+3.874737*T*LN(T)
 $- .16745525 \cdot T^{**2} + 2.398245E-05 \cdot T^{**3} - 217894.75 \cdot T^{**(-1)}$; 600 Y
 $-55000.3392 + 194.236321 \cdot T - 61.99373 \cdot T \cdot \text{LN}(T) - .0947565 \cdot T^{**2}$
 $+ 8.71897167E-06 \cdot T^{**3} + 1869942 \cdot T^{**(-1)}$; 1200 Y
 $-145425.339 + 995.955149 \cdot T - 175.186 \cdot T \cdot \text{LN}(T) - .031046835 \cdot T^{**2}$
 $+ 1.91997333E-06 \cdot T^{**3} + 15573255 \cdot T^{**(-1)}$; 2000 Y
 $-234006.028 + 1523.70103 \cdot T - 245.1252 \cdot T \cdot \text{LN}(T) - .006331555 \cdot T^{**2}$
 $+ 2.72984333E-07 \cdot T^{**3} + 36784840 \cdot T^{**(-1)}$; 3000 N !
 FUNCTION F5670T 298.15 +17823.7974-371.344599*T+30.27895*T*LN(T)
 $- .21539605 \cdot T^{**2} + 3.63464833E-05 \cdot T^{**3} - 151578.95 \cdot T^{**(-1)}$; 600 Y
 $-24422.3503 + 326.276558 \cdot T - 79.56271 \cdot T \cdot \text{LN}(T) - .08687185 \cdot T^{**2}$
 $+ 7.8498E-06 \cdot T^{**3} + 2938210 \cdot T^{**(-1)}$; 1200 Y
 $-114562.636 + 1108.30425 \cdot T - 189.5887 \cdot T \cdot \text{LN}(T) - .02642438 \cdot T^{**2}$
 $+ 1.54113033E-06 \cdot T^{**3} + 16948625 \cdot T^{**(-1)}$; 2250 Y
 $-77182.5939 + 1021.89114 \cdot T - 180.4774 \cdot T \cdot \text{LN}(T) - .02427573 \cdot T^{**2}$
 $+ 1.143287E-06 \cdot T^{**3}$; 3000 N !
 FUNCTION F5696T 298.15 +1028316.51+169.994576*T-62.97185*T*LN(T)
 $- .0317015 \cdot T^{**2} + 4.09694E-06 \cdot T^{**3} + 186275.3 \cdot T^{**(-1)}$; 900 Y
 $+ 999750.247 + 470.150388 \cdot T - 106.5965 \cdot T \cdot \text{LN}(T) - .0014783715 \cdot T^{**2}$
 $+ 7.07236167E-08 \cdot T^{**3} + 3747842.5 \cdot T^{**(-1)}$; 3500 Y
 $+ 990603.918 + 513.736611 \cdot T - 112.1708 \cdot T \cdot \text{LN}(T) - 6.611165E-06 \cdot T^{**2}$
 $+ 1.10554567E-10 \cdot T^{**3} + 6565820 \cdot T^{**(-1)}$; 10000 N !
 FUNCTION F5719T 298.15 +2466802.51+88.4522193*T+10.293*T*LN(T)
 $- 1.15472 \cdot T^{**2} + 1.77008333E-04 \cdot T^{**3} + 4621630 \cdot T^{**(-1)}$; 800 Y

$+1709986.12+9262.28939*T-1356.31*T*LN(T)-.0366229*T**2$
 $+1.98371667E-06*T**3+84578000*T**(-1); 3300 N !$
 FUNCTION F5740T 298.15 +71643.2857-315.496947*T+25.001*T*LN(T)
 $-.2161207*T**2+3.431025E-05*T**3+151720*T**(-1); 600 Y$
 $+13101.0393+567.138312*T-111.518*T*LN(T)-.07424425*T**2$
 $+6.56452833E-06*T**3+4867785*T**(-1); 1300 Y$
 $-109518.172+1531.0277*T-245.03*T*LN(T)-.00845165*T**2$
 $+3.60173333E-07*T**3+26305545*T**(-1); 3500 Y$
 $-158376.968+1751.98658*T-273.057*T*LN(T)-.0015082*T**2$
 $+4.57316667E-08*T**3+41807370*T**(-1); 4000 N !$
 FUNCTION F5748T 298.15 -115232.054-209.218178*T+2.935807*T*LN(T)
 $-.222882*T**2+3.73738333E-05*T**3+285881.45*T**(-1); 600 Y$
 $-166306.578+593.403695*T-122.2293*T*LN(T)-.0853405*T**2$
 $+8.77358E-06*T**3+4226408.5*T**(-1); 900 N !$
 FUNCTION F11215T 298.15 +211801.621+24.4989816*T-20.78611*T*LN(T); 6000
 N
 !
 FUNCTION F11630T 298.15 +192464.748-96.3751151*T-16.12159*T*LN(T)
 $-.019769105*T**2+2.97138167E-06*T**3-147023.6*T**(-1); 800 Y$
 $+178828.93+69.270114*T-40.76914*T*LN(T)+6.024005E-05*T**2$
 $-2.46963833E-08*T**3+1269206.5*T**(-1); 2800 Y$
 $+106642.034+316.320166*T-70.80509*T*LN(T)+.00515165*T**2$
 $-1.59829817E-07*T**3+32167195*T**(-1); 6000 N !$
 FUNCTION F11635T 298.15 +723.159727+85.0011665*T-49.41051*T*LN(T)
 $-.002983041*T**2+1.06815967E-07*T**3+238607.4*T**(-1); 1800 Y$
 $-14646.2096+161.938551*T-59.27522*T*LN(T)-4.589964E-04*T**2$
 $+1.27830317E-08*T**3+4463203.5*T**(-1); 6000 N !$
 FUNCTION F11257T 298.15 +30698.6898+15.9096451*T-29.97699*T*LN(T)
 $+0.001713168*T**2-6.799205E-07*T**3-25503.82*T**(-1); 1000 Y$
 $+31735.5127-12.686636*T-25.42186*T*LN(T)-.003149545*T**2$
 $+1.34404917E-07*T**3+116618.65*T**(-1); 3000 Y$
 $+41016.0783-20.7343256*T-24.94216*T*LN(T)-.0023107985*T**2$
 $+5.91863E-08*T**3-6415210*T**(-1); 8600 Y$
 $-154907.953+370.326117*T-69.24542*T*LN(T)+.0019361405*T**2$
 $-1.47539017E-08*T**3+1.4391015E+08*T**(-1); 18000 Y$
 $+326722.277-65.0792741*T-24.2768*T*LN(T)+6.42189E-05*T**2$
 $-1.30298483E-10*T**3-8.292415E+08*T**(-1); 20000 N !$
 FUNCTION F11478T 298.15 +38833.5298-61.4553091*T-25.08583*T*LN(T)
 $-.021295975*T**2+2.86032667E-06*T**3+6660.06*T**(-1); 800 Y$
 $+24701.0525+100.414687*T-48.95509*T*LN(T)-.0030700765*T**2$
 $+1.908655E-07*T**3+1593906.5*T**(-1); 2300 Y$
 $+26563.2426+117.193958*T-51.63391*T*LN(T)-.0011282815*T**2$
 $+1.99740167E-08*T**3-602425.5*T**(-1); 6000 N !$
 FUNCTION F11483T 298.15 -12074.5083-39.442205*T-28.3291*T*LN(T)
 $-.017353635*T**2+2.546495E-06*T**3+49872.41*T**(-1); 700 Y$

$-15150.1143+17.7050856*T-37.40635*T*LN(T)-.006661085*T**2$
 $+3.289565E-07*T**3+203749.6*T**(-1); 3100 Y$
 $-73720.2397+266.782146*T-68.81657*T*LN(T)+9.10981E-04*T**2$
 $-1.56616617E-08*T**3+21024835*T**(-1); 6000 N !$
 FUNCTION F11704T 298.15 -211011.861+97.08518*T-51.07715*T*LN(T)
 $-.0018230565*T**2-3.713795E-08*T**3+226770.35*T**(-1); 1600 Y$
 $-217144.887+132.05844*T-55.5966*T*LN(T)-7.85282E-04*T**2$
 $-2.62417E-08*T**3+1545066.5*T**(-1); 4800 Y$
 $-160734.305-60.3177521*T-32.15836*T*LN(T)-.004982475*T**2$
 $+1.1111805E-07*T**3-23003520*T**(-1); 6000 N !$
 FUNCTION F11280T 298.15 +1075.64106-55.242048*T-24.45435*T*LN(T)
 $-.018507875*T**2+2.36297E-06*T**3-29469.05*T**(-1); 800 Y$
 $-7932.99164+54.2016233*T-40.775*T*LN(T)-.00501027*T**2$
 $+2.122915E-07*T**3+925845*T**(-1); 3600 Y$
 $-67875.8961+275.406716*T-68.1173*T*LN(T)+6.12331E-04*T**2$
 $-6.573855E-09*T**3+26048030*T**(-1); 6000 N !$
 FUNCTION F11456T 298.15 +130854.682+30.526787*T-34.25937*T*LN(T)
 $+0.00583824*T**2-1.79746E-06*T**3-33304.895*T**(-1); 700 Y$
 $+133769.366-23.7043912*T-25.65337*T*LN(T)-.0042003385*T**2$
 $+2.51694667E-07*T**3-174588.25*T**(-1); 2200 Y$
 $+140179.423-26.6228167*T-25.86682*T*LN(T)-.00276017*T**2$
 $+9.24508333E-08*T**3-3805126*T**(-1); 6000 N !$
 FUNCTION F11767T 298.15 +211140.912-43.6301674*T-24.36669*T*LN(T)
 $-.01080168*T**2+1.61599E-06*T**3-7957.64*T**(-1); 800 Y$
 $+206276.789+21.9054667*T-34.29294*T*LN(T)-.0018393885*T**2$
 $+1.05009867E-07*T**3+436740.95*T**(-1); 3100 Y$
 $+276729.92-164.13142*T-12.69107*T*LN(T)-.0038473845*T**2$
 $+8.15391167E-08*T**3-37046305*T**(-1); 5600 Y$
 $+340796.01-362.685884*T+11.13054*T*LN(T)-.007566195*T**2$
 $+1.86267333E-07*T**3-66454900*T**(-1); 6000 N !$
 FUNCTION F11795T 298.15 +508873.032-56.3652528*T-23.04183*T*LN(T)
 $-.01071154*T**2+1.4689955E-06*T**3-46462.485*T**(-1); 1000 Y$
 $+500139.247+39.1135316*T-37.03719*T*LN(T)-3.8075865E-04*T**2$
 $+2.06460167E-09*T**3+1021210*T**(-1); 6000 N !$
 FUNCTION F11227T 298.15 -9522.97393+78.5273873*T-31.35707*T*LN(T)
 $+0.0027589925*T**2-7.46390667E-07*T**3+56582.3*T**(-1); 1000 Y$
 $+180.10884-15.6128262*T-17.84857*T*LN(T)-.00584168*T**2$
 $+3.14618667E-07*T**3-1280036*T**(-1); 2100 Y$
 $-18840.1661+92.3120249*T-32.05082*T*LN(T)-.0010728235*T**2$
 $+1.14281783E-08*T**3+3561002.5*T**(-1); 6000 N !$
 FUNCTION F11295T 298.15 -250423.434+4.45470312*T-28.40916*T*LN(T)
 $-.00623741*T**2-6.01526167E-08*T**3-64163.45*T**(-1); 1100 Y$
 $-256145.879+30.1894682*T-31.43044*T*LN(T)-.007055445*T**2$
 $+3.05535833E-07*T**3+1246309.5*T**(-1); 2800 Y$
 $-268423.418+116.690197*T-42.96842*T*LN(T)-.003069987*T**2$

$+6.97594167E-08*T^{**3}+2458230.5*T^{**(-1)}$; 8400 Y
 $-489068.882+553.259882*T-92.4077*T*LN(T)+.0016703495*T^{**2}$
 $-1.32333233E-08*T^{**3}+1.765625E+08*T^{**(-1)}$; 18000 Y
 $-165728.771+239.645643*T-59.77872*T*LN(T)+2.213599E-04*T^{**2}$
 $-1.2921095E-09*T^{**3}-4.1931655E+08*T^{**(-1)}$; 20000 N !
 FUNCTION F11488T 298.15 -61018.7584-110.206736*T-15.89155*T*LN(T)
 $-.041483285*T^{**2}+5.65694E-06*T^{**3}-20429.22*T^{**(-1)}$; 700 Y
 $-75894.9894+84.973425*T-45.35345*T*LN(T)-.01526317*T^{**2}$
 $+1.22104317E-06*T^{**3}+1399777*T^{**(-1)}$; 1600 Y
 $-113061.546+340.82609*T-80.07464*T*LN(T)-4.855578E-04*T^{**2}$
 $+1.41639233E-08*T^{**3}+9045045*T^{**(-1)}$; 6000 N !
 FUNCTION F11493T 298.15 -145758.404+2.65845704*T-34.4398*T*LN(T)
 $-.0259218*T^{**2}+3.29976667E-06*T^{**3}+168575.7*T^{**(-1)}$; 700 Y
 $-154483.028+115.388571*T-51.42471*T*LN(T)-.010899305*T^{**2}$
 $+7.38650167E-07*T^{**3}+1022325*T^{**(-1)}$; 2000 Y
 $-190674.476+332.667087*T-80.29469*T*LN(T)-4.119957E-04*T^{**2}$
 $+1.11888783E-08*T^{**3}+9783670*T^{**(-1)}$; 6000 N !
 FUNCTION F11314T 298.15 -147258.971-37.1497212*T-26.10636*T*LN(T)
 $-.036948065*T^{**2}+6.659505E-06*T^{**3}+65357.65*T^{**(-1)}$; 700 Y
 $-156470.505+120.191295*T-50.94271*T*LN(T)-.007931945*T^{**2}$
 $+4.29733833E-07*T^{**3}+684985.5*T^{**(-1)}$; 1500 N !
 FUNCTION F11871T 298.15 -626192.477+287.258861*T-88.19521*T*LN(T)
 $-.0011883405*T^{**2}-4.668365E-07*T^{**3}+456273.05*T^{**(-1)}$; 1300 Y
 $-639612.235+340.042601*T-94.27536*T*LN(T)-.002671967*T^{**2}$
 $+9.71441E-08*T^{**3}+4022410*T^{**(-1)}$; 4300 Y
 $-666861.947+441.763571*T-106.8445*T*LN(T)-1.3221325E-04*T^{**2}$
 $+2.73737E-09*T^{**3}+15095910*T^{**(-1)}$; 6000 N !
 FUNCTION F11498T 298.15 -761674.657+143.621194*T-59.55665*T*LN(T)
 $-.0687444*T^{**2}+1.09779717E-05*T^{**3}+485988.75*T^{**(-1)}$; 750 Y
 $-792877.748+560.495373*T-122.7873*T*LN(T)-.01021921*T^{**2}$
 $+5.72549167E-07*T^{**3}+3456344*T^{**(-1)}$; 2750 Y
 $-851792.667+841.907226*T-159.0106*T*LN(T)+2.152254E-04*T^{**2}$
 $-6.970215E-09*T^{**3}+22853300*T^{**(-1)}$; 6000 N !
 FUNCTION F11467T 298.15 -28637.4626-29.7124465*T-25.37431*T*LN(T)
 $-.012230205*T^{**2}+6.62201E-07*T^{**3}-86459.2*T^{**(-1)}$; 900 Y
 $-38442.2652+51.1969045*T-36.54058*T*LN(T)-.007461545*T^{**2}$
 $+4.40338167E-07*T^{**3}+1395975*T^{**(-1)}$; 2200 Y
 $-65256.7664+203.938596*T-56.66161*T*LN(T)-6.40182E-04*T^{**2}$
 $+2.14147833E-09*T^{**3}+8250950*T^{**(-1)}$; 6000 N !
 FUNCTION F11474T 298.15 -1716.28132+84.8441278*T-51.37952*T*LN(T)
 $-.00808767*T^{**2}+210246*T^{**(-1)}$; 1000 N !
 FUNCTION F12997T 298.15 +418123.955-30.3347885*T-22.06299*T*LN(T)
 $-.005444405*T^{**2}+4.71447833E-07*T^{**3}+102710.1*T^{**(-1)}$; 600 Y
 $+422478.905-85.4786167*T-13.83676*T*LN(T)-.011938995*T^{**2}$
 $+1.33826017E-06*T^{**3}-312130.2*T^{**(-1)}$; 1300 Y

$+400310.17+114.016724*T-42.00406*T*LN(T)+.0037094435*T**2$
 $-2.70261E-07*T**3+2891891*T**(-1); 3200 Y$
 $+493601.747-246.085237*T+2.791973*T*LN(T)-.006002155*T**2$
 $+1.30043383E-07*T**3-34158815*T**(-1); 8200 Y$
 $-96493.044+773.338363*T-111.0188*T*LN(T)+.0037862445*T**2$
 $-2.82257667E-08*T**3+5.418475E+08*T**(-1); 10000 N !$
FUNCTION F13020T 298.15 -124719.967-24.5469489*T-31.53764*T*LN(T)
 $-.0051956*T**2+7.60442333E-07*T**3+103677.85*T**(-1); 900 Y$
 $-126335.849+7.93847572*T-36.65559*T*LN(T)+2.4937065E-04*T**2$
 $-2.05688333E-07*T**3+108868.35*T**(-1); 2500 Y$
 $-130958.323-23.9414483*T-31.58251*T*LN(T)-.003177688*T**2$
 $+6.84986667E-08*T**3+5676870*T**(-1); 5400 Y$
 $-32341.6729-213.786313*T-10.21743*T*LN(T)-.005021225*T**2$
 $+9.162985E-08*T**3-74562000*T**(-1); 10000 N !$
FUNCTION F13037T 298.15 +123600.016-4.19888215*T-36.87727*T*LN(T)
 $-3.3164895E-04*T**2+3.59814167E-08*T**3+102571.4*T**(-1); 1800 Y$
 $+123712.587-2.40996102*T-37.17526*T*LN(T)-3.699702E-05*T**2; 3000 N !$
FUNCTION F13057T 298.15 -22020.3276+46.9195451*T-51.12563*T*LN(T)
 $-.005701935*T**2+8.637425E-07*T**3+212452.95*T**(-1); 1000 Y$
 $-25871.5823+93.9280348*T-58.13034*T*LN(T)-1.332372E-05*T**2$
 $+4.41584333E-10*T**3+616730*T**(-1); 6000 N !$
FUNCTION F13061T 298.15 -611505.065+54.8487779*T-51.72813*T*LN(T)
 $-.028452875*T**2+4.99643833E-06*T**3+271002.95*T**(-1); 700 Y$
 $-626470.385+256.452172*T-82.32033*T*LN(T)-1.8245965E-04*T**2$
 $+6.891315E-09*T**3+1664162*T**(-1); 5100 Y$
 $-641095.137+293.838139*T-86.72291*T*LN(T)+4.319301E-04*T**2$
 $-9.75906E-09*T**3+11187120*T**(-1); 6000 N !$
FUNCTION F13413T 298.15 +276164.054-34.4987551*T-20.786*T*LN(T); 1575 Y
 $+275547.585-29.248057*T-21.52064*T*LN(T)+3.819474E-04*T**2$
 $-3.66030333E-08*T**3+95180.95*T**(-1); 2100 Y$
 $+274521.741-16.384493*T-23.35302*T*LN(T)+.0013469965*T**2$
 $-1.18903067E-07*T**3; 2400 N !$
FUNCTION F13428T 298.15 +151356.092-24.1662503*T-31.02229*T*LN(T)
 $-.005519525*T**2+8.47063667E-07*T**3+97921.9*T**(-1); 900 Y$
 $+146503.882+29.4389958*T-38.90434*T*LN(T)+4.8722855E-04*T**2$
 $-5.46958333E-08*T**3+687003.5*T**(-1); 4100 Y$
 $+163891.797+1.2422565*T-35.94693*T*LN(T)+6.220655E-04*T**2$
 $-7.949125E-08*T**3-12461235*T**(-1); 6000 N !$
FUNCTION F13435T 298.15 +9095.11832-9.18675114*T-36.92694*T*LN(T)
 $-.01944391*T**2+3.43552E-06*T**3+201368.45*T**(-1); 700 Y$
 $-4061.05443+167.414545*T-63.68895*T*LN(T)+.004964408*T**2$
 $-7.80481667E-07*T**3+1423101*T**(-1); 2000 Y$
 $+74138.972-312.782575*T+1.646534*T*LN(T)-.01801756*T**2$
 $+7.59669E-07*T**3-16355180*T**(-1); 3900 Y$
 $-269662.306+860.503282*T-143.1466*T*LN(T)+.008591745*T**2$

$-1.67854167E-07*T^{**3}+1.388169E+08*T^{**(-1)}$; 6000 N !
 FUNCTION F13461T 298.15 +272029.962+.537998086*T-36.95707*T*LN(T)
 $-4.0083575E-04*T^{**2}+1.0645185E-08*T^{**3}+118696.6*T^{**(-1)}$; 2200 Y
 $+280098.89-22.4879433*T-34.31285*T*LN(T)-4.461327E-04*T^{**2}$
 $-2.35506167E-08*T^{**3}-3400330*T^{**(-1)}$; 5800 Y
 $+290313.272-81.9175565*T-26.85443*T*LN(T)-.001945821*T^{**2}$
 $+2.453735E-08*T^{**3}+543722*T^{**(-1)}$; 6000 N !
 FUNCTION F14527T 298.15 -3561.23425-48.0819156*T-25.11393*T*LN(T)
 $-.010079175*T^{**2}+1.56476567E-06*T^{**3}+5439.39*T^{**(-1)}$; 800 Y
 $-7112.74734+7.70326848*T-33.73371*T*LN(T)-.001472197*T^{**2}$
 $+3.03207333E-08*T^{**3}+242592.75*T^{**(-1)}$; 2900 Y
 $-29478.9518+85.9225956*T-43.27841*T*LN(T)+2.1038515E-04*T^{**2}$
 $-1.814365E-08*T^{**3}+9628580*T^{**(-1)}$; 6000 N !
 FUNCTION F14532T 298.15 -70285.9261+1.34023828*T-38.37728*T*LN(T)
 $-.01772857*T^{**2}+3.08948E-06*T^{**3}+141256.25*T^{**(-1)}$; 800 Y
 $-79745.5408+126.983393*T-57.41787*T*LN(T)-2.2150725E-04*T^{**2}$
 $+1.125761E-08*T^{**3}+1053081.5*T^{**(-1)}$; 3400 Y
 $-80760.3244+132.541894*T-58.14045*T*LN(T)-9.364045E-06*T^{**2}$
 $+2.61617833E-10*T^{**3}+1301305.5*T^{**(-1)}$; 6000 N !
 FUNCTION F14596T 298.15 -25476.974+3.04351917*T-34.37623*T*LN(T)
 $-.0026980695*T^{**2}+3.78874167E-07*T^{**3}+120146.05*T^{**(-1)}$; 900 Y
 $-44602.1418+205.651626*T-63.83687*T*LN(T)+.017645965*T^{**2}$
 $-2.284235E-06*T^{**3}+2463047*T^{**(-1)}$; 1800 Y
 $+243278.077-1500.21201*T+161.9497*T*LN(T)-.0612273*T^{**2}$
 $+2.896125E-06*T^{**3}-66468000*T^{**(-1)}$; 2900 Y
 $-571113.316+1685.71588*T-234.6556*T*LN(T)+.024571595*T^{**2}$
 $-5.82819833E-07*T^{**3}+2.468897E+08*T^{**(-1)}$; 4500 Y
 $-14433.8512+256.066958*T-66.76292*T*LN(T)+.002226246*T^{**2}$
 $-2.98498E-08*T^{**3}-97083400*T^{**(-1)}$; 8800 Y
 $+52967.3443+134.904342*T-53.17021*T*LN(T)+.001008387*T^{**2}$
 $-9.46948833E-09*T^{**3}-1.6008755E+08*T^{**(-1)}$; 10000 N !
 FUNCTION F14718T 298.15 -50330.1332-24.7804598*T-30.58571*T*LN(T)
 $-.005797885*T^{**2}+9.044075E-07*T^{**3}+92955.75*T^{**(-1)}$; 900 Y
 $-56752.7506+43.7949237*T-40.60318*T*LN(T)+.0014897095*T^{**2}$
 $-1.41268333E-07*T^{**3}+896318.5*T^{**(-1)}$; 3100 Y
 $+28620.308-236.507016*T-6.632106*T*LN(T)-.004295709*T^{**2}$
 $+3.30261667E-08*T^{**3}-38281150*T^{**(-1)}$; 5900 Y
 $+84089.9265-450.365301*T+19.37683*T*LN(T)-.00859432*T^{**2}$
 $+1.53217517E-07*T^{**3}-45013010*T^{**(-1)}$; 9600 Y
 $-943641.433+1103.17067*T-151.1803*T*LN(T)+.004000447*T^{**2}$
 $-2.13031E-08*T^{**3}+1.118062E+09*T^{**(-1)}$; 10000 N !
 FUNCTION F14734T 298.15 -13143.6008+47.2728177*T-49.14357*T*LN(T)
 $-.007582635*T^{**2}+1.2067E-06*T^{**3}+211591.55*T^{**(-1)}$; 900 Y
 $-17899.898+106.946885*T-58.08361*T*LN(T)-2.2921245E-05*T^{**2}$
 $+7.790445E-10*T^{**3}+695520*T^{**(-1)}$; 6000 N !

FUNCTION F14754T 298.15 +84650.2481-322.81686*T+21.98592*T*LN(T)
 -.10713165*T**2+2.81704E-05*T**3-333363.35*T**(-1); 500 Y
 +42648.3266+404.46472*T-93.37933*T*LN(T)+.03332466*T**2
 -3.80849833E-06*T**3+2526299*T**(-1); 1100 Y
 +84838.7072+11.5277083*T-37.46259*T*LN(T)+9.16682E-05*T**2
 -7.005105E-08*T**3-3491878*T**(-1); 4100 Y
 +106867.647-98.6658678*T-23.49987*T*LN(T)-.00315689*T**2
 +5.93994E-08*T**3-6661880*T**(-1); 9600 Y
 +255442.536-262.961956*T-6.281221*T*LN(T)-.0038787795*T**2
 +6.18786667E-08*T**3-2.2466925E+08*T**(-1); 10000 N !
 FUNCTION F14375T 298.15 -6965.21532-50.5304315*T-22.3649*T*LN(T)
 -.00990912*T**2+1.20026583E-06*T**3-77535.75*T**(-1); 600 Y
 -8807.78237-26.3126811*T-25.99933*T*LN(T)-.00694323*T**2
 +8.04195333E-07*T**3+90022.35*T**(-1); 1000 Y
 -15052.1241+39.5601504*T-35.57101*T*LN(T)-3.708985E-04*T**2
 -4.80521167E-08*T**3+860271.5*T**(-1); 2300 Y
 -8823.65673+3.71926228*T-30.85139*T*LN(T)-.0019495235*T**2
 +5.02773E-08*T**3-670976*T**(-1); 4100 Y
 -7013.9736+6.93103034*T-31.38542*T*LN(T)-.001656954*T**2
 +3.47421833E-08*T**3-3177110*T**(-1); 6000 Y
 +26556.5297-81.8606432*T-20.93747*T*LN(T)-.0030562285*T**2
 +6.90690167E-08*T**3-22459590*T**(-1); 8400 Y
 -414379.34+627.760535*T-99.46439*T*LN(T)+.003184458*T**2
 -2.42980333E-08*T**3+4.4363345E+08*T**(-1); 12000 Y
 -286534.147+496.228104*T-85.70049*T*LN(T)+.002546952*T**2
 -1.90235667E-08*T**3+2.2612925E+08*T**(-1); 16000 Y
 +169868.379+75.3492467*T-42.13511*T*LN(T)+6.93379E-04*T**2
 -4.19646667E-09*T**3-6.73131E+08*T**(-1); 20000 N !
 FUNCTION F14849T 298.15 -306850.417-57.4648268*T-26.25443*T*LN(T)
 -.026896635*T**2+4.38674333E-06*T**3+3287.6615*T**(-1); 800 Y
 -322029.697+136.633618*T-55.46687*T*LN(T)-.0012200165*T**2
 +5.60413333E-08*T**3+1526377.5*T**(-1); 2600 Y
 -325559.066+157.095567*T-58.16429*T*LN(T)-3.140385E-04*T**2
 +2.84143833E-11*T**3+2399356.5*T**(-1); 6000 N !
 FUNCTION F15054T 298.15 -446737.426-119.075067*T-18.39253*T*LN(T)
 -.0584565*T**2+1.73452167E-05*T**3-23894.4*T**(-1); 400 Y
 -454625.634+56.8614783*T-47.76138*T*LN(T)-.00906894*T**2
 +1.52655117E-06*T**3+379683.2*T**(-1); 800 Y
 -459722.562+123.281426*T-57.78518*T*LN(T)-1.2955145E-04*T**2
 +7.39238833E-09*T**3+877074.5*T**(-1); 3100 Y
 -458173.896+119.846881*T-57.4054*T*LN(T)-1.266458E-04*T**2
 +3.65921667E-09*T**3; 6000 N !
 FUNCTION F15060T 298.15 -475494.711+51.404232*T-49.55549*T*LN(T)
 -.030210885*T**2+5.27799667E-06*T**3+255509.3*T**(-1); 700 Y
 -491436.029+265.72401*T-82.06371*T*LN(T)-2.6169375E-04*T**2

$+1.0952625E-08*T^{**3}+1742125.5*T^{*(-1)}$; 4500 Y
 $-494560.763+277.51245*T-83.52789*T*LN(T)+4.9195245E-05*T^{**2}$
 $-1.17628333E-09*T^{**3}+3139224*T^{*(-1)}$; 6000 N !
 FUNCTION F15071T 298.15 $-332610.845+3.22325806*T-38.10718*T*LN(T)$
 $-.01852473*T^{**2}+3.29626E-06*T^{**3}+218721.05*T^{*(-1)}$; 700 Y
 $-342836.09+140.579944*T-58.93983*T*LN(T)+6.65405E-04*T^{**2}$
 $-8.11812167E-08*T^{**3}+1173742*T^{*(-1)}$; 2600 Y
 $-272800.105-96.5265453*T-30.24766*T*LN(T)-.0038011495*T^{**2}$
 $-1.83201667E-11*T^{**3}-28436635*T^{*(-1)}$; 4900 Y
 $-36436.152-803.246488*T+54.45089*T*LN(T)-.017172935*T^{**2}$
 $+3.92562833E-07*T^{**3}-1.509956E+08*T^{*(-1)}$; 6000 N !
 FUNCTION F14415T 298.15 $+134848.008-131.223611*T-12.03048*T*LN(T)$
 $-.05275305*T^{**2}+1.2029595E-05*T^{**3}-102360.9*T^{*(-1)}$; 500 Y
 $+125218.595+47.4797409*T-40.81794*T*LN(T)-.0137036*T^{**2}$
 $+1.90056833E-06*T^{**3}+514086.5*T^{*(-1)}$; 800 Y
 $+116301.963+157.624133*T-57.26249*T*LN(T)-1.3629415E-04*T^{**2}$
 $-2.12367333E-07*T^{**3}+1426255*T^{*(-1)}$; 1200 Y
 $+76721.1518+503.834314*T-106.002*T*LN(T)+.0266356*T^{**2}$
 $-2.98006167E-06*T^{**3}+7474120*T^{*(-1)}$; 1600 Y
 $+48905.4457+717.33371*T-135.3917*T*LN(T)+.040276715*T^{**2}$
 $-4.15597833E-06*T^{**3}+12338385*T^{*(-1)}$; 2100 Y
 $+520719.833-1837.33582*T+198.1425*T*LN(T)-.06465645*T^{**2}$
 $+2.04255167E-06*T^{**3}-1.129672E+08*T^{*(-1)}$; 2500 Y
 $+1271313.19-5388.12786*T+652.5156*T*LN(T)-.18701485*T^{**2}$
 $+8.22613333E-06*T^{**3}-3.456718E+08*T^{*(-1)}$; 3100 Y
 $-58819.7904-242.069298*T+12.85911*T*LN(T)-.05022045*T^{**2}$
 $+2.73771E-06*T^{**3}+1.7323845E+08*T^{*(-1)}$; 3500 Y
 $-1865873.5+6082.45586*T-762.2686*T*LN(T)+.0976441*T^{**2}$
 $-2.554365E-06*T^{**3}+9.636295E+08*T^{*(-1)}$; 4100 Y
 $-1603985.97+5364.29063*T-677.2357*T*LN(T)+.08557655*T^{**2}$
 $-2.24026833E-06*T^{**3}+8.14364E+08*T^{*(-1)}$; 4800 Y
 $-54953.3125+1260.31667*T-193.0202*T*LN(T)+.018228555*T^{**2}$
 $-4.819375E-07*T^{**3}-1.158314E+08*T^{*(-1)}$; 5800 Y
 $-189639.743+1510.18103*T-221.0511*T*LN(T)+.02063245*T^{**2}$
 $-5.15334667E-07*T^{**3}$; 6000 N !
 FUNCTION F15120T 298.15 $-407848.584-56.5330502*T-25.51583*T*LN(T)$
 $-.05275105*T^{**2}+9.862385E-06*T^{**3}+46212.49*T^{*(-1)}$; 600 Y
 $-424606.129+200.97123*T-65.52604*T*LN(T)-.00967297*T^{**2}$
 $+1.02581917E-06*T^{**3}+1378852*T^{*(-1)}$; 1300 Y
 $-438497.867+322.438792*T-82.65325*T*LN(T)-8.210765E-05*T^{**2}$
 $+2.440715E-09*T^{**3}+3548680.5*T^{*(-1)}$; 6000 N !
 FUNCTION F16008T 298.15 $+269797.373+2.28102912*T-25.70471*T*LN(T)$
 $+0.003751372*T^{**2}-5.48887167E-07*T^{**3}+3450.3165*T^{*(-1)}$; 1000 Y
 $+273925.002-38.4958657*T-19.81748*T*LN(T)-2.300353E-04*T^{**2}$
 $-1.18709967E-08*T^{**3}-570436.5*T^{*(-1)}$; 3400 Y

+257401.532-.943967214*T-24.05931*T*LN(T)-5.98546E-07*T**2
 +2.02961167E-09*T**3+9368165*T**(-1); 10000 N !
 FUNCTION F16104T 298.15 +92534.0824+10.011632*T-37.65898*T*LN(T)
 +3.0317985E-04*T**2-1.32384767E-07*T**3+92400.6*T**(-1); 1200 Y
 +89728.3947+58.2757589*T-45.00451*T*LN(T)+.006491675*T**2
 -9.93928E-07*T**3+47395.405*T**(-1); 2100 Y
 +245547.796-807.122389*T+68.4203*T*LN(T)-.030280675*T**2
 +1.24573817E-06*T**3-40178385*T**(-1); 3600 Y
 -231547.443+875.187197*T-137.998*T*LN(T)+.00948989*T**2
 -1.93419667E-07*T**3+1.6704695E+08*T**(-1); 6000 N !
 FUNCTION F16146T 298.15 +149366.708+13.5549074*T-37.7*T*LN(T)
 +6.05E-05*T**2-6.15283333E-08*T**3+133445*T**(-1); 4700 Y
 +183097.622-130.027804*T-19.774*T*LN(T)-.00373305*T**2
 +7.89383333E-08*T**3-9527150*T**(-1); 6000 N !
 FUNCTION F16162T 298.15 +277677.111+210.791158*T-66.67558*T*LN(T)
 +.0042695335*T**2+4.32640167E-06*T**3+859928.5*T**(-1); 500 Y
 +275543.8+297.707653*T-81.95092*T*LN(T)+.034172895*T**2
 -4.959165E-06*T**3+772451*T**(-1); 900 Y
 +302550.103-11.8773201*T-36.34538*T*LN(T)-1.1855935E-04*T**2
 -1.16400417E-07*T**3-2232039*T**(-1); 3300 Y
 +328020.572-149.054313*T-18.61905*T*LN(T)-.00505803*T**2
 +1.26576267E-07*T**3-7678210*T**(-1); 6000 N !
 FUNCTION F16023T 298.15 +117374.548+2.98629558*T-34.09678*T*LN(T)
 -.002325464*T**2+1.85480167E-07*T**3+128593.6*T**(-1); 1000 Y
 +117352.438+2.50383258*T-34.04744*T*LN(T)-.0021150245*T**2
 +9.16602333E-08*T**3+175718.45*T**(-1); 3400 Y
 +124361.091+14.5182895*T-36.1923*T*LN(T)-5.930925E-04*T**2
 -7.54259333E-09*T**3-7484105*T**(-1); 6000 N !
 FUNCTION F16212T 298.15 +76910.4935+93.8496899*T-56.58848*T*LN(T)
 -9.482025E-04*T**2+8.47096E-08*T**3+278152*T**(-1); 1300 Y
 +79425.0396+107.525277*T-59.26268*T*LN(T)+.0032036175*T**2
 -5.74265333E-07*T**3-937326*T**(-1); 2600 Y
 +177551.26-456.275575*T+14.61895*T*LN(T)-.020107145*T**2
 +7.53443333E-07*T**3-22963385*T**(-1); 4600 Y
 -423791.756+1334.03008*T-199.9598*T*LN(T)+.013938185*T**2
 -2.59055167E-07*T**3+2.9345875E+08*T**(-1); 6000 N !
 FUNCTION F16033T 298.15 +126744.316+83.8435679*T-52.94561*T*LN(T)
 -.0043385055*T**2+6.68300333E-07*T**3+276938.3*T**(-1); 1000 Y
 +123958.871+118.720435*T-58.16242*T*LN(T)-7.29079E-06*T**2
 +2.42566833E-10*T**3+558805*T**(-1); 6000 N !
 FUNCTION F16042T 298.15 +109847.439+203.904962*T-72.67966*T*LN(T)
 -.009041155*T**2+1.47148883E-06*T**3+505278*T**(-1); 900 Y
 +104526.08+272.793561*T-83.05028*T*LN(T)-1.828101E-05*T**2
 +6.19803333E-10*T**3+1023588.5*T**(-1); 6000 N !
 FUNCTION F16046T 298.15 +106276.073+170.263397*T-74.99022*T*LN(T)

$-.035336475 * T^{**2} + 5.76872833E-06 * T^{**3} + 227070.6 * T^{**(-1)}$; 900 Y
 $+75139.8853 + 544.891052 * T - 130.537 * T * \text{LN}(T) + .007879015 * T^{**2}$
 $-4.32610333E-07 * T^{**3} + 3425257 * T^{**(-1)}$; 2800 Y
 $+114904.754 + 339.945758 * T - 103.9801 * T * \text{LN}(T) + 2.25877E-05 * T^{**2}$
 $-7.925025E-10 * T^{**3} - 7832715 * T^{**(-1)}$; 6000 N !
 FUNCTION F16051T 298.15 +57214.7955+523.240738*T-130.1838*T*LN(T)
 $-4.152356E-04 * T^{**2} - 4.27131667E-07 * T^{**3} + 779118.5 * T^{**(-1)}$; 1600 Y
 $+8925.72404 + 728.509035 * T - 155.3363 * T * \text{LN}(T) + .002031178 * T^{**2}$
 $-1.776135E-08 * T^{**3} + 14908280 * T^{**(-1)}$; 4200 Y
 $+43158.7845 + 657.511851 * T - 147.3935 * T * \text{LN}(T) + .0015928905 * T^{**2}$
 $-3.34608333E-08 * T^{**3} - 8046775 * T^{**(-1)}$; 6000 N !
 FUNCTION F16056T 298.15 +59623.0035+634.182526*T-153.2939*T*LN(T)
 $-.003102847 * T^{**2} + 3.66153167E-07 * T^{**3} + 940068 * T^{**(-1)}$; 1500 Y
 $+56671.3253 + 666.288103 * T - 157.9591 * T * \text{LN}(T) - 2.441417E-06 * T^{**2}$
 $+7.28532E-11 * T^{**3} + 1284129.5 * T^{**(-1)}$; 6000 N !
 FUNCTION F16060T 298.15 +45619.0286+695.99667*T-166.1987*T*LN(T)
 $-.0109886 * T^{**2} - 1.38875683E-06 * T^{**3} + 753634 * T^{**(-1)}$; 800 Y
 $+22301.5849 + 822.418117 * T - 181.0091 * T * \text{LN}(T) - .020252625 * T^{**2}$
 $+3.04543E-06 * T^{**3} + 4785936 * T^{**(-1)}$; 1500 Y
 $+28125.3362 + 992.470204 * T - 208.7199 * T * \text{LN}(T) + .006139635 * T^{**2}$
 $-2.57977667E-07 * T^{**3} - 2943090 * T^{**(-1)}$; 3900 Y
 $+82396.4106 + 766.112127 * T - 180.3439 * T * \text{LN}(T) - 2.580219E-04 * T^{**2}$
 $+5.17172833E-09 * T^{**3} - 21845450 * T^{**(-1)}$; 6000 N !
 FUNCTION F16551T 298.15 +153602.922-22.5981707*T-20.98549*T*LN(T)
 $+1.951298E-04 * T^{**2} - 3.09095833E-08 * T^{**3} + 4675.2365 * T^{**(-1)}$; 1800 Y
 $+110622.883 + 243.910805 * T - 56.52776 * T * \text{LN}(T) + .0133862 * T^{**2}$
 $-9.57800833E-07 * T^{**3} + 9843260 * T^{**(-1)}$; 3300 Y
 $+770247.913 - 2113.22282 * T + 233.253 * T * \text{LN}(T) - .04337796 * T^{**2}$
 $+1.134592E-06 * T^{**3} - 2.7250735E+08 * T^{**(-1)}$; 4900 Y
 $-197367.294 + 264.872067 * T - 44.45892 * T * \text{LN}(T) - .008078665 * T^{**2}$
 $+2.96671167E-07 * T^{**3} + 3.57637E+08 * T^{**(-1)}$; 6200 Y
 $-949681.502 + 1953.67837 * T - 239.3059 * T * \text{LN}(T) + .01421437 * T^{**2}$
 $-1.79062E-07 * T^{**3} + 8.9842E+08 * T^{**(-1)}$; 9600 Y
 $+33681.1759 + 476.502383 * T - 77.25547 * T * \text{LN}(T) + .00232914 * T^{**2}$
 $-1.54504333E-08 * T^{**3} - 2.2245325E+08 * T^{**(-1)}$; 10000 N !
 FUNCTION F16566T 298.15 +296202.76+61.7700383*T-54.13634*T*LN(T)
 $+ .040485225 * T^{**2} - 9.264165E-06 * T^{**3} - 70453.75 * T^{**(-1)}$; 500 Y
 $+308348.288 - 147.486672 * T - 20.95926 * T * \text{LN}(T) + 1.012636E-04 * T^{**2}$
 $-8.03856667E-09 * T^{**3} - 905190.5 * T^{**(-1)}$; 3000 N !
 FUNCTION F16895T 298.15 +413926.156+43.9423585*T-34.19791*T*LN(T)
 $+ .0122297 * T^{**2} - 2.14534333E-06 * T^{**3} + 97071.5 * T^{**(-1)}$; 700 Y
 $+417505.307 - 13.2762869 * T - 25.29082 * T * \text{LN}(T) + .002768476 * T^{**2}$
 $-3.169895E-07 * T^{**3} - 157006.6 * T^{**(-1)}$; 2000 Y
 $+439627.78 - 100.08208 * T - 14.64876 * T * \text{LN}(T) + .001182233 * T^{**2}$
 $-3.39037833E-07 * T^{**3} - 7693105 * T^{**(-1)}$; 3300 Y

$+656873.926-957.210194*T+92.15071*T*LN(T)-.022050485*T**2$
 $+6.04918167E-07*T**3-90137500*T**(-1); 5500 Y$
 $-81672.0085+877.446828*T-122.4532*T*LN(T)+.005666115*T**2$
 $-6.61492667E-08*T**3+3.865857E+08*T**(-1); 10000 N !$
 FUNCTION F16956T 298.15 +567720.641+85.6851189*T-38.69111*T*LN(T)
 $+0.1152846*T**2-1.693255E-06*T**3+270638.8*T**(-1); 700 Y$
 $+576834.093-14.7850514*T-24.06106*T*LN(T)+.001743641*T**2$
 $-5.94312333E-07*T**3-748947.5*T**(-1); 1300 Y$
 $+574685.474-34.7524557*T-20.46361*T*LN(T)-.002961084*T**2$
 $+1.08391433E-07*T**3+526352.5*T**(-1); 2700 Y$
 $+611588.852-150.697371*T-6.647343*T*LN(T)-.0046738955*T**2$
 $+1.06833583E-07*T**3-15872340*T**(-1); 6600 Y$
 $+485104.072+143.08182*T-40.68801*T*LN(T)-6.38357E-04*T**2$
 $+1.79125333E-08*T**3+71496950*T**(-1); 10000 N !$
 FUNCTION F16975T 298.15 +886779.863-9.29107585*T-37.13672*T*LN(T)
 $-3.2039655E-04*T**2-4.30605167E-09*T**3+85422.15*T**(-1); 3600 Y$
 $+868133.758+14.4701785*T-39.33356*T*LN(T)-.001019669*T**2$
 $+6.09799667E-08*T**3+14065805*T**(-1); 6000 N !$
 FUNCTION F4559T 298.15 -452357.992+535.146046*T-99.1608*T*LN(T); 1500 N !
 FUNCTION F4561T 298.15 -18762.4149+771.690432*T-148.532*T*LN(T); 331 N !
 FUNCTION F4605T 298.15 -262897.462+419.668519*T-81.588*T*LN(T); 400 N !
 FUNCTION F4612T 298.15 -65351.9427+185.223626*T-48.03232*T*LN(T)
 $-.0604588*T**2-282420*T**(-1); 800 N !$
 FUNCTION F4712T 298.15 -930700.284+553.08688*T-92.00616*T*LN(T)
 $-.0194556*T**2+981148*T**(-1); 700 N !$
 FUNCTION F4714T 298.15 -53326.1356+628.18629*T-105.6878*T*LN(T)
 $-.0117152*T**2+851444*T**(-1); 1310 Y$
 $-101750.268+1032.90647*T-158.992*T*LN(T); 1793 N !$
 FUNCTION F4827T 298.15 -1280384.47+914.291127*T-152.0928*T*LN(T)
 $+0.05582535*T**2-1.4874955E-05*T**3+1969584*T**(-1); 1198 Y$
 $-1298766.71+933.349486*T-146*T*LN(T); 1767 Y$
 $-1332339.71+1094.41322*T-165*T*LN(T); 2500 N !$
 FUNCTION F4869T 298.15 +66458.8438+364.2835*T-76.9856*T*LN(T); 1800 N !
 FUNCTION F4932T 298.15 -209000.353+175.01449*T-28.23225*T*LN(T)
 $-.031001765*T**2+6.84174E-06*T**3+229831.3*T**(-1); 600 Y$
 $-216987.597+310.838757*T-49.76366*T*LN(T)-.0045690745*T**2$
 $+6.51418167E-07*T**3+802815.5*T**(-1); 1000 Y$
 $-293590.019+989.897198*T-145.5597*T*LN(T)+.048936275*T**2$
 $-5.03939833E-06*T**3+12267865*T**(-1); 1400 Y$
 $-214492.021+311.123585*T-50.36281*T*LN(T)-.0017572925*T**2$
 $+9.04797E-13*T**3+1.809942*T**(-1); 3805 Y$
 $-236221.304+412.351136*T-62.76*T*LN(T); 6000 N !$
 FUNCTION F5341T 298.15 -520876.535+666.560666*T-123.386*T*LN(T); 500 N !
 FUNCTION F5381T 298.15 -310828.243+585.538554*T-111.4199*T*LN(T); 400 N !
 FUNCTION F5387T 298.15 -484027.237+267.60133*T-47.07*T*LN(T)

$-.1834684*T^{**2}+1.43650667E-05*T^{**3}-23012*T^{**(-1)}$; 800 N !
 FUNCTION F5443T 298.15 -128356.849+906.070625*T-157.1813*T*LN(T)
 $-.029339685*T^{**2}-6.27555E-11*T^{**3}+430101.85*T^{**(-1)}$; 1500 N !
 FUNCTION F5502T 298.15 -98624.7516+396.284574*T-68.6176*T*LN(T)
 $-.0056484*T^{**2}+397480*T^{**(-1)}$; 1000 N !
 FUNCTION F5569T 298.15 -180830.788+1262.22712*T-219.66*T*LN(T)
 $-.050208*T^{**2}$; 1517 N !
 FUNCTION F5722T 298.15 +2232387.45+1624.15871*T-217.988*T*LN(T)
 $-.88971*T^{**2}+1.13199333E-04*T^{**3}+7681900*T^{**(-1)}$; 1000 N !
 FUNCTION F5746T 298.15 +33601.7956+52.9555416*T-20.33424*T*LN(T)
 $-.165268*T^{**2}-761488*T^{**(-1)}$; 800 N !
 FUNCTION F5752T 298.15 -471584.1+3539.04843*T-626.7543*T*LN(T)
 $-.1339635*T^{**2}+4.93775667E-11*T^{**3}+1015027.5*T^{**(-1)}$; 1523 Y
 $-.880272.495+7071.95551*T-1100*T*LN(T)$; 4000 N !
 FUNCTION F3986T 298.15 -16359.4285+175.609805*T-24.31*T*LN(T)
 $-4.723E-04*T^{**2}+2698000*T^{**(-1)}-2.61E+08*T^{**(-2)}+1.11E+10*T^{**(-3)}$; 6000
 N !
 FUNCTION F3970T 298.15 -17368.4408+170.730317*T-24.3*T*LN(T)
 $-4.723E-04*T^{**2}+2562600*T^{**(-1)}-2.643E+08*T^{**(-2)}+1.2E+10*T^{**(-3)}$;
 4765.30 Y
 $-17368.4408+170.730317*T-24.3*T*LN(T)-4.723E-04*T^{**2}+2562600*T^{**(-1)}$
 $-2.643E+08*T^{**(-2)}+1.2E+10*T^{**(-3)}$; 6000 N !
 FUNCTION F11513T 298.15 -2112947.35+1713.59836*T-306.5495*T*LN(T)
 $-.1296359*T^{**2}+1.97452667E-06*T^{**3}-159285.75*T^{**(-1)}$; 700 Y
 $-2115412.62+1757.71334*T-313.5777*T*LN(T)-.12093365*T^{**2}$; 1000 N !
 FUNCTION F11516T 298.15 -2943139.9+4072.88259*T-709.5829*T*LN(T)
 $+.23585815*T^{**2}-9.28319E-05*T^{**3}+2141201*T^{**(-1)}$; 500 Y
 $-2897719.21+3018.62934*T-532.873*T*LN(T)-.06297*T^{**2}$; 1000 N !
 FUNCTION F11644T 298.15 -673866.402+546.691852*T-88.48228*T*LN(T)
 $-.007079465*T^{**2}-3.04339167E-12*T^{**3}+1320222*T^{**(-1)}$; 1000 N !
 FUNCTION F11793T 298.15 -90745.9735+62.2373429*T-12.34*T*LN(T)-.03*T^{**2};
 700 N !
 FUNCTION F11813T 298.15 -213624.764+215.697148*T-39.24592*T*LN(T)
 $-.00757304*T^{**2}$; 1200 N !
 FUNCTION F11833T 298.15 -721883.605+467.480769*T-83.62839*T*LN(T)
 $-.01068517*T^{**2}-2.370405E-10*T^{**3}-7.92334*T^{**(-1)}$; 1000 N !
 FUNCTION F11290T 298.15 -332326.129+1078.74024*T-186.891*T*LN(T)
 $+.2321345*T^{**2}-9.14418333E-05*T^{**3}+978340*T^{**(-1)}$; 496 Y
 $-359544.694+1978.41284*T-344.158*T*LN(T)+.548195*T^{**2}$
 $-1.98468333E-04*T^{**3}+1189260*T^{**(-1)}$; 550 Y
 $-8553683.3+142840.954*T-22663.4*T*LN(T)+27.56365*T^{**2}$
 $-.00632881667*T^{**3}+5.65175E+08*T^{**(-1)}$; 600 Y
 $-331037.834+741.179578*T-117.41*T*LN(T)$; 601 N !
 FUNCTION F11868T 298.15 -994630.009+469.118005*T-80.37768*T*LN(T)
 $-.03375467*T^{**2}+2.61107333E-10*T^{**3}+501615*T^{**(-1)}$; 753 Y

$-1011524.33+795.723052*T-130*T*LN(T)$; 808 Y
 $-1030108.33+972.697979*T-153*T*LN(T)$; 2000 N !
 FUNCTION F11318T 298.15 $-214494.862+488.664597*T-89.3284*T*LN(T)$; 1500 N !
 FUNCTION F11503T 298.15 $-869108.067+897.337162*T-153.8516*T*LN(T)$
 $-.019124105*T**2+1.44695267E-06*T**3+1136712.5*T**(-1)$; 600 Y
 $-863220.126+819.598959*T-141.9156*T*LN(T)-.032402965*T**2$
 $+4.86474E-06*T**3+527638.5*T**(-1)$; 1100 Y
 $-868907.776+959.332775*T-164.0134*T*LN(T)-.009498165*T**2$
 $+1.0877975E-06*T**3$; 1500 N !
 FUNCTION F11472T 298.15 $-43190.6374+401.603166*T-84.0984*T*LN(T)$; 400 N !
 FUNCTION F11476T 298.15 $-43189.8182+401.601487*T-84.098*T*LN(T)$; 350 N !
 FUNCTION F11914T 298.15 $-191672.686+187.433714*T-34.30112*T*LN(T)$
 $-.01626475*T**2-6.885585E-11*T**3-3.804784*T**(-1)$; 1128 Y
 $-212373.824+445.366179*T-71*T*LN(T)-3.218617E-15*T**2$
 $+3.253845E-19*T**3-7.274825E-07*T**(-1)$; 1323 Y
 $-217665.824+478.116808*T-75*T*LN(T)+1.5871265E-16*T**2$
 $-1.3939135E-20*T**3+7.410385E-08*T**(-1)$; 2000 N !
 FUNCTION F11932T 298.15 $-233878.908+189.980573*T-32.803*T*LN(T)$
 $-.0106275*T**2+209000*T**(-1)$; 900 N !
 FUNCTION F11934T 298.15 $-187639.664+231.3843*T-37.54114*T*LN(T)$
 $-.016932115*T**2-6.336835E-09*T**3+818315*T**(-1)$; 960 N !
 FUNCTION F11941T 298.15 $-1451032.62+518.382967*T-88.95254*T*LN(T)$
 $-.06114395*T**2+5.17053E-08*T**3+354629.75*T**(-1)$; 800 N !
 FUNCTION F11961T 298.15 $-277923.603+222.183346*T-38.744*T*LN(T)$
 $-.0077405*T**2$; 686 N !
 FUNCTION F11508T 298.15 $-1179137.97+859.268755*T-151.9723*T*LN(T)$
 $-.0972523*T**2+5.45952667E-06*T**3-320551.1*T**(-1)$; 600 Y
 $-1184456.53+960.421765*T-168.2892*T*LN(T)-.07531175*T**2$; 1000 N !
 FUNCTION F11511T 298.15 $-1490584.39+921.789537*T-164.4024*T*LN(T)$
 $-.1627546*T**2$; 1000 N !
 FUNCTION F11986T 298.15 $-1801200.29+1277.80775*T-229.442*T*LN(T)$
 $-.14709285*T**2+5.13146667E-07*T**3-98125*T**(-1)$; 1000 N !
 FUNCTION F13015T 298.15 $-1466291.67+669.556355*T-117.35*T*LN(T)$
 $-.00825*T**2+815500*T**(-1)$; 675 Y
 $-1466291.67+669.556355*T-117.35*T*LN(T)-.00825*T**2+815500*T**(-1)$;
 2500 N !
 FUNCTION F13040T 298.15 $-470157.03+241.82639*T-46.48424*T*LN(T)$
 $-.0027196*T**2$; 2500 N !
 FUNCTION F13042T 298.15 $-644928.908+378.656583*T-69.036*T*LN(T)$
 $-.01046*T**2$; 1000 N !
 FUNCTION F13066T 298.15 $-1835599.83+674.720454*T-118*T*LN(T)-.008*T**2$
 $+620000*T**(-1)$; 2313 Y
 $-1835599.83+674.720454*T-118*T*LN(T)-.008*T**2+620000*T**(-1)$; 2383 Y
 $-1835599.83+674.720454*T-118*T*LN(T)-.008*T**2+620000*T**(-1)$; 2586 Y

-1993673.15+1359.59688*T-200*T*LN(T); 3500 N !
 FUNCTION F13070T 298.15 -4174282.34+1510.67182*T-256.26*T*LN(T)
 -.016338*T**2+2016400*T**(-1); 2500 N !
 FUNCTION F13072T 298.15 -1257120.63+619.824545*T-116.5244*T*LN(T)
 -.007322*T**2; 2400 N !
 FUNCTION F12993T 298.15 -7968.40253+120.285004*T-26.34*T*LN(T)
 -.0012951655*T**2; 550 Y
 -6473.78487+90.540705*T-21.79186*T*LN(T)-.004045175*T**2
 -5.25864667E-07*T**3; 1134 Y
 -19863.1881+221.907689*T-39.5388*T*LN(T); 1193 Y
 -13623.7981+179.627185*T-34.3088*T*LN(T); 4000 N !
 FUNCTION F13425T 298.15 -399307.296+228.703198*T-42.133*T*LN(T)
 -.0084782*T**2+7.01073333E-07*T**3+120430*T**(-1); 2115 Y
 -413735.572+362.675641*T-60.668*T*LN(T); 2500 N !
 FUNCTION F13433T 298.15 -547056.053+432.954869*T-70.831*T*LN(T)
 -.0038047*T**2+1.40666667E-09*T**3+830445*T**(-1); 800 N !
 FUNCTION F13443T 298.15 -1233982.84-15.8840048*T-11.2837*T*LN(T)
 -.010873*T**2+854955*T**(-1); 2300 N !
 FUNCTION F13449T 298.15 -1515405.3+620.946682*T-105.84*T*LN(T)-.017*T**2
 +669185*T**(-1); 2500 N !
 FUNCTION F13451T 298.15 -1113284.84+735.509373*T-122.4238*T*LN(T)
 -.01866064*T**2+1472768*T**(-1); 973 N !
 FUNCTION F13445T 298.15 -1956747.73+1038.97507*T-160.397*T*LN(T)
 -.013943*T**2+10449550*T**(-1); 2300 N !
 FUNCTION F13459T 298.15 -228755.776+243.505715*T-47.6976*T*LN(T)
 -.0037656*T**2; 1803 Y
 -251215.789+393.467611*T-66.944*T*LN(T); 2200 N !
 FUNCTION F13466T 298.15 -246870.902+374.656719*T-69.70544*T*LN(T)
 -.00882824*T**2+217568*T**(-1); 700 N !
 FUNCTION F13485T 298.15 -993821.582+600.599468*T-103.4703*T*LN(T)
 -.01753096*T**2+675716*T**(-1); 1350 N !
 FUNCTION F13492T 298.15 -2068422.64+989.531692*T-161.9427*T*LN(T)
 -.02898167*T**2+3.34986833E-07*T**3+944525*T**(-1); 900 Y
 -2069966.42+1008.51283*T-164.7673*T*LN(T)-.026730725*T**2
 +4.17358333E-09*T**3+1098684*T**(-1); 2500 N !
 FUNCTION F13497T 298.15 -3003702.35+1507.45781*T-273.234*T*LN(T)
 -.024816*T**2+1899910*T**(-1); 2300 N !
 FUNCTION F13496T 298.15 -808500.498+1508.35111*T-270*T*LN(T); 1000 N !
 FUNCTION F13505T 298.15 -4445199.31+2261.73686*T-386.071*T*LN(T)
 -.035689*T**2+2754865*T**(-1); 2300 N !
 FUNCTION F13507T 298.15 -1434889.46+835.412089*T-144.9338*T*LN(T)
 -.02263544*T**2+460240*T**(-1); 1445 Y
 -1481062.92+1308.55886*T-210.0368*T*LN(T); 1833 N !
 FUNCTION F13510T 298.15 -2275024.66+1258.52313*T-214.793*T*LN(T)
 -.029717*T**2+1944010*T**(-1); 2300 N !

FUNCTION F13517T 298.15 -7047904.15+3513.81636*T-594.028*T*LN(T)
 -.052702*T**2+3989820*T**(-1); 2300 N !
 FUNCTION F13407T 298.15 -8115.2795+130.059572*T-23.4582*T*LN(T)
 -.00734768*T**2+69827.1*T**(-1); 980 Y
 -8053.94509+138.295108*T-24.8785*T*LN(T)-.00583359*T**2
 +70269.1*T**(-1); 1360 Y
 -7858.57375+135.776563*T-24.5177*T*LN(T)-.006*T**2+69600*T**(-1); 1411
 Y
 -9562.87236+133.095001*T-23.7*T*LN(T)-.00744271*T**2+60000*T**(-1);
 1519 Y
 -29211.9952+312.76918*T-48*T*LN(T); 2000 N !
 FUNCTION F14590T 298.15 -606598.04+258.941402*T-46.05318*T*LN(T)
 -.007073085*T**2+1.23145367E-06*T**3+194365.4*T**(-1); 900 Y
 -631347.648+516.486721*T-83.39296*T*LN(T)+.018229075*T**2
 -2.03005167E-06*T**3+3291842*T**(-1); 1700 Y
 -1362818.13+4945.72597*T-671.2812*T*LN(T)+.22717525*T**2
 -1.58762967E-05*T**3+1.731743E+08*T**(-1); 2805 Y
 -678665.767+573.624025*T-84*T*LN(T); 6000 N !
 FUNCTION F14932T 298.15 -657791.613+446.717509*T-79.496*T*LN(T)
 -.0071128*T**2; 600 N !
 FUNCTION F15065T 298.15 -1125582.53+417.508431*T-68.32783*T*LN(T)
 -.0045415885*T**2+1.72444167E-10*T**3+671863.5*T**(-1); 1472 Y
 -1129214.77+484.883106*T-78.1*T*LN(T)-1.0845475E-16*T**2
 +7.81505167E-21*T**3-7.622945E-08*T**(-1); 2620 Y
 -1134192.77+501.737872*T-80*T*LN(T)-2.0126725E-14*T**2
 +9.19196667E-19*T**3-5.127845E-05*T**(-1); 2983 Y
 -1193852.77+681.751568*T-100*T*LN(T); 6000 N !
 FUNCTION F15125T 298.15 -492036.062+1082.23602*T-179.912*T*LN(T); 500 N !
 FUNCTION F15149T 298.15 -1811199.59+719.003629*T-121.252*T*LN(T)
 -.0061085*T**2+1071000*T**(-1); 2000 N !
 FUNCTION F15211T 298.15 -1945493.95+680.542371*T-113.9721*T*LN(T)
 -.012761235*T**2+1.49941783E-06*T**3+813690.5*T**(-1); 1100 Y
 -2012427.82+1275.7521*T-198.0735*T*LN(T)+.03498891*T**2
 -3.688465E-06*T**3+10928115*T**(-1); 2100 Y
 -2274854.51+2766.12582*T-394.0992*T*LN(T)+.10031335*T**2
 -7.78301833E-06*T**3+77093000*T**(-1); 2550 Y
 -2011617.72+1043.70289*T-160*T*LN(T); 2712 Y
 -2120097.72+1399.92055*T-200*T*LN(T); 6000 N !
 FUNCTION F15267T 298.15 -1499119.5+641.39855*T-109.6909*T*LN(T)
 -.026706575*T**2+2.480005E-12*T**3+1049654.5*T**(-1); 1430 Y
 -1529281.2+1062.98509*T-170*T*LN(T); 1880 Y
 -1529281.2+1062.98509*T-170*T*LN(T); 4000 N !
 FUNCTION F15414T 298.15 -4217489.03+1595.57731*T-263.1736*T*LN(T)
 -.0100416*T**2+2405800*T**(-1); 1500 N !
 FUNCTION F15431T 298.15 -2337111.73+2000.06599*T-322.85*T*LN(T)

$+0.04889T^2$; 1050 N !
 FUNCTION F16101T 298.15 -494856.801+253.035367T-47.53265T*LN(T)
 $-0.0038732105T^2+1.43470567E-11T^3+50780.85T^{(-1)}$; 2500 Y
 $-519277.434+405.44225T-67T*LN(T)$; 5200 N !
 FUNCTION F16149T 298.15 -475902.413+266.991868T-48.637T*LN(T)
 $-0.00203355T^2+1.04478333E-07T^3+182775T^{(-1)}$; 2500 N !
 FUNCTION F16209T 298.15 -597018.641+362.969585T-65.28532T*LN(T)
 $-0.006229675T^2-5.06821667E-11T^3+6.51605T^{(-1)}$; 1823 Y
 $-639599.622+635.61647T-100T*LN(T)$; 4000 N !
 FUNCTION F16238T 298.15 -1052341.89+594.307568T-105.9389T*LN(T)
 $-0.017259T^2$; 1200 N !
 FUNCTION F16547T 298.15 -7532.36674+107.183879T-23.905T*LN(T)
 $-0.00461225T^2-1.67477E-07T^3-2055T^{(-1)}$; 820 Y
 $-7807.39361+123.087788T-26.57T*LN(T)-0.0019493T^2-1.7895E-08T^3$
 $+16495T^{(-1)}$; 1050 Y
 $-19123.0899+221.503849T-39.463T*LN(T)$; 1700 N !
 FUNCTION F15998T 298.15 -5198.29365+53.9138545T-10.726T*LN(T)
 $-0.0273801T^2+8.17953667E-06T^3$; 368.30 Y
 $-6126.42216+90.6330606T-17.413T*LN(T)-0.00993935T^2$
 $-7.00616667E-08T^3+1250T^{(-1)}$; 388.30 Y
 $-878435.562+23372.3922T-4028.756T*LN(T)+7.954595T^2$
 $-0.00290851333T^3+33980035T^{(-1)}$; 432.20 Y
 $+451967.08-7809.151T+1237.001T*LN(T)-1.5607295T^2$
 $+3.59883667E-04T^3-31765395T^{(-1)}$; 500 Y
 $+16432.9539-139.376055T+16.535T*LN(T)-0.0454119T^2$
 $+8.32740167E-06T^3-2705030T^{(-1)}$; 700 Y
 $+19121.5192-107.779647T+9.944T*LN(T)-0.0288384T^2+3.791365E-06T^3$
 $-3507570T^{(-1)}$; 900 Y
 $+13996.2416-27.2759999T-2.425T*LN(T)-0.01712545T^2+1.84974E-06T^3$
 $-3215170T^{(-1)}$; 1300 N !
 FUNCTION F16890T 298.15 -8011.08567+128.572399T-25.6657T*LN(T)
 $-0.001757164T^2-4.17561833E-07T^3+26911.51T^{(-1)}$; 1000 Y
 $-7179.70405+114.496589T-23.49418T*LN(T)-0.00382118T^2$
 $-8.25345333E-08T^3$; 1751.10 Y
 $-6184.13783+137.318262T-27.30385T*LN(T)-5.417575E-04T^2$
 $-3.05012167E-07T^3$; 1795.10 Y
 $-29256.7528+266.537676T-43.0952T*LN(T)$; 3700 N !
 FUNCTION F16952T 298.15 -7827.65327+125.650277T-24.162T*LN(T)
 $-0.0043779T^2+34971T^{(-1)}$; 1139.40 Y
 $-4629.21448+128.548393T-25.60741T*LN(T)-3.40084E-04T^2$
 $-9.72897333E-09T^3+25233T^{(-1)}-7.61428917E-11T^4$; 2127.80 Y
 $-33382.4026+267.283165T-42.144T*LN(T)$; 6000 N !
 FUNCTION F877T 298.15 -6197.3787-15.6250179T-20.78611T*LN(T);
 6.00000E+03 N !
 FUNCTION UN_ASS 298.15 +0; 300 N !

\$ End of file.

APPENDIX 2

The La-Sr-Mn-O-Y-Zr-H-Cr Database

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TEMP-LIM 298.15 6000.00 !
$ELEMENT NAME REF. STATE      ATOMIC MASS H0      S0 !
ELEMENT H 1/2_MOLE_H2(G)      1.0079E+00 4.2340E+03 6.5285E+01 !
ELEMENT CR BCC_A2              5.1996E+01 4.0500E+03 2.35429E+01 !
ELEMENT FE BCC_A2              5.5847E+01 4.4890E+03 2.7280E+01 !
ELEMENT LA DOUBLE_HCP(ABAC)   1.3891E+02 6665.112 56.9024 !
ELEMENT MN CBCC_A12           54.938 4996 32.008 !
ELEMENT SR SR_FCC_A1          8.7620E+01 6.5680E+03 5.5694E+01 !
ELEMENT O 1/2_MOLE_O2(G)      1.5999E+01 4.3410E+03 1.0252E+02 !
ELEMENT Y HCP_A3              8.8906E+01 5.9664E+03 4.4434E+01 !
ELEMENT ZR HCP_A3             9.1224E+01 5.5663E+03 3.9181E+01 !
ELEMENT /- ELECTRON_GAS        0.0000E+00 0.0000E+00 0.0000E+00 !
ELEMENT VA VACUUM              0.0000E+00 0.0000E+00 0.0000E+00 !
ELEMENT AR 1_MOLE_AR1(G)      3.9948E+01 0.0000E+00 3.6982E+01 !
$
SPECIE HO                      H1O1 !
SPECIE HO2                     H1O2 !
SPECIE H2                      H2 !
SPECIE H2O                     H2O1 !
SPECIE H2O2                    H2O2 !
SPECIE CR2                     CR2 !
SPECIE CR+2                    CR/+2 !
SPECIE CR+3                    CR/+3 !
SPECIE CR+4                    CR/+4 !
SPECIE CR+5                    CR/+5 !
SPECIE CR+6                    CR/+6 !
SPECIE CRO                     CR1O1 !
SPECIE CRO2                    CR1O2 !
SPECIE CRO3                    CR1O3 !
SPECIE CR2O2                   CR2O2 !
SPECIE CR2O3                   CR2O3 !
SPECIE CR3O4                   CR3O4 !
SPECIE CRH                     CRH1 !
SPECIE CRHO                    CRH1O1 !
SPECIE CRHO2                   CRH1O2 !
SPECIE CRHO3                   CRH1O3 !
SPECIE CRH2O2                  CRH2O2 !
SPECIE CRH2O3                  CRH2O3 !
SPECIE CRH2O4                  CRH2O4 !
SPECIE CRH3O3                  CRH3O3 !
SPECIE CRH3O4                  CRH3O4 !

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SPECIE CRH404	CRH404 !
SPECIE CRH405	CRH405 !
SPECIE CRH505	CRH505 !
SPECIE CRH606	CRH606 !
SPECIE FE+2	FE1/+2 !
SPECIE FE+3	FE1/+3 !
SPECIE FE+4	FE1/+4 !
SPECIE FE1O2	FE1O2 !
SPECIE FE2	FE2 !
SPECIE FEO	FE1O1 !
SPECIE LA+2	LA/+2 !
SPECIE LA+3	LA/+3 !
SPECIE LAO	LA1O1 !
SPECIE LAO2	LA1O2 !
SPECIE LAO15	LA1O1.5 !
SPECIE LA2O1	LA2O1 !
SPECIE LA2O2	LA2O2 !
SPECIE LA2O3	LA2O3 !
SPECIE MN+2	MN/+2 !
SPECIE MN+3	MN/+3 !
SPECIE MN+4	MN/+4 !
SPECIE MNO	MN1O1 !
SPECIE MNO2	MN1O2 !
SPECIE MN2O3	MN2O3 !
SPECIE MN2O7	MN2O7 !
SPECIE MN3O4	MN3O4 !
SPECIE O-2	O/-2 !
SPECIE O2-2	O2/-2 !
SPECIE O2	O2 !
SPECIE O3	O3 !
SPECIE SR+2	SR/+2 !
SPECIE SR2	SR2 !
SPECIE SR2O	SR2O !
SPECIE SRO	SRO !
SPECIE SRO2	SRO2 !
SPECIE Y+3	Y/+3 !
SPECIE YO	O1Y1 !
SPECIE YO2	O2Y1 !
SPECIE YO15	O1.5Y1 !
SPECIE Y2O	O1Y2 !
SPECIE Y2O2	O2Y2 !
SPECIE Y2O3	O3Y2 !
SPECIE ZR+4	ZR1/+4 !
SPECIE ZR2	ZR2 !
SPECIE ZRO	O1ZR1 !

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SPECIE ZRO2          O2ZR1 !
SPECIE LACRO3        LACRO3 !
SPECIE SRCRO3        SRCRO3 !
SPECIE SRCRO4        SRCRO4 !
SPECIE LAMNO3        LAMNO3 !
SPECIE L2Z2O7        LA2O7ZR2 !
SPECIE SRMNO3        SRMNO3 !
SPECIE Y2ZR2O7       O7Y2ZR2 !
SPECIE SZO           SRZRO3 !
SPECIE SRMN3O6       SRMN3O6 !
SPECIE YMN2O5       Y1MN2O5 !
$
DEFAULT-COM DEFINE_SYSTEM_ELEMENT VA /- !
TYPE-DEF Z SEQ * !
TYPE-DEF L GES AMEND_PHASE_DESCRIPTION ION COMP_SET ,, MN+2 : VA
: !
TYPE_DEF B GES AMEND_PHASE_DESCRIPTION @ MAGNETIC -1 0.4 !
TYPE_DEF A GES AMEND_PHASE_DESCRIPTION @ MAGNETIC -3 0.28 !
$
PHASE ION:Y ZL 2 1 1 !
CONST ION:Y : CR+2 CR+3 FE+2 FE+3 LA+3 MN+2 MN+3 Y+3 ZR+4
          SR+2 : O-2 VA SRCRO3 SRCRO4 : !
PAR G(ION,CR+2:VA;0)      298.15 +GCR_L;          6000 N !
PAR G(ION,CR+2:O-2;0)     298.15 +2*GCR1O1_L;      6000 N !
PAR G(ION,CR+3:VA;0)      298.15
+2*GCR_L+GCR2O3_L-3*GCR1O1_L;          6000 N !
PAR G(ION,CR+3:O-2;0)     298.15 +GCR2O3_L;        6000 N !
PAR G(ION,FE+2:VA;0)      298.15 +GFELIQ;          6000 N !
PAR G(ION,FE+2:O-2;0)     298.15 +4*GFEOLIQ;        6000 N !
PAR G(ION,FE+3:VA;0)      298.15 +2*GFELIQ+5*GFEOLIQ
-179638+79.923*T-6*GFEOLIQ;          6000 N !
PAR G(ION,FE+3:O-2;0)     298.15
+5*GFEOLIQ-179638+79.923*T;          6000 N !
PAR G(ION,LA+3:VA)        298.15 +GLALIQ;          3200 N !
PAR G(ION,LA+3:O-2)       298.15 +GLA2O3LIQ;        6000 N !
PAR G(ION,MN+2:VA)        298.15 +GMNLIQ;          3000 N !
PAR G(ION,MN+2:O-2)       298.15 +2*GL11;          3000 N !
PAR G(ION,MN+3:VA)        298.15 +2*GMNLIQ+GL23-3*GL11; 3000 N !
PAR G(ION,MN+3:O-2)       298.15 +GL23;          6000 N !
PAR G(ION,Y+3:VA)         298.15 +GYyliQ;          6000 N !
PAR G(ION,Y+3:O-2)        298.15 +2*GYyliQ+3*GHSEROO
-1824330+245.9*T;          6000 N !
PAR G(ION,ZR+4:VA)        298.15 +GZRLIQ;          6000 N !
PAR G(ION,ZR+4:O-2)       298.15 +2*GZRO2LIQ;        6000 N !
PAR G(ION,SR+2:VA;0)      298.15 +GSRLIQ;          6000 N !

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PAR G(ION,SR+2:O-2;0)	298.15 +2*GSROLIQ;	6000 N !
PAR L(ION,CR+2:O-2,VA;0)	298.15 +121000;	6000 N !
PAR L(ION,CR+3:O-2,VA;0)	298.15 +121000;	6000 N !
PAR L(ION,FE+2:O-2,VA;0)	298.15 +176681-16.368*T;	6000 N !
PAR L(ION,FE+2:O-2,VA;1)	298.15 -65655+30.869*T;	6000 N !
PAR L(ION,FE+2,FE+3:O-2;0)	298.15 -26362;	6000 N !
PAR L(ION,FE+2,FE+3:O-2;1)	298.15 +13353;	6000 N !
PAR L(ION,MN+2:O-2,VA;0)	298.15 +129519;	6000 N !
PAR L(ION,MN+2:O-2,VA;1)	298.15 -45459;	6000 N !
PAR L(ION,MN+2,MN+3:O-2;0)	298.15 -33859;	6000 N !
PAR L(ION,Y+3:O-2,VA;0)	298.15 +6900;	6000 N !
PAR L(ION,Y+3:O-2,VA;1)	298.15 -17000;	6000 N !
PAR L(ION,ZR+4:O-2,VA;0)	298.15 -26500;	6000 N !
PAR L(ION,ZR+4:O-2,VA;1)	298.15 +50000;	6000 N !
PAR L(ION,ZR+4:O-2,VA;2)	298.15 +72000;	6000 N !
\$ The following two are from Povoden,		
\$ but the original source cannot be verified.		
PAR L(ION,CR+2,FE+2:VA;0)	298.15 -17737+7.996546*T;	6000 N !
PAR L(ION,CR+2,FE+2:VA;1)	298.15 +1331;	6000 N !
\$ From Taylor		
PAR L(ION,CR+3,FE+2:VA;0)	298.15 -14550+6.65*T;	6000 N !
PAR L(ION,CR+3,FE+2:O-2;0)	298.15 -7000+10*T;	6000 N !
PAR L(ION,CR+3,FE+2:O-2;1)	298.15 -85000+50*T;	6000 N !
PAR L(ION,CR+3,FE+2:O-2;2)	298.15 +127500-75*T;	6000 N !
PAR L(ION,CR+3,FE+2:O-2,VA;0)	298.15 -604900+290*T;	6000 N !
PAR L(ION,CR+3,FE+2:O-2,VA;1)	298.15 +85000-50*T;	6000 N !
PAR L(ION,CR+3,FE+2:O-2,VA;2)	298.15 -127500+75*T;	6000 N !
\$		
PAR L(ION,CR+2,LA+3:VA;0)	298.15 +60713-5.49*T;	6000 N !
PAR L(ION,CR+2,LA+3:VA;1)	298.15 +64573-23*T;	6000 N !
PAR L(ION,CR+2,LA+3:O-2;0)	298.15 -101850;	6000 N !
PAR L(ION,CR+2,LA+3:O-2;1)	298.15 -39016;	6000 N !
PAR L(ION,CR+3,LA+3:O-2;0)	298.15 -101850;	6000 N !
PAR L(ION,CR+3,LA+3:O-2;1)	298.15 -39016;	6000 N !
PAR L(ION,CR+2,MN+2:VA;0)	298.15 -15009+13.6587*T;	6000 N !
PAR L(ION,CR+2,MN+2:VA;1)	298.15 +504+0.9479*T;	6000 N !
PAR L(ION,CR+3,MN+3:O-2;0)	298.15 -188487.7;	6000 N !
PAR L(ION,CR+2,SR+2:VA;0)	298.15 +200000;	6000 N !
PAR L(ION,CR+2,SR+2:O-2;0)	298.15 -275000;	6000 N !
PAR L(ION,CR+2,SR+2:O-2;1)	298.15 -100000;	6000 N !
PAR L(ION,CR+2,SR+2:O-2;2)	298.15 -250000;	6000 N !
PAR L(ION,CR+3,SR+2:O-2;0)	298.15 -275000;	6000 N !
PAR L(ION,CR+3,SR+2:O-2;1)	298.15 -100000;	6000 N !
PAR L(ION,CR+3,SR+2:O-2;2)	298.15 -250000;	6000 N !
PAR L(ION,CR+2,Y+3:O-2;0)	298.15 -49263;	6000 N !

PAR L(ION,CR+3,Y+3:O-2;0)	298.15 -49263;	6000 N !
PAR L(ION,FE+2,LA+3:VA;0)	298.15 -41+15.2*T;	6000 N !
PAR L(ION,FE+2,LA+3:VA;1)	298.15 -7837+4.9*T;	6000 N !
PAR L(ION,FE+2,LA+3:O-2;0)	298.15 -136242;	6000 N !
PAR L(ION,FE+2,LA+3:O-2;1)	298.15 -9285;	6000 N !
PAR L(ION,FE+3,LA+3:O-2;0)	298.15 -136242;	6000 N !
PAR L(ION,FE+3,LA+3:O-2;1)	298.15 -9285;	6000 N !
PAR L(ION,FE+2,SR+2:O-2;0)	298.15 -281372;	6000 N !
PAR L(ION,FE+3,SR+2:O-2;0)	298.15 -281372;	6000 N !
PAR L(ION,FE+3,SR+2:O-2;1)	298.15 +35000;	6000 N !
PAR L(ION,FE+3,SR+2:O-2;2)	298.15 -35311;	6000 N !
PAR L(ION,LA+3,MN+2:O-2;0)	298.15 -119062;	6000 N !
PAR L(ION,LA+3,MN+3:O-2;0)	298.15 -119062;	6000 N !
PAR L(ION,LA+3,ZR+4:O-2;0)	298.15 -212088;	6000 N !
PAR L(ION,MN+2,Y+3:VA;0)	298.15 -26874.14+2.38277*T;	6000 N !
PAR L(ION,MN+2,Y+3:VA;1)	298.15 -12579.78;	6000 N !
PAR L(ION,MN+2,ZR+4:VA;0)	298.15 -45851.78+5.21718*T;	6000 N !
PAR L(ION,MN+2,ZR+4:VA;1)	298.15 -10658.06+9.26869*T;	6000 N !
PAR L(ION,MN+2,ZR+4:VA;2)	298.15 -11253.58;	6000 N !
PAR L(ION,MN+2,ZR+4:O-2;0)	298.15 -19432;	6000 N !
PAR L(ION,MN+3,ZR+4:O-2;0)	298.15 -19432;	6000 N !
PAR L(ION,Y+3,ZR+4:VA;0)	298.15 +24000;	6000 N !
PAR L(ION,Y+3,ZR+4:VA;1)	298.15 +3000;	6000 N !
PAR L(ION,Y+3,ZR+4:O-2;0)	298.15 +20100;	6000 N !
PAR L(ION,Y+3,ZR+4:O-2;1)	298.15 -13000;	6000 N !
PAR L(ION,Y+3,ZR+4:O-2;2)	298.15 -40000;	6000 N !
PAR L(ION,MN+3,SR+2:O-2;0)	298.15 -1.76300000E+05;	6000 N !
PAR L(ION,MN+2,SR+2:O-2;0)	298.15 -1.76300000E+05;	6000 N !
PAR L(ION,LA+3,SR+2:O-2;0)	298.15 -8.891E+04;	6000 N !
PAR L(ION,LA+3,SR+2:O-2;1)	298.15 -7.368E+04;	6000 N !
\$		
PAR G(ION,SR+2:SRCRO3;0)	298.15 +GS4O+29200-10*T;	6000 N !
PAR G(ION,SR+2:SRCRO4;0)	298.15 +GSCO4+50000-31*T;	6000 N !
PAR G(ION,SR+2:SRCRO3,O-2;0)	298.15 -50000;	6000 N !
PAR G(ION,SR+2:SRCRO4,O-2;0)	298.15 -100000;	6000 N !
\$		
PHASE LIQUID Z 1 1 !		
CONST LIQUID : CR LA MN Y ZR SR : !		
PAR G(LIQUID,CR)	298.15 +GCR_L;	6000 N !
PAR G(LIQUID,LA)	298.15 +GLALIQ;	3200 N !
PAR G(LIQUID,MN)	298.15 +GMNLIQ;	3000 N !
PAR G(LIQUID,Y)	298.15 +GYYLIQ;	6000 N !
PAR G(LIQUID,ZR)	298.15 +GZRLIQ;	6000 N !
PAR G(LIQUID,SR)	298.15 +GSRLIQ;	6000 N !
PAR L(LIQUID,CR,LA;0)	298.15 +60713-5.49*T;	6000 N !


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PAR L(LIQUID,CR,LA;1)      298.15 +64573-23*T;      6000 N !
PAR L(LIQUID,CR,MN;0)      298.15 -15009+13.6587*T;    6000 N !
PAR L(LIQUID,CR,MN;1)      298.15 +504+0.9479*T;      6000 N !
PAR L(LIQUID,CR,SR;0)      298.15 +200000;          6000 N !
PAR L(LIQUID,MN,Y;0)       298.15 -26874.14+2.38277*T;  6000 N !
PAR L(LIQUID,MN,Y;1)       298.15 -12579.78;          6000 N !
PAR L(LIQUID,MN,ZR;0)      298.15 -45851.78+5.21718*T;  6000 N !
PAR L(LIQUID,MN,ZR;1)      298.15 -10658.06+9.26869*T;  6000 N !
PAR L(LIQUID,MN,ZR;2)      298.15 -11253.58;          6000 N !
PAR L(LIQUID,Y,ZR;0)       298.15 +24000;            6000 N !
PAR L(LIQUID,Y,ZR;1)       298.15 +3000;             6000 N !
$
PHASE DHCP Z 2 1 0.5 !
CONST DHCP : LA : VA% O : !
PAR G(DHCP,LA:VA)          298.15 +GHSERLA;          3200 N !
PAR G(DHCP,LA:O)           298.15
+GHSERLA+0.5*GHSEROO-285000+42.4*T;          3200 N !
$
PHASE HCP_A3 Z 2 1 0.5 !
CONST HCP_A3 : CR MN Y% ZR% : VA% O : !
PAR G(HCP_A3,CR:VA;0)      298.15 +GHSERCR+4438;      6000 N !
PAR G(HCP_A3,CR:O)         298.15
+GHSERCR+4438+0.5*GHSEROO;          6000 N !
PAR TC(HCP_A3,CR:VA;0)     298.15 -1109;             6000 N !
PAR BMAGN(HCP_A3,CR:VA;0)  298.15 -2.46;             6000 N !
PAR G(HCP_A3,MN:VA)        298.15 +GMNHCP;            2000 N !
PAR G(HCP_A3,MN:O)         298.15 +GMNHCP+0.5*GHSEROO; 6000 N !
PAR TC(HCP_A3,MN:VA;0)     298.15 -1620;             6000 N !
PAR BMAGN(HCP_A3,MN:VA;0)  298.15 -1.86;             6000 N !
PAR G(HCP_A3,Y:VA)         298.15 +GHSERYYY;          3700 N !
PAR G(HCP_A3,Y:O)          298.15 +GHSERYYY+0.5*GHSEROO
-303600+37.5*T;          6000 N !
PAR G(HCP_A3,ZR:VA)        298.15 +GHSERZR;          6000 N !
PAR G(HCP_A3,ZR:O)         298.15 +GHSERZR+0.5*GHSEROO
-280300+41*T;          6000 N !
PAR L(HCP_A3,Y:O,VA;0)     298.15 +3500;             6000 N !
PAR L(HCP_A3,ZR:O,VA;0)    298.15 -29100+15.5*T;      6000 N !
PAR L(HCP_A3,ZR:O,VA;1)    298.15 -9150+3*T;         6000 N !
PAR L(HCP_A3,CR,MN:VA;0)   298.15 +60000;            6000 N !
PAR L(HCP_A3,MN,Y:VA;0)    298.15 +19000;            6000 N !
PAR L(HCP_A3,MN,ZR:VA;0)   298.15 -8123.31;          6000 N !
PAR L(HCP_A3,Y,ZR:VA;0)    298.15 +50000;            6000 N !
$
PHASE BCC_A2 ZB 2 1 1.5 !
CONST BCC_A2 : CR LA MN Y ZR SR : VA% O : !

```

PAR TC(BCC_A2,CR:VA;0)	298.15 -311.5;	6000 N !
PAR TC(BCC_A2,MN:VA)	298.15 -580;	2000 N !
PAR TC(BCC_A2,CR,MN:VA;0)	298.15 -1325;	6000 N !
PAR TC(BCC_A2,CR,MN:VA;2)	298.15 -1133;	6000 N !
PAR TC(BCC_A2,CR,MN:VA;4)	298.15 -10294;	6000 N !
PAR TC(BCC_A2,CR,MN:VA;6)	298.15 +26706;	6000 N !
PAR TC(BCC_A2,CR,MN:VA;8)	298.15 -28117;	6000 N !
PAR BMAGN(BCC_A2,CR:VA;0)	298.15 -0.008;	6000 N !
PAR BMAGN(BCC_A2,MN:VA)	298.15 -0.27;	2000 N !
PAR BMAGN(BCC_A2,CR,MN:VA;0)	298.15 +0.48643;	6000 N !
PAR BMAGN(BCC_A2,CR,MN:VA;2)	298.15 -0.72035;	6000 N !
PAR BMAGN(BCC_A2,CR,MN:VA;4)	298.15 -1.93265;	6000 N !
PAR G(BCC_A2,CR:VA;0)	298.15 +GHSERCR;	6000 N !
PAR G(BCC_A2,CR:O;0)	298.15	
	+GHSERCR+1.5*GHSEROO+113.17755*T;	6000 N !
PAR G(BCC_A2,LA:VA)	298.15 +GLABCC;	3200 N !
PAR G(BCC_A2,LA:O)	298.15	
	+GLABCC+1.5*GHSEROO-855000+142.5*T;	3200 N !
PAR G(BCC_A2,MN:VA)	298.15 +GMNBCC;	2000 N !
PAR G(BCC_A2,MN:O)	298.15	
	+GMNBCC+1.5*GHSEROO+50*T;	6000 N !
PAR G(BCC_A2,SR:VA;0)	298.15 +GSRBCC;	3000 N !
PAR G(BCC_A2,SR:O;0)	298.15 +GSRBCC+1.5*GHSEROO;	3000 N !
PAR G(BCC_A2,Y:VA)	298.15 +GYYBCC;	3700 N !
PAR G(BCC_A2,Y:O)	298.15 +GYYBCC+1.5*GHSEROO	
	-899200+123*T;	6000 N !
PAR G(BCC_A2,ZR:VA)	298.15 +GZRBCC;	6000 N !
PAR G(BCC_A2,ZR:O)	298.15 +GZRBCC+1.5*GHSEROO;	6000 N !
PAR L(BCC_A2,CR:O,VA;0)	298.15 -355151.422;	6000 N !
PAR L(BCC_A2,Y:O,VA;0)	298.15 -5000;	3300 N !
PAR L(BCC_A2,ZR:O,VA;0)	298.15 -1102000+155.4*T;	6000 N !
PAR L(BCC_A2,ZR:O,VA;1)	298.15 -235000;	6000 N !
PAR L(BCC_A2,CR,LA:VA;0)	298.15 +99571;	6000 N !
PAR L(BCC_A2,CR,MN:VA;0)	298.15 -20328+18.7339*T;	6000 N !
PAR L(BCC_A2,CR,MN:VA;1)	298.15 -9162+4.4183*T;	6000 N !
PAR L(BCC_A2,MN,Y:VA;0)	298.15 +25000;	3300 N !
PAR L(BCC_A2,MN,ZR:VA;0)	298.15 -54491.27+30.8108*T;	6000 N !
PAR L(BCC_A2,MN,ZR:VA;1)	298.15 -6418.27+0.51346*T;	6000 N !
PAR L(BCC_A2,Y,ZR:VA;0)	298.15 +40000;	6000 N !
PAR L(BCC_A2,Y,ZR:VA;1)	298.15 -9000;	6000 N !
\$		
PHASE CBCC_A12 ZA 2 1 1 !		
CONST CBCC_A12 : CR MN : VA : !		
PAR TC(CBCC_A12,MN:VA)	298.15 -285;	2000 N !
PAR BMAGN(CBCC_A12,MN:VA)	298.15 -0.66;	2000 N !

PAR G(CBCC_A12,CR:VA;0) 298.15 +GHSERCR+11087+2.7196*T; 6000 N !
 PAR G(CBCC_A12,MN:VA;0) 298.15 +GHSERMN; 2000 N !
 PAR L(CBCC_A12,CR,MN:VA;0) 298.15 -38349+22.6925*T; 6000 N !
 \$
 PHASE FCC_A1 ZA 2 1 1 !
 CONST FCC_A1 : CR LA% MN% ZR SR : VA% O : !
 PAR G(FCC_A1,CR:VA;0) 298.15 +GCRFCC; 6000 N !
 PAR G(FCC_A1,CR:O;0) 298.15 +GCRFCC+GHSEROO; 6000 N !
 PAR TC(FCC_A1,CR:VA;0) 298.15 -1109; 6000 N !
 PAR BMAGN(FCC_A1,CR:VA;0) 298.15 -2.46; 6000 N !
 PAR G(FCC_A1,LA:VA) 298.15 +GLAFCC; 3200 N !
 PAR G(FCC_A1,LA:O) 298.15
 +GLAFCC+GHSEROO-570000+91.4*T; 3200 N !
 PAR G(FCC_A1,MN:VA) 298.15 +GMNFCC; 2000 N !
 PAR G(FCC_A1,MN:O) 298.15 +GMNFCC+GHSEROO; 2000 N !
 PAR TC(FCC_A1,MN:VA) 298.15 -1620; 2000 N !
 PAR BMAGN(FCC_A1,MN:VA) 298.15 -1.86; 2000 N !
 PAR G(FCC_A1,ZR:VA) 130.00 +GHSERZR+7600-0.9*T; 6000 N !
 PAR G(FCC_A1,ZR:O) 130.00
 +GHSERZR+7600-0.9*T+GHSEROO; 6000 N !
 PAR G(FCC_A1,SR:VA;0) 298.15 +GHSERSR; 3000 N !
 PAR G(FCC_A1,SR:O;0) 298.15 +GHSERSR+GHSEROO; 3000 N !
 \$ The parameter below is to keep Cr solubility in fcc La zero.
 PAR L(FCC_A1,CR,LA:VA;0) 298.15 +100000; 6000 N !
 \$
 PAR L(FCC_A1,CR,MN:VA;0) 298.15 -19088+17.5423*T; 6000 N !
 PAR L(FCC_A1,MN,ZR:VA;0) 298.15 +5059.03-0.40472*T; 6000 N !
 PAR L(FCC_A1,MN,ZR:VA;1) 298.15 -26984.11+2.15873*T; 6000 N !
 \$
 PHASE CUB_A13 Z 2 1 1 !
 CONST CUB_A13 : CR MN : VA : !
 PAR G(CUB_A13,CR:VA;0) 298.15 +GHSERCR+15899+0.6276*T; 6000 N !
 PAR G(CUB_A13,MN:VA) 298.15 +GMNCUB; 2000 N !
 PAR L(CUB_A13,CR,MN:VA;0) 298.15 -31260+16.4919*T; 6000 N !
 \$ SIGMA ALLOY
 PHASE SIGMA Z 3 8 4 18 !
 CONST SIGMA : MN : CR : CR MN : !
 PAR G(SIGMA,MN:CR:CR;0) 298.15
 +8*GMNFCC+22*GHSERCR+65859.5; 6000 N !
 PAR G(SIGMA,MN:CR:MN;0) 298.15
 +8*GMNFCC+4*GHSERCR+18*GMNBCC-172946+69.0245*T; 6000 N !
 PAR L(SIGMA,MN:CR:CR,MN;0) 298.15 -1095771+862.0312*T; 6000 N !
 \$ H_SIGMA ALLOY
 PHASE HSIGMA Z 3 8 4 18 !
 CONST HSIGMA : MN : CR : CR MN : !

PAR G(HSIGMA,MN:CR:CR;0) 298.15
 +8*GMNFCC+22*GHSECR-192369+152.4742*T; 6000 N !
 PAR G(HSIGMA,MN:CR:MN;0) 298.15
 +8*GMNFCC+4*GHSECR+18*GMNBCC-74263-10.7082*T; 6000 N !
 PAR L(HSIGMA,MN:CR:CR,MN;0) 298.15 +90000; 6000 N !
 \$ ALPHA'_ALLOY
 PHASE ALPHA Z 2 3 5 !
 CONST ALPHA : CR : MN : !
 PAR G(ALPHA,CR:MN;0) 298.15
 +3*GHSECR+5*GHSERMN-72550+21.1732*T; 6000 N !
 \$
 PHASE MN12Y Z 2 12 1 !
 CONST MN12Y : MN : Y : !
 PAR G(MN12Y,MN:Y) 298.15 +GMN12Y; 2000 N !
 \$
 PHASE MN23Y6 Z 2 23 6 !
 CONST MN23Y6 : MN : Y : !
 PAR G(MN23Y6,MN:Y) 298.15 +GMN23Y6; 2000 N !
 \$
 PHASE MN2Y Z 2 2 1 !
 CONST MN2Y : MN : Y : !
 PAR G(MN2Y,MN:Y) 298.15 +GMN2Y; 2000 N !
 \$
 PHASE MN2ZR Z 2 2 1 !
 CONST MN2ZR : MN : ZR% VA : !
 PAR G(MN2ZR,MN:ZR) 298.15 +2*GHSERMN+GHSEZR
 -120013.95+36.9305*T; 6000 N !
 PAR G(MN2ZR,MN:VA) 298.15 +2*GHSERMN+15000; 6000 N !
 PAR L(MN2ZR,MN:ZR,VA;0) 298.15 -2029.39+0.16235*T; 6000 N !
 \$
 \$ (CrFe)2O3 with Mn solubility
 \$ Cr-Mn-O fully optimized
 \$ Cr-Fe-O from Taylor, 1993
 PHASE CFCORU:I ZA 3 2 1 3 !
 CONST CFCORU:I : CR+2 CR+3 FE+3 MN+3 : CR+3 VA : O-2: !
 PAR TC(CFCORU,CR+2:CR+3:O-2;0) 298.15 +308.6; 6000 N !
 PAR TC(CFCORU,CR+2:VA:O-2;0) 298.15 +308.6; 6000 N !
 PAR TC(CFCORU,CR+3:CR+3:O-2;0) 298.15 +308.6; 6000 N !
 PAR TC(CFCORU,CR+3:VA:O-2;0) 298.15 +308.6; 6000 N !
 PAR TC(CFCORU,FE+3:CR+3:O-2;0) 298.15 -2867; 6000 N !
 PAR TC(CFCORU,FE+3:VA:O-2;0) 298.15 -2867; 6000 N !
 PAR TC(CFCORU,MN+3:CR+3:O-2;0) 298.15 +309; 6000 N !
 PAR TC(CFCORU,MN+3:VA:O-2;0) 298.15 +309; 6000 N !
 PAR BMAGN(CFCORU,CR+2:CR+3:O-2;0) 298.15 +3; 6000 N !
 PAR BMAGN(CFCORU,CR+2:VA:O-2;0) 298.15 +3; 6000 N !

PAR BMAGN(CFCORU,CR+3:CR+3:O-2;0) 298.15 +3; 6000 N !
 PAR BMAGN(CFCORU,CR+3:VA:O-2;0) 298.15 +3; 6000 N !
 PAR BMAGN(CFCORU,FE+3:CR+3:O-2;0) 298.15 -25.1; 6000 N !
 PAR BMAGN(CFCORU,FE+3:VA:O-2;0) 298.15 -25.1; 6000 N !
 PAR BMAGN(CFCORU,MN+3:CR+3:O-2;0) 298.15 +0.59; 6000 N !
 PAR BMAGN(CFCORU,MN+3:VA:O-2;0) 298.15 +0.59; 6000 N !
 PAR G(CFCORU,CR+2:CR+3:O-2;0) 298.15
 +GCRO0+.33333333334*GHSECR-5.2923*T; 6000 N !
 PAR G(CFCORU,CR+2:VA:O-2;0) 298.15
 +GCRO0-0.66666666667*GHSECR-5.2923*T; 6000 N !
 PAR G(CFCORU,CR+3:CR+3:O-2;0) 298.15 +GCR2O3+GHSECR; 6000 N !
 PAR G(CFCORU,CR+3:VA:O-2;0) 298.15 +GCR2O3; 6000 N !
 PAR G(CFCORU,FE+3:CR+3:O-2;0) 298.15 +GFE2O3+300000; 6000 N !
 PAR G(CFCORU,FE+3:VA:O-2;0) 298.15 +GFE2O3; 6000 N !
 PAR G(CFCORU,MN+3:CR+3:O-2;0) 298.15 +GMN2O3+GHSECR+39503; 6000 N !
 PAR G(CFCORU,MN+3:VA:O-2;0) 298.15 +GMN2O3+39503; 6000 N !
 PAR L(CFCORU,CR+3,FE+3:VA:O-2;1) 298.15 -16250+12.5*T; 6000 N !
 \$
 \$ ESKOLAITE, NONSTOICHIOMETRIC CR2O3 SOLID SOLUTION
 PHASE CR2O3:I ZA 3 2 1 3 !
 CONST CR2O3:I : MN+3 CR+2 CR+3 : CR+3 VA : O-2: !
 PAR TC(CR2O3,MN+3:CR+3:O-2;0) 298.15 +309; 6000 N !
 PAR TC(CR2O3,MN+3:VA:O-2;0) 298.15 +309; 6000 N !
 PAR TC(CR2O3,CR+2:CR+3:O-2;0) 298.15 +308.6; 6000 N !
 PAR TC(CR2O3,CR+2:VA:O-2;0) 298.15 +308.6; 6000 N !
 PAR TC(CR2O3,CR+3:CR+3:O-2;0) 298.15 +308.6; 6000 N !
 PAR TC(CR2O3,CR+3:VA:O-2;0) 298.15 +308.6; 6000 N !
 PAR BMAGN(CR2O3,MN+3:CR+3:O-2;0) 298.15 +0.59; 6000 N !
 PAR BMAGN(CR2O3,MN+3:VA:O-2;0) 298.15 +0.59; 6000 N !
 PAR BMAGN(CR2O3,CR+2:CR+3:O-2;0) 298.15 +3; 6000 N !
 PAR BMAGN(CR2O3,CR+2:VA:O-2;0) 298.15 +3; 6000 N !
 PAR BMAGN(CR2O3,CR+3:CR+3:O-2;0) 298.15 +3; 6000 N !
 PAR BMAGN(CR2O3,CR+3:VA:O-2;0) 298.15 +3; 6000 N !
 PAR G(CR2O3,MN+3:CR+3:O-2;0) 298.15 +GMN2O3+GHSECR+39503; 6000 N !
 PAR G(CR2O3,MN+3:VA:O-2;0) 298.15 +GMN2O3+39503; 6000 N !
 PAR G(CR2O3,CR+2:CR+3:O-2;0) 298.15
 +GCRO0+.33333333334*GHSECR-5.2923*T; 6000 N !
 PAR G(CR2O3,CR+2:VA:O-2;0) 298.15
 +GCRO0-0.66666666667*GHSECR-5.2923*T; 6000 N !
 PAR G(CR2O3,CR+3:CR+3:O-2;0) 298.15 +GCR2O3+GHSECR; 6000 N !
 PAR G(CR2O3,CR+3:VA:O-2;0) 298.15 +GCR2O3; 6000 N !
 \$
 \$ Fe2O3 Corundum, to be combined with Cr2O3 in the future!

PHASE COR:I ZA 3 2 1 3 !
 CONST COR:I : FE+3 : VA : O-2 : !
 PAR TC(COR,FE+3:VA:O-2;0) 298.15 -2867; 6000 N !
 PAR BMAGN(COR,FE+3:VA:O-2;0) 298.15 -25.1; 6000 N !
 PAR G(COR,FE+3:VA:O-2;0) 298.15 +GFE2O3; 6000 N !
 \$
 \$ Monoxide containing FeO and MnO with Cr solubility
 \$ Only Mn-Cr-O fully optimized
 \$ FeO-MnO to be optimized in the future!
 \$ FeO-CrO, interaction parameters taken from Taylor, 1993
 PHASE MONOX:I Z 2 1 1 !
 CONST MONOX:I : CR+3 FE+2 FE+3 MN+2 MN+3 VA : O-2 : !
 PAR G(MONOX,CR+3:O-2;0) 298.15
 +0.5*GCR2O3-7.93845*T+71549.3; 6000 N !
 PAR G(MONOX,FE+2:O-2;0) 298.15 +GFEO; 6000 N !
 PAR G(MONOX,FE+3:O-2;0) 298.15 +1.25*GFEO+1.25*GAFeO; 6000 N !
 PAR G(MONOX,MN+2:O-2) 298.15 +GMN1O1; 6000 N !
 PAR G(MONOX,MN+3:O-2) 298.15 +GMN1O1-21884-22.185*T; 6000 N !
 PAR G(MONOX,VA:O-2) 298.15 0; 6000 N !
 PAR L(MONOX,FE+2,FE+3:O-2;0) 298.15 -12324; 6000 N !
 PAR L(MONOX,FE+2,FE+3:O-2;1) 298.15 +20070; 6000 N !
 PAR L(MONOX,MN+2,MN+3:O-2;0) 298.15 -42105; 6000 N !
 PAR L(MONOX,MN+2,MN+3:O-2;1) 298.15 +46513; 6000 N !
 PAR L(MONOX,CR+3,FE+2:O-2;0) 298.15 +12500; 6000 N !
 \$
 \$ (CrFe)3O4 spinel from Taylor, 1993
 \$ In the future: simply the model and include Co3O4, Mn3O4.
 \$
 PHASE CFSPIN:I ZA 4 1 2 2 4 !
 CONST CFSPIN:I : CR+2 CR+3 FE+2 FE+3 : CR+3 FE+2 FE+3 VA : FE+2 VA : O-2 :
 !
 PAR TC(CFSPIN,FE+2:FE+2:FE+2:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,FE+2:FE+2:VA:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,FE+2:FE+3:FE+2:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,FE+2:FE+3:VA:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,FE+2:CR+3:FE+2:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,FE+2:CR+3:VA:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,FE+2:VA:FE+2:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,FE+2:VA:VA:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,FE+3:FE+2:FE+2:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,FE+3:FE+2:VA:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,FE+3:FE+3:FE+2:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,FE+3:FE+3:VA:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,FE+3:CR+3:FE+2:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,FE+3:CR+3:VA:O-2;0) 298.15 +100; 6000 N !

PAR TC(CFSPIN,FE+3:VA:FE+2:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,FE+3:VA:VA:O-2;0) 298.15 +848; 6000 N !
 PAR TC(CFSPIN,CR+2:FE+2:FE+2:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,CR+2:FE+2:VA:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,CR+2:FE+3:FE+2:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,CR+2:FE+3:VA:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,CR+2:CR+3:FE+2:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,CR+2:VA:FE+2:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,CR+3:FE+2:FE+2:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,CR+3:FE+3:FE+2:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,CR+3:CR+3:FE+2:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,CR+3:FE+2:VA:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,CR+3:FE+3:VA:O-2;0) 298.15 +100; 6000 N !
 PAR TC(CFSPIN,CR+3:VA:FE+2:O-2;0) 298.15 +100; 6000 N !
 PAR BMAGN(CFSPIN,FE+2:FE+2:FE+2:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,FE+2:FE+2:VA:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,FE+2:FE+3:FE+2:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,FE+2:FE+3:VA:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,FE+2:CR+3:FE+2:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,FE+2:CR+3:VA:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,FE+2:VA:FE+2:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,FE+2:VA:VA:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,FE+3:FE+2:FE+2:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,FE+3:FE+2:VA:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,FE+3:FE+3:FE+2:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,FE+3:FE+3:VA:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,FE+3:CR+3:FE+2:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,FE+3:CR+3:VA:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,FE+3:VA:FE+2:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,FE+3:VA:VA:O-2;0) 298.15 +44.54; 6000 N !
 PAR BMAGN(CFSPIN,CR+2:FE+2:FE+2:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,CR+2:FE+2:VA:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,CR+2:FE+3:FE+2:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,CR+2:FE+3:VA:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,CR+2:CR+3:FE+2:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,CR+2:VA:FE+2:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,CR+3:FE+2:FE+2:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,CR+3:FE+3:FE+2:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,CR+3:CR+3:FE+2:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,CR+3:FE+2:VA:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,CR+3:FE+3:VA:O-2;0) 298.15 +0.9; 6000 N !
 PAR BMAGN(CFSPIN,CR+3:VA:FE+2:O-2;0) 298.15 +0.9; 6000 N !
 PAR G(CFSPIN,FE+2:FE+2:FE+2:O-2;0) 298.15 +9*GFE3O4+DFE3O4; 6000 N !
 PAR G(CFSPIN,FE+2:FE+2:VA:O-2;0) 298.15 +7*GFE3O4+BFE3O4; 6000 N !
 PAR G(CFSPIN,FE+2:FE+3:FE+2:O-2;0) 298.15

+9*GFE3O4+DFE3O4-BFE3O4; 6000 N !
 PAR G(CFSPIN,FE+2:VA:FE+2:O-2;0) 298.15
 +7*GFE3O4+DFE3O4+CFE3O4-BFE3O4; 6000 N !
 PAR G(CFSPIN,FE+2:FE+3:VA:O-2;0) 298.15 +7*GFE3O4; 6000 N !
 PAR G(CFSPIN,FE+2:VA:VA:O-2;0) 298.15 +5*GFE3O4+CFE3O4; 6000 N !
 PAR G(CFSPIN,FE+2:CR+3:FE+2:O-2;0) 298.15
 +7*FSPIN+2*GFE3O4+DFE3O4-BFE3O4; 6000 N !
 PAR G(CFSPIN,FE+2:CR+3:VA:O-2;0) 298.15 +7*FSPIN; 6000 N !
 PAR G(CFSPIN,FE+3:FE+2:FE+2:O-2;0) 298.15
 +9*GFE3O4+DFE3O4-BFE3O4; 6000 N !
 PAR G(CFSPIN,FE+3:FE+3:FE+2:O-2;0) 298.15
 +9*GFE3O4+DFE3O4-2*BFE3O4; 6000 N !
 PAR G(CFSPIN,FE+3:VA:FE+2:O-2;0) 298.15
 +7*GFE3O4+DFE3O4+CFE3O4-2*BFE3O4; 6000 N !
 PAR G(CFSPIN,FE+3:FE+2:VA:O-2;0) 298.15 +7*GFE3O4; 6000 N !
 PAR G(CFSPIN,FE+3:VA:VA:O-2;0) 298.15
 +5*GFE3O4+CFE3O4-BFE3O4; 6000 N !
 PAR G(CFSPIN,FE+3:CR+3:FE+2:O-2;0) 298.15
 +7*FSPIN+2*GFE3O4+DFE3O4-2*BFE3O4; 6000 N !
 PAR G(CFSPIN,FE+3:CR+3:VA:O-2;0) 298.15 +7*FSPIN-BFE3O4; 6000 N !
 PAR G(CFSPIN,FE+3:FE+3:VA:O-2;0) 298.15 +7*GFE3O4-BFE3O4; 6000 N !
 PAR G(CFSPIN,CR+2:FE+2:FE+2:O-2;0) 298.15
 +3.5*FSPIN+5.5*GFE3O4-.5*BFE3O4+RSPIN+SSPIN+DFE3O4; 6000 N !
 PAR G(CFSPIN,CR+2:FE+3:FE+2:O-2;0) 298.15
 +3.5*FSPIN+5.5*GFE3O4-1.5*BFE3O4+RSPIN+SSPIN+DFE3O4; 6000 N !
 PAR G(CFSPIN,CR+2:VA:FE+2:O-2;0) 298.15
 +3.5*FSPIN+3.5*GFE3O4-1.5*BFE3O4+RSPIN+SSPIN+CFE3O4+DFE3O4;
 6000 N !
 PAR G(CFSPIN,CR+2:FE+2:VA:O-2;0) 298.15
 +3.5*FSPIN+3.5*GFE3O4+.5*BFE3O4+RSPIN+SSPIN; 6000 N !
 PAR G(CFSPIN,CR+2:FE+3:VA:O-2;0) 298.15
 +3.5*FSPIN+3.5*GFE3O4-.5*BFE3O4+RSPIN+SSPIN; 6000 N !
 PAR G(CFSPIN,CR+2:VA:VA:O-2;0) 298.15
 +3.5*FSPIN+1.5*GFE3O4-.5*BFE3O4+RSPIN+SSPIN+CFE3O4; 6000 N !
 PAR G(CFSPIN,CR+2:CR+3:FE+2:O-2;0) 298.15
 +10.5*FSPIN-1.5*GFE3O4-1.5*BFE3O4+RSPIN+SSPIN+DFE3O4; 6000 N !
 PAR G(CFSPIN,CR+2:CR+3:VA:O-2;0) 298.15
 +10.5*FSPIN-3.5*GFE3O4-.5*BFE3O4+RSPIN+SSPIN; 6000 N !
 PAR G(CFSPIN,CR+3:FE+2:FE+2:O-2;0) 298.15
 +3.5*FSPIN+5.5*GFE3O4+RSPIN-.5*BFE3O4+DFE3O4; 6000 N !
 PAR G(CFSPIN,CR+3:FE+3:FE+2:O-2;0) 298.15
 +3.5*FSPIN+5.5*GFE3O4+RSPIN-1.5*BFE3O4+DFE3O4; 6000 N !
 PAR G(CFSPIN,CR+3:VA:FE+2:O-2;0) 298.15
 +3.5*FSPIN+3.5*GFE3O4+RSPIN-1.5*BFE3O4+DFE3O4+CFE3O4; 6000 N !
 PAR G(CFSPIN,CR+3:FE+2:VA:O-2;0) 298.15

+3.5*FSPIN+3.5*GFE3O4+RSPIN+.5*BFE3O4; 6000 N !
 PAR G(CFSPIN,CR+3:FE+3:VA:O-2;0) 298.15
 +3.5*FSPIN+3.5*GFE3O4+RSPIN-.5*BFE3O4; 6000 N !
 PAR G(CFSPIN,CR+3:VA:VA:O-2;0) 298.15
 +3.5*FSPIN+1.5*GFE3O4+RSPIN-.5*BFE3O4+CFE3O4; 6000 N !
 PAR G(CFSPIN,CR+3:CR+3:FE+2:O-2;0) 298.15
 +10.5*FSPIN-1.5*GFE3O4+DFE3O4-1.5*BFE3O4+RSPIN; 6000 N !
 PAR G(CFSPIN,CR+3:CR+3:VA:O-2;0) 298.15
 +10.5*FSPIN-3.5*GFE3O4+RSPIN-.5*BFE3O4; 6000 N !
 PAR L(CFSPIN,FE+2:CR+3,FE+2:VA:O-2;0) 298.15 +152380-60*T; 6000 N !
 PAR L(CFSPIN,FE+2:CR+3,FE+3:VA:O-2;0) 298.15 -24942+28.5714*T; 6000 N !
 PAR L(CFSPIN,FE+2:CR+3,VA:VA:O-2;0) 298.15 +5000; 6000 N !
 PAR L(CFSPIN,FE+2:CR+3,VA:VA:O-2;1) 298.15 +150000; 6000 N !
 PAR L(CFSPIN,FE+3:CR+3,FE+2:VA:O-2;0) 298.15 +152380-60*T; 6000 N !
 PAR L(CFSPIN,FE+3:CR+3,VA:VA:O-2;0) 298.15 +5000; 6000 N !
 PAR L(CFSPIN,FE+3:CR+3,VA:VA:O-2;1) 298.15 +150000; 6000 N !
 PAR L(CFSPIN,CR+3,FE+2:FE+2:VA:O-2;0) 298.15 +20000; 6000 N !
 PAR L(CFSPIN,CR+3,FE+2:FE+3:VA:O-2;0) 298.15 +20000; 6000 N !
 PAR L(CFSPIN,CR+3,FE+2:VA:VA:O-2;0) 298.15 +20000; 6000 N !
 PAR L(CFSPIN,CR+3,FE+2:CR+3:VA:O-2;0) 298.15 +20000; 6000 N !
 \$

PHASE SPINEL:I ZA 4 1 2 2 4 !

CONST SPINEL:I :FE+2 FE+3 : FE+2 FE+3 VA : FE+2 VA : O-2 : !

PAR TC(SPINEL,FE+2:FE+2:FE+2:O-2;0) 298.15 848; 6000 N !
 PAR TC(SPINEL,FE+3:FE+2:FE+2:O-2;0) 298.15 848; 6000 N !
 PAR TC(SPINEL,FE+2:FE+3:FE+2:O-2;0) 298.15 848; 6000 N !
 PAR TC(SPINEL,FE+3:FE+3:FE+2:O-2;0) 298.15 848; 6000 N !
 PAR TC(SPINEL,FE+2:VA:FE+2:O-2;0) 298.15 848; 6000 N !
 PAR TC(SPINEL,FE+3:VA:FE+2:O-2;0) 298.15 848; 6000 N !
 PAR TC(SPINEL,FE+2:FE+2:VA:O-2;0) 298.15 848; 6000 N !
 PAR TC(SPINEL,FE+3:FE+2:VA:O-2;0) 298.15 848; 6000 N !
 PAR TC(SPINEL,FE+2:FE+3:VA:O-2;0) 298.15 848; 6000 N !
 PAR TC(SPINEL,FE+3:FE+3:VA:O-2;0) 298.15 848; 6000 N !
 PAR TC(SPINEL,FE+2:VA:VA:O-2;0) 298.15 848; 6000 N !
 PAR TC(SPINEL,FE+3:VA:VA:O-2;0) 298.15 848; 6000 N !
 PAR BMAGN(SPINEL,FE+2:FE+2:FE+2:O-2;0) 298.15 44.54; 6000 N !
 PAR BMAGN(SPINEL,FE+3:FE+2:FE+2:O-2;0) 298.15 44.54; 6000 N !
 PAR BMAGN(SPINEL,FE+2:FE+3:FE+2:O-2;0) 298.15 44.54; 6000 N !
 PAR BMAGN(SPINEL,FE+3:FE+3:FE+2:O-2;0) 298.15 44.54; 6000 N !
 PAR BMAGN(SPINEL,FE+2:VA:FE+2:O-2;0) 298.15 44.54; 6000 N !
 PAR BMAGN(SPINEL,FE+3:VA:FE+2:O-2;0) 298.15 44.54; 6000 N !
 PAR BMAGN(SPINEL,FE+2:FE+2:VA:O-2;0) 298.15 44.54; 6000 N !
 PAR BMAGN(SPINEL,FE+3:FE+2:VA:O-2;0) 298.15 44.54; 6000 N !
 PAR BMAGN(SPINEL,FE+2:FE+3:VA:O-2;0) 298.15 44.54; 6000 N !
 PAR BMAGN(SPINEL,FE+3:FE+3:VA:O-2;0) 298.15 44.54; 6000 N !

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PAR BMAGN(SPINEL,FE+2:VA:O-2;0) 298.15 44.54; 6000 N !
PAR BMAGN(SPINEL,FE+3:VA:O-2;0) 298.15 44.54; 6000 N !
PAR G(SPINEL,FE+2:FE+2:FE+2:O-2;0) 298.15 +9*GFE3O4+DFE3O4; 6000 N !
PAR G(SPINEL,FE+3:FE+2:FE+2:O-2;0) 298.15
+9*GFE3O4+DFE3O4-BFE3O4; 6000 N !
PAR G(SPINEL,FE+2:FE+3:FE+2:O-2;0) 298.15
+9*GFE3O4+DFE3O4-BFE3O4; 6000 N !
PAR G(SPINEL,FE+3:FE+3:FE+2:O-2;0) 298.15
+9*GFE3O4+DFE3O4-2*BFE3O4; 6000 N !
PAR G(SPINEL,FE+2:VA:FE+2:O-2;0) 298.15
+7*GFE3O4+DFE3O4+CFE3O4-BFE3O4; 6000 N !
PAR G(SPINEL,FE+3:VA:FE+2:O-2;0) 298.15
+7*GFE3O4+DFE3O4+CFE3O4-2*BFE3O4; 6000 N !
PAR G(SPINEL,FE+2:FE+2:VA:O-2;0) 298.15 +7*GFE3O4+BFE3O4; 6000 N !
PAR G(SPINEL,FE+3:FE+2:VA:O-2;0) 298.15 +7*GFE3O4; 6000 N !
PAR G(SPINEL,FE+2:FE+3:VA:O-2;0) 298.15 +7*GFE3O4; 6000 N !
PAR G(SPINEL,FE+3:FE+3:VA:O-2;0) 298.15 +7*GFE3O4-BFE3O4; 6000 N !
PAR G(SPINEL,FE+2:VA:VA:O-2;0) 298.15 +5*GFE3O4+CFE3O4; 6000 N !
PAR G(SPINEL,FE+3:VA:VA:O-2;0) 298.15
+5*GFE3O4+CFE3O4-BFE3O4; 6000 N !
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
PHASE MNO:I Z 2 1 1 !
CONST MNO:I : CR+3 MN+2 MN+3 VA : O-2 : !
PAR G(MNO,CR+3:O-2;0) 298.15
+0.5*GCR2O3-7.93845*T+71549.3; 6000 N !
PAR G(MNO,MN+2:O-2) 298.15 +GMN1O1; 6000 N !
PAR G(MNO,MN+3:O-2) 298.15 +GMN1O1-21884-22.185*T; 6000 N !
PAR G(MNO,VA:O-2) 298.15 0; 6000 N !
PAR L(MNO,MN+2,MN+3:O-2;0) 298.15 -42105; 6000 N !
PAR L(MNO,MN+2,MN+3:O-2;1) 298.15 +46513; 6000 N !
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$
PHASE TSPINEL:I Z 3 1 2 4 !
CONST TSPINEL:I : MN+2 : CR+3 MN+3 : O-2 : !
PAR G(TSPINEL,MN+2:CR+3:O-2;0) 298.15 +GTSPINEL; 6000 N !
PAR G(TSPINEL,MN+2:MN+3:O-2) 298.15 +GMN3O4; 6000 N !
$
PHASE CSPINEL:I Z 3 1 2 4 !
CONST CSPINEL:I : CR+2 MN+2 : CR+3 MN+3 : O-2 : !
PAR G(CSPINEL,MN+2:MN+3:O-2) 298.15 +GMN3O4B; 6000 N !
PAR G(CSPINEL,MN+2:CR+3:O-2;0) 298.15 +GSPINEL; 6000 N !
PAR G(CSPINEL,CR+2:CR+3:O-2;0) 298.15 +GCR3O4; 6000 N !
PAR G(CSPINEL,CR+2:MN+3:O-2;0) 298.15 +GCR3O4+GMN3O4B-GSPINEL;
6000 N !

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 PHASE MNO2:I Z 2 1 2 !
 CONST MNO2:I : MN+4 : O-2 : !
 PAR G(MNO2,MN+4:O-2) 298.15 +GMN1O2; 6000 N !
 \$
 PHASE LA2O3_A:I Z 3 2 3 1 !
 CONST LA2O3_A:I : LA LA+3% Y+3 ZR+4 SR+2 : O-2% VA : O-2 VA% : !
 PAR G(LA2O3_A,LA:VA:VA) 298.15 +2*GHSERLA+204124; 6000 N !
 PAR G(LA2O3_A,LA:O-2:O-2) 298.15
 +2*GHSERLA+4*GHSEROO+304124+15.87691*T; 6000 N !
 PAR G(LA2O3_A,LA:O-2:VA) 298.15
 +2*GHSERLA+3*GHSEROO+204124; 6000 N !
 PAR G(LA2O3_A,LA:VA:O-2) 298.15
 +2*GHSERLA+GHSEROO+304124+15.87691*T; 6000 N !
 PAR G(LA2O3_A,LA+3:O-2:VA) 298.15 +GLA2O3A; 6000 N !
 PAR G(LA2O3_A,LA+3:VA:VA) 298.15 +GLA2O3A-3*GHSEROO; 6000 N !
 !
 PAR G(LA2O3_A,LA+3:VA:O-2) 298.15
 +GLA2O3A-2*GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(LA2O3_A,LA+3:O-2:O-2) 298.15
 +GLA2O3A+GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(LA2O3_A,Y+3:O-2:VA) 298.15 +2*GAAYO15; 6000 N !
 PAR G(LA2O3_A,Y+3:VA:VA) 298.15 +2*GAAYO15-3*GHSEROO; 6000 N !
 !
 PAR G(LA2O3_A,Y+3:VA:O-2) 298.15
 +2*GAAYO15-2*GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(LA2O3_A,Y+3:O-2:O-2) 298.15
 +2*GAAYO15+GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(LA2O3_A,ZR+4:VA:VA) 298.15
 +2*GMAZRO2-4*GHSEROO-100000-15.87691*T; 6000 N !
 PAR G(LA2O3_A,ZR+4:O-2:O-2) 298.15 +2*GMAZRO2; 6000 N !
 PAR G(LA2O3_A,ZR+4:O-2:VA) 298.15
 +2*GMAZRO2-GHSEROO-100000-15.87691*T; 6000 N !
 PAR G(LA2O3_A,ZR+4:VA:O-2) 298.15 +2*GMAZRO2-3*GHSEROO; 6000 N !
 !
 PAR G(LA2O3_A,SR+2:O-2:VA;0) 298.15
 +SR_ALPHA+GHSEROO+15.87691*T; 6000 N !
 PAR G(LA2O3_A,SR+2:VA:VA;0) 298.15
 +SR_ALPHA-2*GHSEROO+15.87691*T; 6000 N !
 PAR G(LA2O3_A,SR+2:O-2:O-2;0) 298.15
 +SR_ALPHA+GHSEROO+15.87691*T+GHSEROO+100000+15.87691*T; 6000 N !
 !
 PAR G(LA2O3_A,SR+2:VA:O-2;0) 298.15
 +SR_ALPHA-2*GHSEROO+15.87691*T+GHSEROO+100000+15.87691*T;
 6000 N !

PAR L(LA2O3_A,LA+3,Y+3:O-2:O-2;0) 298.15 +36269; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:O-2:VA;0) 298.15 +36269; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:VA:O-2;0) 298.15 +36269; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:VA:VA;0) 298.15 +36269; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:O-2:O-2;1) 298.15 +18981; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:O-2:VA;1) 298.15 +18981; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:VA:O-2;1) 298.15 +18981; 6000 N !
 PAR L(LA2O3_A,LA+3,Y+3:VA:VA;1) 298.15 +18981; 6000 N !
 PAR L(LA2O3_A,LA+3,ZR+4:VA:VA;0) 298.15 -101793; 6000 N !
 PAR L(LA2O3_A,LA+3,ZR+4:O-2:O-2;0) 298.15 -101793; 6000 N !
 PAR L(LA2O3_A,LA+3,ZR+4:O-2:VA;0) 298.15 -101793; 6000 N !
 PAR L(LA2O3_A,LA+3,ZR+4:VA:O-2;0) 298.15 -101793; 6000 N !
 PAR L(LA2O3_A,LA+3,SR+2:O-2:O-2;0) 298.15 +2.149E+05-7.81E+01*T; 6000 N !
 PAR L(LA2O3_A,LA+3,SR+2:O-2:VA;0) 298.15 +2.149E+05-7.81E+01*T; 6000 N !
 PAR L(LA2O3_A,LA+3,SR+2:VA:O-2;0) 298.15 +2.149E+05-7.81E+01*T; 6000 N !
 PAR L(LA2O3_A,LA+3,SR+2:VA:VA;0) 298.15 +2.149E+05-7.81E+01*T; 6000 N !
 !
 \$
 PHASE LA2O3_B:I Z 3 2 3 1 !
 CONST LA2O3_B:I : LA+3 Y+3 : O-2% VA : O-2 VA% : !
 PAR G(LA2O3_B,LA+3:O-2:VA) 298.15 +GLA2O3B; 6000 N !
 PAR G(LA2O3_B,LA+3:VA:VA) 298.15 +GLA2O3B-3*GHSEROO; 6000 N !
 !
 PAR G(LA2O3_B,LA+3:VA:O-2) 298.15
 +GLA2O3B-2*GHSEROO+15.87691*T+100000; 6000 N !
 PAR G(LA2O3_B,LA+3:O-2:O-2) 298.15
 +GLA2O3B+GHSEROO+15.87691*T+100000; 6000 N !
 PAR G(LA2O3_B,Y+3:O-2:VA) 298.15 +2*GBBYO15; 6000 N !
 PAR G(LA2O3_B,Y+3:VA:VA) 298.15 +2*GBBYO15-3*GHSEROO; 6000 N !
 !
 PAR G(LA2O3_B,Y+3:VA:O-2) 298.15
 +2*GBBYO15-2*GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(LA2O3_B,Y+3:O-2:O-2) 298.15
 +2*GBBYO15+GHSEROO+100000+15.87691*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:O-2:O-2;0) 298.15 -21475+26.2*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:O-2:VA;0) 298.15 -21475+26.2*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:VA:O-2;0) 298.15 -21475+26.2*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:VA:VA;0) 298.15 -21475+26.2*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:O-2:O-2;1) 298.15 -60190+31.5*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:O-2:VA;1) 298.15 -60190+31.5*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:VA:O-2;1) 298.15 -60190+31.5*T; 6000 N !
 PAR L(LA2O3_B,LA+3,Y+3:VA:VA;1) 298.15 -60190+31.5*T; 6000 N !
 \$
 PHASE Y2O3_CUB:I Z 3 2 3 1 !

CONST Y2O3_CUB:I : CR+3 LA+3 MN+3% Y Y+3% ZR+4 : O-2% VA : O-2 VA% :
 !
 \$ This is essentially an ordered fluorite structure
 \$ This is also Mn2O3
 PAR G(Y2O3_CUB,CR+3:O-2:VA;0) 298.15 +GCR2O3+3459; 6000 N !
 PAR G(Y2O3_CUB,CR+3:O-2:O-2;0) 298.15
 +GCR2O3+3459+GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(Y2O3_CUB,CR+3:VA:O-2;0) 298.15
 +GCR2O3+3459-2*GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(Y2O3_CUB,CR+3:VA:VA;0) 298.15
 +GCR2O3+3459-3*GHSEROO; 6000 N !
 PAR G(Y2O3_CUB,LA+3:O-2:VA) 298.15 +GLA2O3C; 6000 N !
 PAR G(Y2O3_CUB,LA+3:VA:VA) 298.15 +GLA2O3C-3*GHSEROO; 6000 N
 !
 PAR G(Y2O3_CUB,LA+3:VA:O-2) 298.15
 +GLA2O3C-2*GHSEROO+15.87691*T+100000; 6000 N !
 PAR G(Y2O3_CUB,LA+3:O-2:O-2) 298.15
 +GLA2O3C+GHSEROO+15.87691*T+100000; 6000 N !
 PAR G(Y2O3_CUB,MN+3:O-2:VA) 298.15 +GMN2O3; 6000 N !
 PAR G(Y2O3_CUB,MN+3:VA:VA) 298.15 +GMN2O3-3*GHSEROO; 6000 N
 !
 PAR G(Y2O3_CUB,MN+3:VA:O-2) 298.15 +GMN2O3-2*GHSEROO
 +15.87691*T+100000; 6000 N !
 PAR G(Y2O3_CUB,MN+3:O-2:O-2) 298.15 +GMN2O3+GHSEROO
 +15.87691*T+100000; 6000 N !
 PAR G(Y2O3_CUB,Y:VA:VA) 298.15 +2*GHSERYY+245600; 6000 N !
 PAR G(Y2O3_CUB,Y:O-2:O-2) 298.15 +2*GHSERYY+245600
 +4*GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(Y2O3_CUB,Y:O-2:VA) 298.15 +2*GHSERYY+245600
 +3*GHSEROO; 6000 N !
 PAR G(Y2O3_CUB,Y:VA:O-2) 298.15 +2*GHSERYY+245600
 +GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(Y2O3_CUB,Y+3:O-2:VA) 298.15 +2*GCCYO15; 6000 N !
 PAR G(Y2O3_CUB,Y+3:VA:VA) 298.15 +2*GCCYO15-3*GHSEROO; 6000 N
 !
 PAR G(Y2O3_CUB,Y+3:VA:O-2) 298.15 +2*GCCYO15-2*GHSEROO
 +15.87691*T+100000; 6000 N !
 PAR G(Y2O3_CUB,Y+3:O-2:O-2) 298.15 +2*GCCYO15+GHSEROO
 +15.87691*T+100000; 6000 N !
 PAR G(Y2O3_CUB,ZR+4:VA:VA) 298.15 +2*GMCZRO2-4*GHSEROO
 -100000-15.87691*T; 6000 N !
 PAR G(Y2O3_CUB,ZR+4:O-2:O-2) 298.15 +2*GMCZRO2; 6000 N !
 PAR G(Y2O3_CUB,ZR+4:O-2:VA) 298.15 +2*GMCZRO2-GHSEROO
 -100000-15.87691*T; 6000 N !

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PAR G(Y2O3_CUB,ZR+4:VA:O-2) 298.15 +2*GMCZRO2-3*GHSEROO; 6000
N !
$
PAR L(Y2O3_CUB,CR+3,Y+3:VA:VA;0) 298.15 +200000; 6000 N !
PAR L(Y2O3_CUB,CR+3,Y+3:O-2:O-2;0) 298.15 +200000; 6000 N !
PAR L(Y2O3_CUB,CR+3,Y+3:O-2:VA;0) 298.15 +200000; 6000 N !
PAR L(Y2O3_CUB,CR+3,Y+3:VA:O-2;0) 298.15 +200000; 6000 N !
PAR L(Y2O3_CUB,CR+3,ZR+4:VA:VA;0) 298.15 +200000; 6000 N !
PAR L(Y2O3_CUB,CR+3,ZR+4:O-2:O-2;0) 298.15 +200000; 6000 N !
PAR L(Y2O3_CUB,CR+3,ZR+4:O-2:VA;0) 298.15 +200000; 6000 N !
PAR L(Y2O3_CUB,CR+3,ZR+4:VA:O-2;0) 298.15 +200000; 6000 N !
$
PAR L(Y2O3_CUB,LA+3,Y+3:O-2:O-2;0) 298.15 +31866; 6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:O-2:VA;0) 298.15 +31866; 6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:VA:O-2;0) 298.15 +31866; 6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:VA:VA;0) 298.15 +31866; 6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:O-2:O-2;1) 298.15 +29838; 6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:O-2:VA;1) 298.15 +29838; 6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:VA:O-2;1) 298.15 +29838; 6000 N !
PAR L(Y2O3_CUB,LA+3,Y+3:VA:VA;1) 298.15 +29838; 6000 N !
PAR L(Y2O3_CUB,MN+3,Y+3:VA:VA;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_CUB,MN+3,Y+3:O-2:O-2;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_CUB,MN+3,Y+3:O-2:VA;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_CUB,MN+3,Y+3:VA:O-2;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_CUB,MN+3,ZR+4:VA:VA;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_CUB,MN+3,ZR+4:O-2:O-2;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_CUB,MN+3,ZR+4:O-2:VA;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_CUB,MN+3,ZR+4:VA:O-2;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_CUB,Y+3,ZR+4:VA:VA;0) 298.15 -88700+13*T; 6000 N !
PAR L(Y2O3_CUB,Y+3,ZR+4:O-2:O-2;0) 298.15 -88700+13*T; 6000 N !
PAR L(Y2O3_CUB,Y+3,ZR+4:O-2:VA;0) 298.15 -88700+13*T; 6000 N !
PAR L(Y2O3_CUB,Y+3,ZR+4:VA:O-2;0) 298.15 -88700+13*T; 6000 N !
$
PHASE Y2O3_HEX:I Z 3 2 3 1 !
CONST Y2O3_HEX:I : LA LA+3% MN+3 Y Y+3% ZR+4 SR+2 : O-2% VA : O-2 VA%
: !
$ This is beta-Y2O3 (alias H-Y2O3)
$ This is also H-La2O3
PAR G(Y2O3_HEX,LA:VA:VA) 298.15 +2*GHSERLA+204124; 6000 N !
PAR G(Y2O3_HEX,LA:O-2:O-2) 298.15
+2*GHSERLA+4*GHSEROO+304124+15.87691*T; 6000 N !
PAR G(Y2O3_HEX,LA:O-2:VA) 298.15
+2*GHSERLA+3*GHSEROO+204124; 6000 N !
PAR G(Y2O3_HEX,LA:VA:O-2) 298.15
+2*GHSERLA+GHSEROO+304124+15.87691*T; 6000 N !

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PAR G(Y2O3_HEX,LA+3:O-2:VA) 298.15 +GLA2O3H; 6000 N !
 PAR G(Y2O3_HEX,LA+3:VA:VA) 298.15 +GLA2O3H-3*GHSEROO; 6000 N !
 PAR G(Y2O3_HEX,LA+3:VA:O-2) 298.15
 +GLA2O3H-2*GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(Y2O3_HEX,LA+3:O-2:O-2) 298.15
 +GLA2O3H+GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(Y2O3_HEX,MN+3:O-2:VA) 298.15 +GMHNMN2O3; 6000 N !
 PAR G(Y2O3_HEX,MN+3:VA:VA) 298.15 +GMHNMN2O3-3*GHSEROO; 6000 N !
 PAR G(Y2O3_HEX,MN+3:VA:O-2) 298.15 +GMHNMN2O3-2*GHSEROO
 +15.87691*T+100000; 6000 N !
 PAR G(Y2O3_HEX,MN+3:O-2:O-2) 298.15 +GMHNMN2O3+GHSEROO
 +15.87691*T+100000; 6000 N !
 PAR G(Y2O3_HEX,Y:VA:VA) 298.15 +2*GHSERYY+245600; 6000 N !
 PAR G(Y2O3_HEX,Y:O-2:O-2) 298.15 +2*GHSERYY+245600
 +4*GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(Y2O3_HEX,Y:O-2:VA) 298.15 +2*GHSERYY+245600
 +3*GHSEROO; 6000 N !
 PAR G(Y2O3_HEX,Y:VA:O-2) 298.15 +2*GHSERYY+245600
 +GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(Y2O3_HEX,Y+3:O-2:VA) 298.15 +2*GHHYO15; 6000 N !
 PAR G(Y2O3_HEX,Y+3:VA:VA) 298.15 +2*GHHYO15-3*GHSEROO; 6000 N !
 PAR G(Y2O3_HEX,Y+3:VA:O-2) 298.15 +2*GHHYO15-2*GHSEROO
 +15.87691*T+100000; 6000 N !
 PAR G(Y2O3_HEX,Y+3:O-2:O-2) 298.15 +2*GHHYO15+GHSEROO
 +15.87691*T+100000; 6000 N !
 PAR G(Y2O3_HEX,ZR+4:VA:VA) 298.15 +2*GMHZRO2-4*GHSEROO
 -100000-15.87691*T; 6000 N !
 PAR G(Y2O3_HEX,ZR+4:O-2:O-2) 298.15 +2*GMHZRO2; 6000 N !
 PAR G(Y2O3_HEX,ZR+4:O-2:VA) 298.15 +2*GMHZRO2-GHSEROO
 -100000-15.87691*T; 6000 N !
 PAR G(Y2O3_HEX,ZR+4:VA:O-2) 298.15 +2*GMHZRO2-3*GHSEROO; 6000 N !
 PAR G(Y2O3_HEX,SR+2:O-2:VA;0) 298.15
 +SRH_ALPH+GHSEROO+15.87691*T; 6000 N !
 PAR G(Y2O3_HEX,SR+2:VA:VA;0) 298.15
 +SRH_ALPH-2*GHSEROO+15.87691*T; 6000 N !
 PAR G(Y2O3_HEX,SR+2:O-2:O-2;0) 298.15
 +SRH_ALPH+GHSEROO+15.87691*T+GHSEROO+100000+15.87691*T; 6000 N !
 PAR G(Y2O3_HEX,SR+2:VA:O-2;0) 298.15
 +SRH_ALPH-2*GHSEROO+15.87691*T+GHSEROO+100000+15.87691*T; 6000 N !

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PAR L(Y2O3_HEX,LA+3,Y+3:O-2:O-2;0) 298.15 +27920; 6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:O-2:VA;0) 298.15 +27920; 6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:VA:O-2;0) 298.15 +27920; 6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:VA:VA;0) 298.15 +27920; 6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:O-2:O-2;1) 298.15 +12879; 6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:O-2:VA;1) 298.15 +12879; 6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:VA:O-2;1) 298.15 +12879; 6000 N !
PAR L(Y2O3_HEX,LA+3,Y+3:VA:VA;1) 298.15 +12879; 6000 N !
PAR L(Y2O3_HEX,LA+3,ZR+4:VA:VA;0) 298.15 -144923; 6000 N !
PAR L(Y2O3_HEX,LA+3,ZR+4:O-2:O-2;0) 298.15 -144923; 6000 N !
PAR L(Y2O3_HEX,LA+3,ZR+4:O-2:VA;0) 298.15 -144923; 6000 N !
PAR L(Y2O3_HEX,LA+3,ZR+4:VA:O-2;0) 298.15 -144923; 6000 N !
PAR L(Y2O3_HEX,MN+3,Y+3:VA:VA;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_HEX,MN+3,Y+3:O-2:O-2;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_HEX,MN+3,Y+3:O-2:VA;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_HEX,MN+3,Y+3:VA:O-2;0) 298.15 +100000; 6000 N !
PAR L(Y2O3_HEX,LA+3,SR+2:O-2:O-2;0) 298.15 1.936E+05-7.81E+01*T; 6000 N !
PAR L(Y2O3_HEX,LA+3,SR+2:O-2:VA;0) 298.15 1.936E+05-7.81E+01*T; 6000 N !
PAR L(Y2O3_HEX,LA+3,SR+2:VA:O-2;0) 298.15 1.936E+05-7.81E+01*T; 6000 N !
PAR L(Y2O3_HEX,LA+3,SR+2:VA:VA;0) 298.15 1.936E+05-7.81E+01*T; 6000 N
!
$
PHASE ZRO2_MONO:I Z 2 1 2 !
CONST ZRO2_MONO:I : Y+3 ZR+4% : O-2% VA : !
PAR G(ZRO2_MONO,Y+3:O-2) 298.15 +GMMYO15+0.5*GHSEROO
+9.3511*T; 6000 N !
PAR G(ZRO2_MONO,Y+3:VA) 298.15 +GMMYO15-1.5*GHSEROO
+9.3511*T; 6000 N !
PAR G(ZRO2_MONO,ZR+4:O-2) 298.15 +GMMZRO2; 6000 N !
PAR G(ZRO2_MONO,ZR+4:VA) 298.15 +GMMZRO2-2*GHSEROO; 6000 N
!
$
PHASE ZRO2_TETR:I Z 2 1 2 !
CONST ZRO2_TETR:I : LA+3 MN+2 MN+3 Y+3 ZR+4% : O-2% VA : !
PAR G(ZRO2_TETR,LA+3:O-2) 298.15
+0.5*GMTLA2O3+0.5*GHSEROO+9.3511*T; 6000 N !
PAR G(ZRO2_TETR,LA+3:VA) 298.15
+0.5*GMTLA2O3-1.5*GHSEROO+9.3511*T; 6000 N !
PAR G(ZRO2_TETR,MN+2:O-2) 298.15 +GMTMN1O1+GHSEROO
+11.5264*T; 6000 N !
PAR G(ZRO2_TETR,MN+2:VA) 298.15 +GMTMN1O1-GHSEROO
+11.5264*T; 6000 N !
PAR G(ZRO2_TETR,MN+3:O-2) 298.15 +0.5*GMTMN2O3+0.5*GHSEROO
+9.3511*T; 6000 N !
PAR G(ZRO2_TETR,MN+3:VA) 298.15 +0.5*GMTMN2O3-1.5*GHSEROO

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+9.3511*T; 6000 N !
PAR G(ZRO2_TETR,Y+3:O-2) 298.15 +GMTYO15+0.5*GHSEROO
+9.3511*T; 6000 N !
PAR G(ZRO2_TETR,Y+3:VA) 298.15 +GMTYO15-1.5*GHSEROO
+9.3511*T; 6000 N !
PAR G(ZRO2_TETR,ZR+4:O-2) 298.15 +GTTZRO2; 6000 N !
PAR G(ZRO2_TETR,ZR+4:VA) 298.15 +GTTZRO2-2*GHSEROO; 6000 N !
PAR L(ZRO2_TETR,LA+3,ZR+4:O-2;0) 298.15 -23609; 6000 N !
PAR L(ZRO2_TETR,LA+3,ZR+4:VA;0) 298.15 -23609; 6000 N !
PAR L(ZRO2_TETR,MN+2,ZR+4:O-2;0) 298.15 +20863; 6000 N !
PAR L(ZRO2_TETR,MN+2,ZR+4:VA;0) 298.15 +20863; 6000 N !
PAR L(ZRO2_TETR,MN+3,ZR+4:O-2;0) 298.15 +20863; 6000 N !
PAR L(ZRO2_TETR,MN+3,ZR+4:VA;0) 298.15 +20863; 6000 N !
PAR L(ZRO2_TETR,Y+3,ZR+4:O-2;0) 298.15 -48800+18.4*T; 6000 N !
PAR L(ZRO2_TETR,Y+3,ZR+4:VA;0) 298.15 -48800+18.4*T; 6000 N !
$
PHASE ZRO2_CUB:I Z 2 1 2 !
CONST ZRO2_CUB:I : CR+3 LA LA+3% MN+2 MN+3 Y Y+3% ZR ZR+4% SR+2 :
O-2 VA : !
$ This is also X-La2O3
PAR G(ZRO2_CUB,CR+3:O-2;0) 298.15
+0.5*GMCCR2O3+0.5*GHSEROO+9.3511*T; 6000 N !
PAR G(ZRO2_CUB,CR+3:VA;0) 298.15
+0.5*GMCCR2O3-1.5*GHSEROO+9.3511*T; 6000 N !
PAR G(ZRO2_CUB,LA:O-2) 298.15
+GHSERLA+2*GHSEROO+102062; 6000 N !
PAR G(ZRO2_CUB,LA:VA) 298.15 +GHSERLA+102062; 6000 N !
PAR G(ZRO2_CUB,LA+3:O-2) 298.15
+0.5*GLA2O3X+0.5*GHSEROO+9.3511*T; 6000 N !
PAR G(ZRO2_CUB,LA+3:VA) 298.15
+0.5*GLA2O3X-1.5*GHSEROO+9.3511*T; 6000 N !
PAR G(ZRO2_CUB,MN+2:O-2) 298.15 +GMFMN1O1+GHSEROO
+11.5264*T; 6000 N !
PAR G(ZRO2_CUB,MN+2:VA) 298.15 +GMFMN1O1-GHSEROO
+11.5264*T; 6000 N !
PAR G(ZRO2_CUB,MN+3:O-2) 298.15 +0.5*GMFMN2O3+0.5*GHSEROO
+9.3511*T; 6000 N !
PAR G(ZRO2_CUB,MN+3:VA) 298.15 +0.5*GMFMN2O3-1.5*GHSEROO
+9.3511*T; 6000 N !
PAR G(ZRO2_CUB,Y:O-2) 298.15 +GHSERYY+2*GHSEROO
+122800; 6000 N !
PAR G(ZRO2_CUB,Y:VA) 298.15 +GHSERYY+122800; 6000 N !
PAR G(ZRO2_CUB,Y+3:O-2) 298.15 +GXXYO15+0.5*GHSEROO
+9.3511*T; 6000 N !
PAR G(ZRO2_CUB,Y+3:VA) 298.15 +GXXYO15-1.5*GHSEROO

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PAR L(ZRO2_CUB,MN+2,ZR+4:VA;0) 298.15 +60656; 6000 N !
PAR L(ZRO2_CUB,MN+2,ZR+4:O-2;1) 298.15 +64538; 6000 N !
PAR L(ZRO2_CUB,MN+2,ZR+4:VA;1) 298.15 +64538; 6000 N !
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$$$$
PAR L(ZRO2_CUB,MN+3,ZR+4:O-2;0) 298.15 +51416; 6000 N !
PAR L(ZRO2_CUB,MN+3,ZR+4:VA;0) 298.15 +51416; 6000 N !
PAR L(ZRO2_CUB,MN+3,ZR+4:O-2;1) 298.15 +43282; 6000 N !
PAR L(ZRO2_CUB,MN+3,ZR+4:VA;1) 298.15 +43282; 6000 N !
PAR L(ZRO2_CUB,Y+3,ZR+4:O-2;0) 298.15 -84750+34.41*T; 6000 N !
PAR L(ZRO2_CUB,Y+3,ZR+4:VA;0) 298.15 -84750+34.41*T; 6000 N !
PAR L(ZRO2_CUB,Y+3,ZR+4:O-2;1) 298.15 +29880-7.69*T; 6000 N !
PAR L(ZRO2_CUB,Y+3,ZR+4:VA;1) 298.15 +29880-7.69*T; 6000 N !
PAR L(ZRO2_CUB,MN+2,Y+3,ZR+4:O-2;0) 298.15 -141939; 6000 N !
PAR L(ZRO2_CUB,MN+2,Y+3,ZR+4:VA;0) 298.15 -141939; 6000 N !
PAR L(ZRO2_CUB,MN+3,Y+3,ZR+4:O-2;0) 298.15 -141939; 6000 N !
PAR L(ZRO2_CUB,MN+3,Y+3,ZR+4:VA;0) 298.15 -141939; 6000 N !
PAR L(ZRO2_CUB,LA+3,SR+2:O-2;0) 298.15 +1.687E+05-7.81E+01*T; 6000 N !
PAR L(ZRO2_CUB,LA+3,SR+2:VA;0) 298.15 +1.687E+05-7.81E+01*T; 6000 N !
PAR L(ZRO2_CUB,LA+3,SR+2:O-2;1) 298.14 -2E+04; 6000 N !
PAR L(ZRO2_CUB,LA+3,SR+2:VA;1) 298.14 -2E+04; 6000 N !
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ X-La2O3 with SrO solubility only
$ PHASE LA2O3_CUB:I Z 2 2 3 !
$ CONST LA2O3_CUB:I : LA+3 SR+2 : O-2 VA : !
$ PAR G(LA2O3_CUB,LA+3:O-2;0) 298.15 +GLA2O3X; 6000 N !
$ PAR G(LA2O3_CUB,LA+3:VA;0) 298.15 +GLA2O3X-3*GHSEROO; 6000 N
!
$ PAR G(LA2O3_CUB,SR+2:O-2;0) 298.15
$ +SRX_ALPH+GHSEROO+15.87691*T; 6000 N !
$ PAR G(LA2O3_CUB,SR+2:VA;0) 298.15
$ +SRX_ALPH-2*GHSEROO+15.87691*T; 6000 N !
$ PAR L(LA2O3_CUB,LA+3,SR+2:O-2;0) 298.15 +1.687E+05-7.81E+01*T; 6000 N
!
$ PAR L(LA2O3_CUB,LA+3,SR+2:VA;0) 298.15 +1.687E+05-7.81E+01*T; 6000 N
!
$ PAR L(LA2O3_CUB,LA+3,SR+2:O-2;1) 298.15 -2E+04; 6000 N !
$ PAR L(LA2O3_CUB,LA+3,SR+2:VA;1) 298.15 -2E+04; 6000 N !
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$
$ SrO with La2O3 solubility
PHASE SRO:I Z 2 1 1 !
CONST SRO:I : LA+3 SR+2 VA : O-2 : !
PAR G(SRO,SR+2:O-2;0) 298.15 +GSROSOL; 6000 N !

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PAR G(SRO,LA+3:O-2;0) 298.15 +0.5*GLA2O3A+1.137E+05; 6000 N !
 PAR G(SRO,VA:O-2;0) 298.15 0; 6000 N !
 \$
 PHASE SRO2:I Z 2 1 2 !
 CONST SRO2:I : SR : O : !
 PAR G(SRO2,SR:O;0) 298.15 +GSRO2SOL; 6000 N !
 \$
 \$ Cr-Y-O, Ming Chen
 \$ CrYO3
 PHASE YCRO3:I Z 3 1 1 3 !
 CONST YCRO3:I : Y+3 : CR+3 : O-2 : !
 PAR G(YCRO3,Y+3:CR+3:O-2;0) 298.15 +GYCRO3; 6000 N !
 \$
 \$ LA-CR-O, Povoden
 \$ STOICHIOMETRIC LA2CRO6
 PHASE LA2CRO6:I Z 3 2 1 6 !
 CONST LA2CRO6:I : LA+3 : CR+6 : O-2 : !
 PAR G(LA2CRO6,LA+3:CR+6:O-2;0) 298.15 +GLA2CRO6; 6000 N !
 \$ STOICHIOMETRIC LA2CR3O12
 PHASE LA2CR3:I Z 3 2 3 12 !
 CONST LA2CR3:I : LA+3 : CR+6 : O-2 : !
 PAR G(LA2CR3,LA+3:CR+6:O-2;0) 298.15 +GLA2CR3; 6000 N !
 \$ SR-CR-O, Povoden
 \$ SRCR2O4
 PHASE SC2O4:I Z 3 1 2 4 !
 CONST SC2O4:I : SR+2 : CR+3 : O-2 : !
 PAR G(SC2O4,SR+2:CR+3:O-2;0) 298.15 +GSC2O4; 6000 N !
 \$ SR2CRO4
 PHASE S2CO4:I Z 3 2 1 4 !
 CONST S2CO4:I : SR+2 : CR+4 : O-2 : !
 PAR G(S2CO4,SR+2:CR+4:O-2;0) 298.15 +GS2CO4; 6000 N !
 \$ SR2.67CR2O8
 PHASE S3C2N:I Z 3 2.666667 2 8 !
 CONST S3C2N:I : SR : CR : O : !
 PAR G(S3C2N,SR:CR:O;0) 298.15 +GS3C2O8; 6000 N !
 \$ SRCRO4
 PHASE SCO4:I Z 3 1 1 4 !
 CONST SCO4:I : SR+2 : CR+6 : O-2 : !
 PAR G(SCO4,SR+2:CR+6:O-2;0) 298.15 +GSCO4; 6000 N !
 \$ La-Sr-Fe-O
 \$ Sr2FeO4 with La solubility
 PHASE SR2FEO4 Z 6 1 1 1 3 1 !
 CONST SR2FEO4 : SR+2 : LA+3 SR+2 : FE+4 : O-2 : O-2 : O-2 VA : !
 PAR G(SR2FEO4,SR+2:LA+3:FE+4:O-2:O-2:O-2;0) 298.15
 +GSRPRVOX+.5*GLA2O3A+.5*GHSEROO+38200-69.9*T; 6000 N !

PAR G(SR2FEO4,SR+2:LA+3:FE+4:O-2:O-2:VA;0) 298.15
 +GSRPRVOX+.5*GLA2O3A-.5*GHSEROO+38200-69.9*T; 6000 N !
 PAR G(SR2FEO4,SR+2:SR+2:FE+4:O-2:O-2:O-2;0) 298.15
 +GSM4_RP1+GHSEROO; 6000 N !
 PAR G(SR2FEO4,SR+2:SR+2:FE+4:O-2:O-2:VA;0) 298.15
 +GSM4_RP1; 6000 N !
 PAR L(SR2FEO4,SR+2:LA+3,SR+2:FE+4:O-2:O-2:O-2;1)
 298.15 -150000; 6000 N !
 \$
 \$ Sr3Fe2O7 with La solubility
 PHASE SR3FE2O7 Z 5 1 2 2 6 1 !
 CONST SR3FE2O7 : LA+3 SR+2 : LA+3 SR+2 : FE+3 FE+4 : O-2 VA : O-2 : !
 PAR G(SR3FE2O7,LA+3:LA+3:FE+3:O-2:O-2;0) 298.15
 +GLF3O-300000+115*T; 6000 N !
 PAR G(SR3FE2O7,LA+3:LA+3:FE+3:VA:O-2;0) 298.15
 +GSF4V+GLF3O-GSF4O-300000+115*T; 6000 N !
 PAR G(SR3FE2O7,SR+2:LA+3:FE+3:O-2:O-2;0) 298.15 +GLF3O; 6000 N !
 PAR G(SR3FE2O7,SR+2:LA+3:FE+3:VA:O-2;0) 298.15
 +GSF4V+GLF3O-GSF4O; 6000 N !
 PAR G(SR3FE2O7,LA+3:SR+2:FE+3:O-2:O-2;0) 298.15
 +GSR3FE2O+22.4772*T+GHSEROO-300000+115*T; 6000 N !
 PAR G(SR3FE2O7,LA+3:SR+2:FE+3:VA:O-2;0) 298.15
 +GSR3FE2O+22.4772*T-5*GHSEROO-300000+115*T; 6000 N !
 PAR G(SR3FE2O7,SR+2:SR+2:FE+3:O-2:O-2;0) 298.15
 +GSR3FE2O+22.4772*T+GHSEROO; 6000 N !
 PAR G(SR3FE2O7,SR+2:SR+2:FE+3:VA:O-2;0) 298.15
 +GSR3FE2O+22.4772*T-5*GHSEROO; 6000 N !
 PAR G(SR3FE2O7,LA+3:LA+3:FE+4:O-2:O-2;0) 298.15
 +GLF3O+GSF4O-GSF3O-300000+115*T; 6000 N !
 PAR G(SR3FE2O7,LA+3:LA+3:FE+4:VA:O-2;0) 298.15
 +GSF4V+GLF3O+GSF4O-GSF3O-GSF4O-300000+115*T; 6000 N !
 PAR G(SR3FE2O7,SR+2:LA+3:FE+4:O-2:O-2;0) 298.15
 +GLF3O+GSF4O-GSF3O; 6000 N !
 PAR G(SR3FE2O7,SR+2:LA+3:FE+4:VA:O-2;0) 298.15
 +GSF4V+GLF3O+GSF4O-GSF3O-GSF4O; 6000 N !
 PAR G(SR3FE2O7,LA+3:SR+2:FE+4:O-2:O-2;0) 298.15
 +GSF4O-300000+115*T; 6000 N !
 PAR G(SR3FE2O7,LA+3:SR+2:FE+4:VA:O-2;0) 298.15
 +GSF4O-6*GHSEROO-300000+115*T; 6000 N !
 PAR G(SR3FE2O7,SR+2:SR+2:FE+4:O-2:O-2;0) 298.15 +GSF4O; 6000 N !
 PAR G(SR3FE2O7,SR+2:SR+2:FE+4:VA:O-2;0) 298.15
 +GSF4O-6*GHSEROO; 6000 N !
 PAR L(SR3FE2O7,SR+2:LA+3,SR+2:FE+3:O-2:O-2;0) 298.15 -150000; 6000 N !
 PAR L(SR3FE2O7,SR+2:LA+3,SR+2:FE+3:O-2:O-2;1) 298.15 +200000; 6000 N !
 \$

\$ La₂SrFe₂O₇
 PHASE L2SF2O7 Z 5 1 2 2 6 1 !
 CONST L2SF2O7 : SR+2 : LA+3 SR+2 : FE+3 FE+4 : O-2 : O-2 : !
 PAR G(L2SF2O7,SR+2:LA+3:FE+3:O-2:O-2;0) 298.15 +GLF3O-20*T; 6000 N !
 PAR G(L2SF2O7,SR+2:LA+3:FE+4:O-2:O-2;0) 298.15
 +GLF3O-20*T+GSF4O-GSF3O; 6000 N !
 PAR G(L2SF2O7,SR+2:SR+2:FE+3:O-2:O-2;0) 298.15
 +GSR3FE2O+22.4772*T+GHSEROO; 6000 N !
 PAR G(L2SF2O7,SR+2:SR+2:FE+4:O-2:O-2;0) 298.15 +GSF4O; 6000 N !
 \$
 \$ Sr₄Fe₃O₁₀ with La solubility
 PHASE SR4FE3O10 Z 5 1 3 3 9 1 !
 CONST SR4FE3O10 : LA+3 SR+2 : LA+3 SR+2 : FE+3 FE+4 : O-2 VA : O-2 : !
 PAR G(SR4FE3O10,LA+3:LA+3:FE+3:O-2:O-2;0) 298.15
 +GSL3+GLS3-GSS3; 6000 N !
 PAR G(SR4FE3O10,LA+3:LA+3:FE+3:VA:O-2;0) 298.15
 +9*GLS3OV-9*GLS3+234.93*T+GLL3; 6000 N !
 PAR G(SR4FE3O10,SR+2:LA+3:FE+3:O-2:O-2;0) 298.15 +GSL3; 6000 N !
 PAR G(SR4FE3O10,SR+2:LA+3:FE+3:VA:O-2;0) 298.15
 +GSS3OV-6*GSS3+202.295*T+GSL3; 6000 N !
 PAR G(SR4FE3O10,LA+3:SR+2:FE+3:O-2:O-2;0) 298.15 +GLS3; 6000 N !
 PAR G(SR4FE3O10,LA+3:SR+2:FE+3:VA:O-2;0) 298.15
 +9*GLS3OV-8*GLS3+234.93*T; 6000 N !
 PAR G(SR4FE3O10,SR+2:SR+2:FE+3:O-2:O-2;0) 298.15
 +.5*GLS3+.5*GSS4; 6000 N !
 PAR G(SR4FE3O10,SR+2:SR+2:FE+3:VA:O-2;0) 298.15
 +GSS3OV-5*GSS3+202.295*T; 6000 N !
 PAR G(SR4FE3O10,LA+3:LA+3:FE+4:O-2:O-2;0) 298.15
 +GSL4+GLS4-GSS4; 6000 N !
 PAR G(SR4FE3O10,LA+3:LA+3:FE+4:VA:O-2;0) 298.15
 +9*GLS3OV-9*GLS3+234.93*T+GLL4; 6000 N !
 PAR G(SR4FE3O10,SR+2:LA+3:FE+4:O-2:O-2;0) 298.15
 +GSS4+GSL3-GSS3; 6000 N !
 PAR G(SR4FE3O10,SR+2:LA+3:FE+4:VA:O-2;0) 298.15
 +GSS3OV-6*GSS3+202.295*T+GSL4; 6000 N !
 PAR G(SR4FE3O10,LA+3:SR+2:FE+4:O-2:O-2;0) 298.15
 +.5*GLS3+.5*GSS4; 6000 N !
 PAR G(SR4FE3O10,LA+3:SR+2:FE+4:VA:O-2;0) 298.15
 +9*GLS3OV-9*GLS3+234.93*T+GLS4; 6000 N !
 PAR G(SR4FE3O10,SR+2:SR+2:FE+4:O-2:O-2;0) 298.15 +GSS4; 6000 N !
 PAR G(SR4FE3O10,SR+2:SR+2:FE+4:VA:O-2;0) 298.15
 +GSS3OV-6*GSS3+202.295*T+GSS4; 6000 N !
 \$
 \$ Sr₄Fe₆O₁₃ with La solubility
 PHASE SR4FE6O13 Z 5 4 4 2 12 2 !

CONST SR4FE6O13 : LA+3 SR+2 : FE+3 : FE+2 FE+3 FE+4 : O-2 : O-2 VA : !
 PAR G(SR4FE6O13,LA+3:FE+3:FE+2:O-2:O-2;0) 298.15
 +GLAYREF-900000; 6000 N !
 PAR G(SR4FE6O13,SR+2:FE+3:FE+2:O-2:O-2;0) 298.15 +GLAYREF; 6000 N !
 PAR G(SR4FE6O13,LA+3:FE+3:FE+3:O-2:O-2;0) 298.15
 +GLAYS-.5*GLAYRED+.5*GLAYREF+11.5264*T-900000; 6000 N !
 PAR G(SR4FE6O13,SR+2:FE+3:FE+3:O-2:O-2;0) 298.15
 +GLAYS-.5*GLAYRED+.5*GLAYREF+11.5264*T; 6000 N !
 PAR G(SR4FE6O13,LA+3:FE+3:FE+4:O-2:O-2;0) 298.15
 +GLAYOX-900000; 6000 N !
 PAR G(SR4FE6O13,SR+2:FE+3:FE+4:O-2:O-2;0) 298.15 +GLAYOX; 6000 N !
 PAR G(SR4FE6O13,LA+3:FE+3:FE+2:O-2:VA;0) 298.15
 +GLAYRED-900000; 6000 N !
 PAR G(SR4FE6O13,SR+2:FE+3:FE+2:O-2:VA;0) 298.15 +GLAYRED; 6000 N !
 PAR G(SR4FE6O13,LA+3:FE+3:FE+3:O-2:VA;0) 298.15
 +.5*GLAYRED-.5*GLAYREF+GLAYS+11.5264*T-900000; 6000 N !
 PAR G(SR4FE6O13,SR+2:FE+3:FE+3:O-2:VA;0) 298.15
 +.5*GLAYRED-.5*GLAYREF+GLAYS+11.5264*T; 6000 N !
 PAR G(SR4FE6O13,LA+3:FE+3:FE+4:O-2:VA;0) 298.15
 +GLAYOX+GLAYRED-GLAYREF-900000; 6000 N !
 PAR G(SR4FE6O13,SR+2:FE+3:FE+4:O-2:VA;0) 298.15
 +GLAYOX+GLAYRED-GLAYREF; 6000 N !
 PAR L(SR4FE6O13,SR+2:FE+3:FE+3,FE+4:O-2:O-2;0) 298.15 9982; 6000 N !
 PAR L(SR4FE6O13,SR+2:FE+3:FE+3:O-2:O-2,VA;0) 298.15 15000; 6000 N !
 PAR L(SR4FE6O13,SR+2:FE+3:FE+4:O-2:O-2,VA;0) 298.15 15000; 6000 N !
 PAR L(SR4FE6O13,SR+2:FE+3:FE+3,FE+4:O-2:VA;0) 298.15 9982; 6000 N !

\$

\$ (LaSr)1Fe12O19

PHASE SRFE12O19 Z 4 1 1 11 19 !

CONST SRFE12O19 : LA+3 SR+2 : FE+2 FE+3 : FE+3 : O-2 : !
 PAR G(SRFE12O19,LA+3:FE+2:FE+3:O-2;0) 298.15 +GHEXLA; 6000 N !
 PAR G(SRFE12O19,SR+2:FE+2:FE+3:O-2;0) 298.15 +G2HEX; 6000 N !
 PAR G(SRFE12O19,LA+3:FE+3:FE+3:O-2;0) 298.15
 +GHEX+GHEXLA-G2HEX; 6000 N !
 PAR G(SRFE12O19,SR+2:FE+3:FE+3:O-2;0) 298.15 +GHEX; 6000 N !
 PAR G(SRFE12O19,LA+3,SR+2:FE+2:FE+3:O-2;0) 298.15 53400; 6000 N !
 PAR G(SRFE12O19,LA+3,SR+2:FE+3:FE+3:O-2;0) 298.15 53400; 6000 N !

\$

\$ LaMnO3 perovskite

\$ with vacancies on both cation sub-lattices and antisite defects

\$

PHASE PEROV:I Z 3 1 1 3 !

CONST PEROV:I : MN+3 LA+3% VA : MN+2 MN+3% MN+4 VA : O-2% VA : !
 PAR G(PEROV,LA+3:MN+3:O-2) 298.15 +GL3OR; 6000 N !
 PAR G(PEROV,LA+3:MN+3:VA) 298.15 +GL3OR-3*GHSEROO; 6000 N !

PAR G(PEROV,LA+3:MN+4:O-2) 298.15
 +0.66667*GL4O+0.5*GV4O-0.166667*GVVV-0.5*GHSEROO+5.76318*T; 6000
 N !
 PAR G(PEROV,LA+3:MN+4:VA) 298.15
 +0.66667*GL4O+0.5*GV4O-0.166667*GVVV-3.5*GHSEROO+5.76318*T; 6000
 N !
 PAR G(PEROV,LA+3:MN+2:O-2) 298.15
 +GL2O+0.5*GHSEROO+11.2386*T; 6000 N !
 PAR G(PEROV,LA+3:MN+2:VA) 298.15
 +GL2O-2.5*GHSEROO+11.2386*T; 6000 N !
 PAR G(PEROV,LA+3:VA:O-2) 298.15
 +2*GL4O-1.5*GV4O+0.5*GVVV+1.5*GHSEROO+1.41263*T; 6000 N !
 PAR G(PEROV,LA+3:VA:VA) 298.15
 +2*GL4O+0.5*GVVV-1.5*GV4O-1.5*GHSEROO+1.41263*T; 6000 N !
 \$
 PAR G(PEROV,MN+3:MN+3:O-2) 298.15 +GL3OR+ANTI; 6000 N !
 PAR G(PEROV,MN+3:MN+3:VA) 298.15 +GL3OR-3*GHSEROO+ANTI; 6000
 N !
 PAR G(PEROV,MN+3:MN+4:O-2) 298.15
 +0.66667*GL4O+0.5*GV4O-0.166667*GVVV-0.5*GHSEROO+5.76318*T+ANTI;
 6000 N !
 PAR G(PEROV,MN+3:MN+4:VA) 298.15
 +0.66667*GL4O+0.5*GV4O-0.166667*GVVV-3.5*GHSEROO+5.76318*T+ANTI;
 6000 N !
 PAR G(PEROV,MN+3:MN+2:O-2) 298.15
 +GL2O+0.5*GHSEROO+11.2386*T+ANTI; 6000 N !
 PAR G(PEROV,MN+3:MN+2:VA) 298.15
 +GL2O-2.5*GHSEROO+11.2386*T+ANTI; 6000 N !
 PAR G(PEROV,MN+3:VA:O-2) 298.15
 +2*GL4O-1.5*GV4O+0.5*GVVV+1.5*GHSEROO+1.41263*T+ANTI; 6000 N
 !
 PAR G(PEROV,MN+3:VA:VA) 298.15
 +2*GL4O+0.5*GVVV-1.5*GV4O-1.5*GHSEROO+1.41263*T+ANTI; 6000 N
 !
 \$
 PAR G(PEROV,VA:MN+3:O-2) 298.15
 +GL3OR+1.5*GV4O+0.5*GVVV-2*GL4O+1.5*GHSEROO-1.41263*T; 6000 N
 !
 PAR G(PEROV,VA:MN+3:VA) 298.15
 +GL3OR+1.5*GV4O+0.5*GVVV-2*GL4O-1.5*GHSEROO-1.41263*T; 6000 N
 !
 PAR G(PEROV,VA:MN+4:O-2) 298.15
 +2*GV4O+0.33333*GVVV-1.33333*GL4O+GHSEROO+4.35056*T; 6000 N !
 PAR G(PEROV,VA:MN+4:VA) 298.15
 +2*GV4O+0.3333*GVVV-1.333*GL4O-2*GHSEROO+4.35056*T; 6000 N !

PAR G(PEROV,VA:MN+2:O-2) 298.15
 +GL2O+1.5*GV4O+0.5*GVVV-2*GL4O+2*GHSEROO+9.82596*T; 6000 N
 !
 PAR G(PEROV,VA:MN+2:VA) 298.15
 +GL2O+1.5*GV4O+0.5*GVVV-2*GL4O-GHSEROO+9.82596*T; 6000 N !
 PAR G(PEROV,VA:VA:O-2) 298.15 +GVVV+3*GHSEROO; 6000 N !
 PAR G(PEROV,VA:VA:VA) 298.15 +GVVV; 6000 N !
 \$
 PHASE L2MNO4:I Z 3 2 1 4 !
 CONST L2MNO4:I : LA+3 : MN+2 : O-2 : !
 PAR G(L2MNO4,LA+3:MN+2:O-2) 298.15 +GL2MNO4; 6000 N !
 \$
 PHASE LAYO3:I Z 3 1 1 3 !
 CONST LAYO3:I : LA+3 : Y+3 : O-2 : !
 PAR G(LAYO3,LA+3:Y+3:O-2) 298.15 +GLAYO3; 6000 N !
 \$ La2Zr2O7
 PHASE L2Z2O7:I Z 4 2 2 6 1 !
 CONST L2Z2O7:I : LA+3% ZR+4 VA : ZR+4% LA+3 : O-2% VA : O-2 : !
 PAR G(L2Z2O7,LA+3:ZR+4:O-2:O-2) 298.15 +GL2Z2O7; 6000 N !
 PAR G(L2Z2O7,LA+3:LA+3:O-2:O-2) 298.15
 +2*GL2Z2O7-4*GFFZRO2+GHSEROO+RV71+RV72*T
 -1.333*RV75-1.333*RV76*T-12.468*T; 6000 N !
 PAR G(L2Z2O7,LA+3:ZR+4:VA:O-2) 298.15
 -11*GL2Z2O7+24*GFFZRO2+12*GLA2O3X-6*GHSEROO-6*RV71-6*RV72*T
 +6*RV73+6*RV74*T+7.998*RV75+7.998*RV76*T+209.832*T; 6000 N !
 PAR G(L2Z2O7,LA+3:LA+3:VA:O-2) 298.15
 -10*GL2Z2O7+20*GFFZRO2+12*GLA2O3X-5*GHSEROO-5*RV71-5*RV72*T
 +6*RV73+6*RV74*T+6.665*RV75+6.665*RV76*T+197.364*T; 6000 N !
 PAR G(L2Z2O7,ZR+4:ZR+4:O-2:O-2) 298.15
 +4*GFFZRO2-GHSEROO+1.333*RV75+1.333*RV76*T+12.468*T; 6000 N !
 PAR G(L2Z2O7,ZR+4:LA+3:O-2:O-2) 298.15 +GL2Z2O7+RV71+RV72*T; 6000 N
 !
 PAR G(L2Z2O7,ZR+4:ZR+4:VA:O-2) 298.15
 -12*GL2Z2O7+28*GFFZRO2+12*GLA2O3X-7*GHSEROO-6*RV71-6*RV72*T
 +6*RV73+6*RV74*T+9.331*RV75+9.331*RV76*T+222.3*T; 6000 N !
 PAR G(L2Z2O7,ZR+4:LA+3:VA:O-2) 298.15
 -11*GL2Z2O7+24*GFFZRO2+12*GLA2O3X-6*GHSEROO-5*RV71-5*RV72*T
 +6*RV73+6*RV74*T+7.998*RV75+7.998*RV76*T+209.832*T; 6000 N !
 PAR G(L2Z2O7,VA:ZR+4:O-2:O-2) 298.15 +2*GFFZRO2+3*GHSEROO; 6000 N
 !
 PAR G(L2Z2O7,VA:LA+3:O-2:O-2) 298.15
 +GL2Z2O7-2*GFFZRO2+4*GHSEROO+RV71+RV72*T
 -1.333*RV75-1.333*RV76*T-12.468*T; 6000 N !
 PAR G(L2Z2O7,VA:ZR+4:VA:O-2) 298.15
 -12*GL2Z2O7+26*GFFZRO2+12*GLA2O3X-3*GHSEROO-6*RV71-6*RV72*T

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+6*RV73+6*RV74*T+7.998*RV75+7.998*RV76*T+209.832*T;          6000 N !
PAR G(L2Z2O7,VA:LA+3:VA:O-2) 298.15
-11*GL2Z2O7+22*GFFZRO2+12*GLA2O3X-2*GHSEROO-5*RV71-5*RV72*T
+6*RV73+6*RV74*T+6.665*RV75+6.665*RV76*T+197.364*T;          6000 N !
$ C2
PHASE C2:I Z 3 2 1 5 !
CONST C2:I : LA+3 : ZR+4 : O-2 : !
PAR G(C2,LA+3:ZR+4:O-2) 298.15 +GC2;          6000 N !
$
PHASE YMNO3H:I Z 3 1 1 3 !
CONST YMNO3H:I : Y+3 : MN+3 : O-2 : !
PAR G(YMNO3H,Y+3:MN+3:O-2) 298.15 +GYMNO3H;          6000 N !
$
PHASE YMN2O5:I Z 4 1 1 1 5 !
CONST YMN2O5:I : Y+3 : MN+3 : MN+4 : O-2 : !
PAR G(YMN2O5,Y+3:MN+3:MN+4:O-2) 298.15 +GYMN2O5;          6000 N !
$
PHASE ZR3Y4O12:I Z 3 3 4 12 !
CONST ZR3Y4O12:I : ZR+4 : Y+3 : O-2 : !
PAR G(ZR3Y4O12,ZR+4:Y+3:O-2) 298.15 +7*GZYO;          6000 N !
$
$ phases from the La-Sr-O system
$
PHASE BETA:I Z 2 2 3 !
CONST BETA:I : LA+3 SR+2 : O-2 VA : !
PAR G(BETA,LA+3:O-2;0) 298.15 +LA_BETA;          6000 N !
PAR G(BETA,LA+3:VA;0) 298.15 +LA_BETA-3*GHSEROO;          6000 N !
PAR G(BETA,SR+2:O-2;0) 298.15
+SR_ALPHA+4.161E+05+GHSEROO+15.87691*T;          6000 N !
PAR G(BETA,SR+2:VA;0) 298.15
+SR_ALPHA+4.161E+05-2*GHSEROO+15.87691*T;          6000 N !
PAR L(BETA,LA+3,SR+2:O-2;0) 298.15 -1.21E+05-2.378E+02*T;          6000 N !
PAR L(BETA,LA+3,SR+2:VA;0) 298.15 -1.21E+05-2.378E+02*T;          6000 N !
$
PHASE LA4SR3O9:I Z 3 4 3 9 !
CONST LA4SR3O9:I : LA+3 : SR+2 : O-2 : !
PAR G(LA4SR3O9,LA+3:SR+2:O-2;0) 298.15
+2*GLA2O3A+3*GSROSOL+2.298E+05-1.3675E+02*T;          6000 N !
$
$ phases from the Sr-Mn-O system
$
PHASE SRMN3O6:I Z 5 1 2 3 1 3 !
CONST SRMN3O6:I : SR+2 : MN+3 : O-2 : MN+3 MN+4 : O-2 VA : !
PAR G(SRMN3O6,SR+2:MN+3:O-2:MN+4:O-2;0) 298.15 GSM4OZ;          6000 N !

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PAR G(SRMN3O6,SR+2:MN+3:O-2:MN+4:VA;0) 298.15 GSM4OZ-3*GHSEROO;
 6000 N !
 PAR G(SRMN3O6,SR+2:MN+3:O-2:MN+3:O-2;0) 298.15
 +GSM3OZ+0.5*GHSEROO+11.23859*T; 6000 N !
 PAR G(SRMN3O6,SR+2:MN+3:O-2:MN+3:VA;0) 298.15
 +GSM3OZ-2.5*GHSEROO+11.23859*T; 6000 N !
 \$
 PHASE SR7MN4O15:I Z 3 7 4 15 !
 CONST SR7MN4O15:I : SR+2 : MN+4 : O-2 : !
 PAR G(SR7MN4O15,SR+2:MN+4:O-2;0) 298.15 +GS7M4; 6000 N !
 \$
 PHASE SR4MN3O10:I Z 3 4 3 10 !
 CONST SR4MN3O10:I : SR+2 : MN+4 : O-2 : !
 PAR G(SR4MN3O10,SR+2:MN+4:O-2;0) 298.15 +GSM4_RP3; 6000 N !
 \$
 PHASE SRMNO3_HEX:I Z 3 1 1 3 !
 CONST SRMNO3_HEX:I : SR+2 : MN+3 MN+4 : O-2 VA : !
 PAR G(SRMNO3_HEX,SR+2:MN+4:O-2;0) 298.15 GSM4_HEX; 6000 N !
 PAR G(SRMNO3_HEX,SR+2:MN+4:VA;0) 298.15 GSM4_HEX-3*GHSEROO;
 6000 N !
 PAR G(SRMNO3_HEX,SR+2:MN+3:O-2;0) 298.15
 +GSM3_HEX+0.5*GHSEROO+11.23859*T; 6000 N !
 PAR G(SRMNO3_HEX,SR+2:MN+3:VA;0) 298.15
 +GSM3_HEX-2.5*GHSEROO+11.23859*T; 6000 N !
 \$ RP2, Grundy modified it in LSM modeling
 PHASE RP2:I Z 4 1 2 2 7 !
 CONST RP2:I : SR+2: SR+2: MN+3 MN+4: O-2: !
 PAR G(RP2,SR+2:SR+2:MN+3:O-2;0) 298.15
 +3*GSROSOL+GMN2O3+GHSEROO; 6000 N !
 PAR G(RP2,SR+2:SR+2:MN+4:O-2;0) 298.15 +GS4O_RP2; 6000 N !
 \$
 \$ perovskite without antisite defects
 PHASE PERV:I ZA 3 1 1 3 !
 CONST PERV:I : LA+3 SR+2 VA : CR+3 CR+4 FE+2 FE+3 FE+4 MN+2 MN+3
 MN+4 VA : O-2 VA : !
 \$
 PAR TC(PERV,LA+3:FE+2:O-2;0) 298.15 742.88; 6000 N !
 PAR TC(PERV,LA+3:FE+3:O-2;0) 298.15 742.88; 6000 N !
 PAR TC(PERV,LA+3:FE+4:O-2;0) 298.15 742.88; 6000 N !
 PAR TC(PERV,LA+3:FE+2:VA;0) 298.15 742.88; 6000 N !
 PAR TC(PERV,LA+3:FE+3:VA;0) 298.15 742.88; 6000 N !
 PAR TC(PERV,LA+3:FE+4:VA;0) 298.15 742.88; 6000 N !
 \$
 PAR BMAGN(PERV,LA+3:FE+2:O-2;0) 298.15 .779; 6000 N !
 PAR BMAGN(PERV,LA+3:FE+3:O-2;0) 298.15 .779; 6000 N !

PAR BMAGN(PERV,LA+3:FE+4:O-2;0) 298.15 .779; 6000 N !
 PAR BMAGN(PERV,LA+3:FE+2:VA;0) 298.15 .779; 6000 N !
 PAR BMAGN(PERV,LA+3:FE+3:VA;0) 298.15 .779; 6000 N !
 PAR BMAGN(PERV,LA+3:FE+4:VA;0) 298.15 .779; 6000 N !
 \$
 PAR G(PERV,LA+3:CR+3:O-2;0) 298.15 +GLACRO3; 6000 N !
 PAR G(PERV,LA+3:CR+3:VA;0) 298.15 +GLACRO3-3*GHSEROO; 6000 N !
 !
 PAR G(PERV,LA+3:CR+4:O-2;0) 298.15
 +GS4O+GLACRO3-GN-0.1666667*GS4O+0.16666667*GS4V; 6000 N !
 PAR G(PERV,LA+3:CR+4:VA;0) 298.15
 +GS4O-GN-0.1666667*GS4O+0.16666667*GS4V+GLACRO3-3*GHSEROO;
 6000 N !
 PAR G(PERV,LA+3:FE+2:O-2;0) 298.15
 +GRPRVRED+.5*GHSEROO+11.2386*T; 6000 N !
 PAR G(PERV,LA+3:FE+2:VA;0) 298.15
 +GRPRVRED-2.5*GHSEROO+11.2386*T; 6000 N !
 PAR G(PERV,LA+3:FE+3:O-2;0) 298.15 +GRPRV; 6000 N !
 PAR G(PERV,LA+3:FE+3:VA;0) 298.15
 +GRPRV-3*GHSEROO; 6000 N !
 PAR G(PERV,LA+3:FE+4:O-2;0) 298.15 +.66667*GLAFE4O
 +.5*GVFE4O-.166667*GVVV-.5*GHSEROO+5.76318*T; 6000 N !
 PAR G(PERV,LA+3:FE+4:VA;0) 298.15 +.66667*GLAFE4O
 +.5*GVFE4O-.166667*GVVV-3.5*GHSEROO+5.76318*T; 6000 N !
 PAR G(PERV,LA+3:MN+3:O-2;0) 298.15 GL3OR; 6000 N !
 PAR G(PERV,LA+3:MN+3:VA;0) 298.15 GL3OR-3*GHSEROO; 6000 N !
 PAR G(PERV,LA+3:MN+4:O-2;0) 298.15
 0.66667*GL4O+0.5*GV4O-0.166667*GVVV-0.5*GHSEROO+5.76318*T; 6000
 N !
 PAR G(PERV,LA+3:MN+4:VA;0) 298.15
 0.66667*GL4O+0.5*GV4O-0.166667*GVVV-3.5*GHSEROO+5.76318*T; 6000
 N !
 PAR G(PERV,LA+3:MN+2:O-2;0) 298.15 GL2O+0.5*GHSEROO+11.2386*T; 6000
 N !
 PAR G(PERV,LA+3:MN+2:VA;0) 298.15 GL2O-2.5*GHSEROO+11.2386*T; 6000
 N !
 PAR G(PERV,LA+3:VA:O-2;0) 298.15
 2*GL4O-1.5*GV4O+0.5*GVVV+1.5*GHSEROO+1.41263*T; 6000 N !
 PAR G(PERV,LA+3:VA:VA;0) 298.15
 2*GL4O+0.5*GVVV-1.5*GV4O-1.5*GHSEROO+1.41263*T; 6000 N !
 PAR G(PERV,SR+2:CR+3:O-2;0) 298.15
 +GN+0.1666667*GS4O-0.16666667*GS4V; 6000 N !
 PAR G(PERV,SR+2:CR+3:VA;0) 298.15
 +GN-0.8333333*GS4O+0.8333333*GS4V; 6000 N !
 PAR G(PERV,SR+2:CR+4:O-2;0) 298.15 +GS4O; 6000 N !

PAR G(PERV,SR+2:CR+4:VA;0) 298.15 +GS4V; 6000 N !
 PAR G(PERV,SR+2:FE+2:O-2;0) 298.15
 +GSRPRVR+15.8769*T+GHSEROO; 6000 N !
 PAR G(PERV,SR+2:FE+2:VA;0) 298.15
 +GSRPRVR+15.8769*T-2*GHSEROO; 6000 N !
 PAR G(PERV,SR+2:FE+3:O-2;0) 298.15
 +GSRPRV+5*GHSEROO+11.2386*T; 6000 N !
 PAR G(PERV,SR+2:FE+3:VA;0) 298.15
 +GSRPRV-2.5*GHSEROO+11.2386*T; 6000 N !
 PAR G(PERV,SR+2:FE+4:O-2;0) 298.15 +GSRPRVOX; 6000 N !
 PAR G(PERV,SR+2:FE+4:VA;0) 298.15
 +GSRPRVOX-3*GHSEROO; 6000 N !
 \$PAR G(PERV,MN+3:MN+3:O-2;0) 298.15 GL3OR+ANTI; 6000 N !
 \$PAR G(PERV,MN+3:MN+3:VA;0) 298.15 GL3OR-3*GHSEROO+ANTI; 6000
 N !
 \$PAR G(PERV,MN+3:MN+4:O-2;0) 298.15
 \$ 0.66667*GL4O+0.5*GV4O-0.166667*GVVV-0.5*GHSEROO+5.76318*T+ANTI;
 6000 N !
 \$PAR G(PERV,MN+3:MN+4:VA;0) 298.15
 \$ 0.66667*GL4O+0.5*GV4O-0.166667*GVVV-3.5*GHSEROO+5.76318*T+ANTI;
 6000 N !
 \$PAR G(PERV,MN+3:MN+2:O-2;0) 298.15
 \$ GL2O+0.5*GHSEROO+11.2386*T+ANTI; 6000 N !
 \$PAR G(PERV,MN+3:MN+2:VA;0) 298.15
 \$ GL2O-2.5*GHSEROO+11.2386*T+ANTI; 6000 N !
 \$PAR G(PERV,MN+3:VA:O-2;0) 298.15
 \$ 2*GL4O-1.5*GV4O+0.5*GVVV+1.5*GHSEROO+1.41263*T+ANTI; 6000 N
 !
 \$PAR G(PERV,MN+3:VA:VA;0) 298.15
 \$ 2*GL4O+0.5*GVVV-1.5*GV4O-1.5*GHSEROO+1.41263*T+ANTI; 6000 N
 !
 PAR G(PERV,SR+2:MN+2:O-2;0) 298.15
 GMS3O+GL2O-GL3OR+GHSEROO+22.47717*T; 6000 N !
 PAR G(PERV,SR+2:MN+2:VA;0) 298.15
 GMS3O+GL2O-GL3OR-2*GHSEROO+22.47717*T; 6000 N !
 PAR G(PERV,SR+2:MN+3:O-2;0) 298.15
 GMS3O+0.5*GHSEROO+11.23859*T; 6000 N !
 PAR G(PERV,SR+2:MN+3:VA;0) 298.15 GMS3O-2.5*GHSEROO+11.23859*T;
 6000 N !
 PAR G(PERV,SR+2:MN+4:O-2;0) 298.15 GMS4O; 6000 N !
 PAR G(PERV,SR+2:MN+4:VA;0) 298.15 GMS4O-3*GHSEROO; 6000 N !
 PAR G(PERV,SR+2:VA:O-2;0) 298.15
 GMS3O-GL3OR+2*GL4O-1.5*GV4O+0.5*GVVV+2*GHSEROO+12.62121*T;
 6000 N !
 PAR G(PERV,SR+2:VA:VA;0) 298.15

GMS3O+2*GL4O-1.5*GV4O+0.5*GVVV-GL3OR-GHSEROO+12.62121*T;
 6000 N !
 PAR G(PERV,VA:CR+3:O-2;0) 298.15
 +GLACRO3+1.5*GVCR4O+0.5*GVVV-2*GLACR4O+1.5*GHSEROO-1.41263*T;
 6000 N !
 PAR G(PERV,VA:CR+3:VA;0) 298.15
 +GLACRO3+1.5*GVCR4O+0.5*GVVV-2*GLACR4O-1.5*GHSEROO-1.41263*T;
 6000 N !
 PAR G(PERV,VA:CR+4:O-2;0) 298.15
 +2*GVCR4O+0.33333*GVVV-1.33333*GLACR4O+GHSEROO+4.35056*T;
 6000 N !
 PAR G(PERV,VA:CR+4:VA;0) 298.15
 +2*GVCR4O+0.3333*GVVV-1.333*GLACR4O-2*GHSEROO+4.35057*T; 6000
 N !
 PAR G(PERV,VA:FE+2:O-2;0) 298.15 +GRPRVRED+1.5*GVFE4O
 +.5*GVVV-2*GLAFE4O+2*GHSEROO+9.82596*T; 6000 N !
 PAR G(PERV,VA:FE+2:VA;0) 298.15 +GRPRVRED+1.5*GVFE4O
 +.5*GVVV-2*GLAFE4O-GHSEROO+9.82596*T; 6000 N !
 PAR G(PERV,VA:FE+3:O-2;0) 298.15 +GRPRV+1.5*GVFE4O+.5*GVVV
 -2*GLAFE4O+1.5*GHSEROO-1.41263*T; 6000 N !
 PAR G(PERV,VA:FE+3:VA;0) 298.15 +GRPRV+1.5*GVFE4O+.5*GVVV
 -2*GLAFE4O-1.5*GHSEROO-1.41263*T; 6000 N !
 PAR G(PERV,VA:FE+4:O-2;0) 298.15 +2*GVFE4O+.33333*GVVV
 -1.33333*GLAFE4O+GHSEROO+4.35056*T; 6000 N !
 PAR G(PERV,VA:FE+4:VA;0) 298.15 +2*GVFE4O+.33333*GVVV
 -1.33333*GLAFE4O-2*GHSEROO+4.35056*T; 6000 N !
 PAR G(PERV,VA:MN+2:O-2;0) 298.15
 GL2O+1.5*GV4O+0.5*GVVV-2*GL4O+2*GHSEROO+9.82596*T; 6000 N
 !
 PAR G(PERV,VA:MN+2:VA;0) 298.15
 GL2O+1.5*GV4O+0.5*GVVV-2*GL4O-GHSEROO+9.82596*T; 6000 N !
 PAR G(PERV,VA:MN+3:O-2;0) 298.15
 GL3OR+1.5*GV4O+0.5*GVVV-2*GL4O+1.5*GHSEROO-1.41263*T; 6000 N
 !
 PAR G(PERV,VA:MN+3:VA;0) 298.15
 GL3OR+1.5*GV4O+0.5*GVVV-2*GL4O-1.5*GHSEROO-1.41263*T; 6000 N
 !
 PAR G(PERV,VA:MN+4:O-2;0) 298.15
 2*GV4O+0.33333*GVVV-1.33333*GL4O+GHSEROO+4.35056*T; 6000 N !
 PAR G(PERV,VA:MN+4:VA;0) 298.15
 2*GV4O+0.3333*GVVV-1.333*GL4O-2*GHSEROO+4.35057*T; 6000 N !
 PAR G(PERV,VA:VA:O-2;0) 298.15 GVVV+3*GHSEROO; 6000 N !
 PAR G(PERV,VA:VA:VA;0) 298.15 GVVV; 6000 N !
 \$ Interaction Parameters for Mn+2 / Mn+3
 PAR L(PERV,LA+3:MN+3,MN+2:O-2;0) 298.15 0; 6000 N !

PAR L(PERV,LA+3:MN+3,MN+2:O-2;1) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+3,MN+2:O-2;0) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+3,MN+2:O-2;1) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+3,MN+2:O-2;0) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+3,MN+2:O-2;1) 298.15 0; 6000 N !
 PAR L(PERV,LA+3:MN+3,MN+2:VA;0) 298.15 0; 6000 N !
 PAR L(PERV,LA+3:MN+3,MN+2:VA;1) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+3,MN+2:VA;0) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+3,MN+2:VA;1) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+3,MN+2:VA;0) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+3,MN+2:VA;1) 298.15 0; 6000 N !

\$ Interaction Parameters for O-2/Va

PAR L(PERV,LA+3:MN+4:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,LA+3:MN+4:O-2,VA;1) 298.15 0; 6000 N !
 PAR L(PERV,LA+3:MN+3:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,LA+3:MN+3:O-2,VA;1) 298.15 0; 6000 N !
 PAR L(PERV,LA+3:MN+2:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,LA+3:MN+2:O-2,VA;1) 298.15 0; 6000 N !
 PAR L(PERV,LA+3:VA:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,LA+3:VA:O-2,VA;1) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+4:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+4:O-2,VA;1) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+3:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+3:O-2,VA;1) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+2:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+2:O-2,VA;1) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:VA:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:VA:O-2,VA;1) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+4:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+4:O-2,VA;1) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+3:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+3:O-2,VA;1) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+2:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+2:O-2,VA;1) 298.15 0; 6000 N !
 PAR L(PERV,VA:VA:O-2,VA;0) 298.15 0; 6000 N !
 PAR L(PERV,VA:VA:O-2,VA;1) 298.15 0; 6000 N !

\$ Interaction Parameters for Mn+2/Mn+4

PAR L(PERV,LA+3:MN+4,MN+2:O-2;0) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+4,MN+2:O-2;0) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+4,MN+2:O-2;0) 298.15 0; 6000 N !
 PAR L(PERV,LA+3:MN+4,MN+2:VA;0) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+4,MN+2:VA;0) 298.15 0; 6000 N !
 PAR L(PERV,SR+2:MN+4,MN+2:VA;0) 298.15 0; 6000 N !
 PAR L(PERV,LA+3:MN+4,MN+2:O-2;1) 298.15 0; 6000 N !
 PAR L(PERV,VA:MN+4,MN+2:O-2;1) 298.15 0; 6000 N !

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PAR L(PERV,SR+2:MN+4,MN+2:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3:MN+4,MN+2:VA;1) 298.15 0; 6000 N !
PAR L(PERV,VA:MN+4,MN+2:VA;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2:MN+4,MN+2:VA;1) 298.15 0; 6000 N !
$ Interaction Parameters for Mn+3 / Mn+4
PAR L(PERV,LA+3:MN+4,MN+3:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3:MN+4,MN+3:O-2;1) 298.15 +185; 6000 N !
PAR L(PERV,VA:MN+4,MN+3:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,VA:MN+4,MN+3:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2:MN+4,MN+3:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2:MN+4,MN+3:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,VA:MN+4,MN+3:VA;0) 298.15 0; 6000 N !
PAR L(PERV,VA:MN+4,MN+3:VA;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3:MN+4,MN+3:VA;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3:MN+4,MN+3:VA;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2:MN+4,MN+3:VA;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2:MN+4,MN+3:VA;1) 298.15 0; 6000 N !
$ Interaction parameters for Va/La+3
PAR L(PERV,LA+3,VA:MN+4:O-2;0) 298.15 +20; 6000 N !
PAR L(PERV,LA+3,VA:MN+4:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:MN+3:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:MN+3:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:MN+2:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:MN+2:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:VA:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:VA:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:MN+4:VA;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:MN+4:VA;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:MN+3:VA;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:MN+3:VA;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:MN+2:VA;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:MN+2:VA;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:VA:VA;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,VA:VA:VA;1) 298.15 0; 6000 N !
$ Interaction parameters for La+3/Sr+2
PAR L(PERV,LA+3,SR+2:CR+3:O-2;0) 298.15 -39.5*T; 6000 N !
PAR L(PERV,LA+3,SR+2:CR+4:O-2;0) 298.15 -39.5*T; 6000 N !
PAR L(PERV,LA+3,SR+2:MN+4:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,SR+2:MN+4:O-2;1) 298.15 -117000; 6000 N !
PAR L(PERV,LA+3,SR+2:MN+3:O-2;0) 298.15 -1.5*T; 6000 N !
PAR L(PERV,LA+3,SR+2:MN+3:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3,SR+2:MN+2:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,SR+2:MN+2:O-2;1) 298.15 -136600; 6000 N !
PAR L(PERV,LA+3,SR+2:VA:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,SR+2:VA:O-2;1) 298.15 0; 6000 N !

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PAR L(PERV,LA+3,SR+2:MN+4:VA;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,SR+2:MN+4:VA;1) 298.15 -117000; 6000 N !
PAR L(PERV,LA+3,SR+2:MN+3:VA;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,SR+2:MN+3:VA;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3,SR+2:MN+2:VA;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,SR+2:MN+2:VA;1) 298.15 -136600; 6000 N !
PAR L(PERV,LA+3,SR+2:VA:VA;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3,SR+2:VA:VA;1) 298.15 0; 6000 N !
$ Interaction parameters for Va/Sr+2
PAR L(PERV,SR+2,VA:MN+4:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:MN+4:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:MN+3:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:MN+3:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:MN+2:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:MN+2:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:VA:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:VA:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:MN+4:VA;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:MN+4:VA;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:MN+3:VA;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:MN+3:VA;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:MN+2:VA;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:MN+2:VA;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:VA:VA;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2,VA:VA:VA;1) 298.15 0; 6000 N !
$ Interaction parameters for Va/Mn+4
PAR L(PERV,LA+3:MN+4,VA:O-2;0) 298.15 -2; 6000 N !
PAR L(PERV,LA+3:MN+4,VA:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,VA:MN+4,VA:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,VA:MN+4,VA:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2:MN+4,VA:O-2;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2:MN+4,VA:O-2;1) 298.15 0; 6000 N !
PAR L(PERV,VA:MN+4,VA:VA;0) 298.15 0; 6000 N !
PAR L(PERV,VA:MN+4,VA:VA;1) 298.15 0; 6000 N !
PAR L(PERV,LA+3:MN+4,VA:VA;0) 298.15 0; 6000 N !
PAR L(PERV,LA+3:MN+4,VA:VA;1) 298.15 0; 6000 N !
PAR L(PERV,SR+2:MN+4,VA:VA;0) 298.15 0; 6000 N !
PAR L(PERV,SR+2:MN+4,VA:VA;1) 298.15 0; 6000 N !
$
PAR L(PERV,LA+3:CR+3,VA:O-2;0) 298.15 250000; 6000 N !
PAR L(PERV,LA+3:CR+4,VA:O-2;0) 298.15 250000; 6000 N !
$
$PAR L(PERV,LA+3:CR+3,MN+3:O-2;0) 298.15 8500; 6000 N !
PAR L(PERV,LA+3:CR+3,MN+3:O-2;0) 298.15 3766; 6000 N !
PAR L(PERV,LA+3:CR+3,MN+3:O-2;1) 298.15 -1297; 6000 N !

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PAR L(LS3MN2O7,SR+2:LA+3:MN+3,MN+4:O-2;1) 298.15 0; 6000 N !
 \$ Sr-Zr-O
 \$ SrZrO3 from Factsage
 PHASE SZOF:I Z 3 1 1 3 !
 CONST SZOF:I : SR+2 : ZR+4 : O-2 : !
 PAR G(SZOF,SR+2:ZR+4:O-2;0) 298.15 +GSZOF; 6000 N !
 \$ SrZrO3 from Yokokawa
 PHASE SZOY:I Z 3 1 1 3 !
 CONST SZOY:I : SR+2 : ZR+4 : O-2 : !
 PAR G(SZOY,SR+2:ZR+4:O-2;0) 298.15 +GSZOY; 6000 N !
 \$ Stoichiometric phases, used as references
 \$ A-La2O3
 PHASE RLA2O3:I Z 2 2 3 !
 CONST RLA2O3:I : LA+3 : O-2 : !
 PAR G(RLA2O3,LA+3:O-2) 298.15 +GLA2O3A; 6000 N !
 \$ Mn1O1
 PHASE RMN1O1:I Z 2 1 1 !
 CONST RMN1O1:I : MN+2 : O-2 : !
 PAR G(RMN1O1,MN+2:O-2) 298.15 +GMN1O1; 6000 N !
 \$ Mn2O3
 PHASE RMN2O3:I Z 2 2 3 !
 CONST RMN2O3:I : MN+3 : O-2 : !
 PAR G(RMN2O3,MN+3:O-2) 298.15 +GMN2O3; 6000 N !
 \$ c-Y2O3
 PHASE RY2O3:I Z 2 2 3 !
 CONST RY2O3:I : Y+3 : O-2 : !
 PAR G(RY2O3,Y+3:O-2) 298.15 +2*GCCYO15; 6000 N !
 \$ m-ZrO2
 PHASE RMZRO2:I Z 2 1 2 !
 CONST RMZRO2:I : ZR+4 : O-2 : !
 PAR G(RMZRO2,ZR+4:O-2) 298.15 +GMMZRO2; 6000 N !
 \$ t-ZrO2
 PHASE RTZRO2:I Z 2 1 2 !
 CONST RTZRO2:I : ZR+4 : O-2 : !
 PAR G(RTZRO2,ZR+4:O-2) 298.15 +GTTZRO2; 6000 N !
 \$ c-ZrO2 (fluorite)
 PHASE RFZRO2:I Z 2 1 2 !
 CONST RFZRO2:I : ZR+4 : O-2 : !
 PAR G(RFZRO2,ZR+4:O-2) 298.15 +GFFZRO2; 6000 N !
 \$ LaMnO3
 PHASE RLMNO3:I Z 3 1 1 3 !
 CONST RLMNO3:I : LA+3 : MN+3 : O-2 : !
 PAR G(RLMNO3,LA+3:MN+3:O-2) 298.15 +GL3O; 6000 N !
 \$ La2Zr2O7
 PHASE RL2Z2O7:I Z 3 2 2 7 !

```

CONST RL2Z2O7:I : LA+3 : ZR+4 : O-2 : !
PAR  G(RL2Z2O7,LA+3:ZR+4:O-2)  298.15  +GL2Z2O7;          6000 N !
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ La2Zr2O7 from Ming Chen with different enthalpy of formation
$
PHASE RLZOA:I Z 3 2 2 7 !
CONST RLZOA:I : LA+3 : ZR+4 : O-2 : !
PAR  G(RLZOA,LA+3:ZR+4:O-2)  298.15  +GLZOA;          6000 N !
$
PHASE RLZOB:I Z 3 2 2 7 !
CONST RLZOB:I : LA+3 : ZR+4 : O-2 : !
PAR  G(RLZOB,LA+3:ZR+4:O-2)  298.15  +GLZOB;          6000 N !
$
PHASE RLZOC:I Z 3 2 2 7 !
CONST RLZOC:I : LA+3 : ZR+4 : O-2 : !
PAR  G(RLZOC,LA+3:ZR+4:O-2)  298.15  +GLZOC;          6000 N !
$
PHASE RLZOD:I Z 3 2 2 7 !
CONST RLZOD:I : LA+3 : ZR+4 : O-2 : !
PAR  G(RLZOD,LA+3:ZR+4:O-2)  298.15  +GLZOD;          6000 N !
$
PHASE RLZOE:I Z 3 2 2 7 !
CONST RLZOE:I : LA+3 : ZR+4 : O-2 : !
PAR  G(RLZOE,LA+3:ZR+4:O-2)  298.15  +GLZOE;          6000 N !
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ La2Zr2O7 from Wang Chong 20060814
PHASE RLZOW:I Z 3 2 2 7 !
CONST RLZOW:I : LA+3 : ZR+4 : O-2 : !
PAR  G(RLZOW,LA+3:ZR+4:O-2)  298.15  +GLZOW;          6000 N !
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ La2Zr2O7 from Yokokawa
PHASE RLZOY:I Z 3 2 2 7 !
CONST RLZOY:I : LA+3 : ZR+4 : O-2 : !
PAR  G(RLZOY,LA+3:ZR+4:O-2)  298.15  +GLZOY;          6000 N !
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$
PHASE O2_GAS Z 1 1.0 !
CONSTITUENT O2_GAS :O2 :!
PAR  G(O2_GAS,O2)  298.15  +2*GHSEROO+RTLNP;          6000 N !
$
PHASE H2GAS Z 1 1 !
CONST H2GAS : H2 : !
PAR  G(H2GAS,H2;0)  298.15  +H2GAS+RTLNP;          6000 N !
$

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PHASE CRO3GAS Z 1 1 !
 CONST CRO3GAS : CRO3 : !
 PAR G(CRO3GAS,CRO3;0) 298.15 +F7726T+RTLNP; 6000 N !
 \$
 PHASE H2OGAS Z 1 1 !
 CONST H2OGAS : H2O : !
 PAR G(H2OGAS,H2O;0) 298.15 +F10963T+RTLNP; 20000 N !
 \$
 PHASE GAS:G Z 1 1 !
 CONST GAS:G : CR CR2 CRO CRO2 CRO3 CRH CRHO CRHO2 CRHO3
 CRH2O2 CRH2O3 CRH2O4 CRH3O3 CRH3O4 CRH4O4 CRH4O5 CRH5O5
 CRH6O6
 H HO HO2 H2 H2O H2O2 LA LAO LA2O1 LA2O2
 MN MNO MNO2 O O2 O3 Y Y2O YO Y2O2 YO2 ZR ZR2 ZRO ZRO2 SR SR2 SRO
 AR: !
 PAR G(GAS,CR;0) 298.15 +F7491T+RTLNP; 6000 N !
 PAR G(GAS,CR2;0) 298.15 +F7763T+RTLNP; 6000 N !
 PAR G(GAS,CRH;0) 298.15 +F7586T+RTLNP; 6000 N !
 PAR G(GAS,CRO;0) 298.15 +F7705T+RTLNP; 6000 N !
 PAR G(GAS,CRO2;0) 298.15 +F7713T+RTLNP; 6000 N !
 PAR G(GAS,CRO3;0) 298.15 +F7726T+RTLNP; 6000 N !
 PAR G(GAS,CRHO;0) 298.15 +F7592T+RTLNP; 6000 N !
 PAR G(GAS,CRHO2;0) 298.15 +F7597T+RTLNP; 6000 N !
 PAR G(GAS,CRHO3;0) 298.15 +F7602T+RTLNP; 6000 N !
 PAR G(GAS,CRH2O2;0) 298.15 +F7607T+RTLNP; 6000 N !
 PAR G(GAS,CRH2O3;0) 298.15 +F7612T+RTLNP; 6000 N !
 PAR G(GAS,CRH2O4;0) 298.15 +F7617T+RTLNP; 6000 N !
 PAR G(GAS,CRH3O3;0) 298.15 +F7622T+RTLNP; 6000 N !
 PAR G(GAS,CRH3O4;0) 298.15 +F7627T+RTLNP; 6000 N !
 PAR G(GAS,CRH4O4;0) 298.15 +F7632T+RTLNP; 6000 N !
 PAR G(GAS,CRH4O5;0) 298.15 +F7637T+RTLNP; 6000 N !
 PAR G(GAS,CRO;0) 298.15 +GCR1O1G+RTLNP; 6000 N !
 PAR G(GAS,CRO2;0) 298.15 +GCR1O2G+RTLNP; 6000 N !
 PAR G(GAS,CRO3;0) 298.15 +GCR1O3G+RTLNP; 6000 N !
 PAR G(GAS,CRHO;0) 298.15 +GCRH1O1G+RTLNP; 6000 N !
 PAR G(GAS,CRHO2;0) 298.15 +GCRH1O2G+RTLNP; 6000 N !
 PAR G(GAS,CRHO3;0) 298.15 +GCRH1O3G+RTLNP; 6000 N !
 PAR G(GAS,CRH2O2;0) 298.15 +GCRH2O2G+RTLNP; 6000 N !
 PAR G(GAS,CRH2O3;0) 298.15 +GCRH2O3G+RTLNP; 6000 N !
 PAR G(GAS,CRH2O4;0) 298.15 +GCRH2O4G+RTLNP; 6000 N !
 PAR G(GAS,CRH3O3;0) 298.15 +GCRH3O3G+RTLNP; 6000 N !
 PAR G(GAS,CRH3O4;0) 298.15 +GCRH3O4G+RTLNP; 6000 N !
 PAR G(GAS,CRH4O4;0) 298.15 +GCRH4O4G+RTLNP; 6000 N !
 PAR G(GAS,CRH4O5;0) 298.15 +GCRH4O5G+RTLNP; 6000 N !
 PAR G(GAS,CRH5O5;0) 298.15 +GCRH5O5G+RTLNP; 6000 N !

PAR G(GAS,CRH6O6;0)	298.15 +GCRH6O6G+RTLNP;	6000 N !
PAR G(GAS,H;0)	298.15 +HGAS+RTLNP;	6000 N !
PAR G(GAS,HO;0)	298.15 +F10666T+RTLNP;	20000 N !
PAR G(GAS,HO2;0)	298.15 +F10729T+RTLNP;	6000 N !
PAR G(GAS,H2;0)	298.15 +H2GAS+RTLNP;	6000 N !
PAR G(GAS,H2O;0)	298.15 +F10963T+RTLNP;	20000 N !
PAR G(GAS,H2O2;0)	298.15 +F10983T+RTLNP;	1500 N !
PAR G(GAS,LA)	298.15 +F12026T+RTLNP;	6000 N !
PAR G(GAS,LAO)	298.15 +F12049T+RTLNP;	6000 N !
PAR G(GAS,LA2O1)	298.15 +F12085T+RTLNP;	6000 N !
PAR G(GAS,LA2O2)	298.15 +F12089T+RTLNP;	6000 N !
PAR G(GAS,MN)	298.15 +F12439T+RTLNP;	6000 N !
PAR G(GAS,MNO)	298.15 +F12454T+RTLNP;	6000 N !
PAR G(GAS,MNO2)	298.15 +F12461T+RTLNP;	6000 N !
PAR G(GAS,O)	298.15 +F7397T+RTLNP;	6000 N !
PAR G(GAS,O2)	298.15 +2*GHSEROO+RTLNP;	6000 N !
PAR G(GAS,O3)	298.15 +F7683T+RTLNP;	6000 N !
PAR G(GAS,Y)	298.15 +F14722T+RTLNP;	6000 N !
PAR G(GAS,Y2O)	298.15 +F12945T+RTLNP;	6000 N !
PAR G(GAS,YO)	298.15 +F12929T+RTLNP;	6000 N !
PAR G(GAS,Y2O2)	298.15 +F13270T+RTLNP;	6000 N !
PAR G(GAS,YO2)	298.15 +F13266T+RTLNP;	6000 N !
PAR G(GAS,ZR)	298.15 +GZRGAS+RTLNP;	6000 N !
PAR G(GAS,ZR2)	298.15 +F15702T+RTLNP;	6000 N !
PAR G(GAS,ZRO)	298.15 +F12964T+RTLNP;	6000 N !
PAR G(GAS,ZRO2)	298.15 +F13281T+RTLNP;	6000 N !
PAR G(GAS,SR;0)	298.15 +F14450T+RTLNP;	6000 N !
PAR G(GAS,SR2;0)	298.15 +F14465T+RTLNP;	6000 N !
PAR G(GAS,SRO;0)	298.15 +F12810T+RTLNP;	6000 N !
PAR G(GAS,AR;0)	298.15 +F877T+RTLNP;	6000 N !

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FUNCTION GHSERCR 298.15 -8856.94+157.48*T-26.908*T*LN(T)
+0.00189435*T**2-1.47721E-06*T**3+139250*T**(-1);
2180.00 Y -34869.344+344.18*T-50.0*T*LN(T)-2.88526E+32*T**(-9);
6000.00 N !
FUNCTION GCRFCC 298.15 +GHSERCR+7284+0.163*T;
1519.00 N !
FUNCTION GCRHCP 298.15 -4418.94+157.48*T-26.908*T*LN(T)
+0.00189435*T**2-1.47721E-06*T**3+139250*T**(-1);
2180.00 Y -30431.344+344.18*T-50*T*LN(T)-2.88526E+32*T**(-9);
6000.00 N !

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FUNCTION GCRCUB 298.15 +7042.06+158.1076*T-26.908*T*LN(T)
    +0.00189435*T**2-1.47721E-06*T**3+139250*T**(-1);
2180.00 Y -18970.344+344.8076*T-50*T*LN(T)-2.88526E+32*T**(-9);
6000.00 N !
FUNCTION GCRBCCA12 298.15 +2230.06+160.1996*T-26.908*T*LN(T)
    +0.00189435*T**2-1.47721E-06*T**3+139250*T**(-1);
2180.00 Y -23782.344+346.8996*T-50*T*LN(T)-2.88526E+32*T**(-9);
6000.00 N !
FUNCTION GCR_L 298.15 +15483.015+146.059775*T-26.908*T*LN(T)
    +.00189435*T**2-1.47721E-06*T**3+139250*T**(-1)+2.37615E-21*T**7;
2180.00 Y -16459.984+335.616317*T-50*T*LN(T);
6000.00 N !
$
FUNCTION GFELIQ 298.15 +13265.87+117.5757*T-23.5143*T*LN(T)
    -.00439752*T**2-5.89269E-08*T**3+77358.5*T**(-1)-3.6751551E-21*T**7;
1811.00 Y -10838.83+291.302*T-46*T*LN(T);
3000.00 N !
$
FUNCTION GHSERLA
298.15 -7968.403+120.284604*T-26.34*T*LN(T)-.001295165*T**2;
550 Y -3381.413+59.06113*T-17.1659411*T*LN(T)-.008371705*T**2
    +6.8932E-07*T**3-399448*T**(-1);
2000 Y -15608.882+181.390071*T-34.3088*T*LN(T);
4000 N !
FUNCTION GLABCC
298.15 -3952.161+88.072353*T-21.7919*T*LN(T)-0.004045175*T**2
    -5.25865E-07*T**3;
800 Y +321682.673-3565.08252*T+513.440708*T*LN(T)-0.387295093*T**2
    +4.9547989E-05*T**3-36581228*T**(-1);
1134 Y -16377.894+218.492988*T-39.5388*T*LN(T);
1193 Y -136609.91+1123.34397*T-163.413074*T*LN(T)+0.053968535*T**2
    -4.056395E-06*T**3+21167204*T**(-1);
2000 Y -8205.988+174.836315*T-34.3088*T*LN(T);
4000 N !
FUNCTION GLAFCC
298.15 -6109.797+89.878761*T-21.7919*T*LN(T)
    -0.004045175*T**2-5.25865E-07*T**3;
1134 Y -124598.976+955.878375*T-139.346741*T*LN(T)+0.042032405*T**2
    -3.066199E-06*T**3+20994153*T**(-1);
2000 Y -12599.386+178.54399*T-34.3088*T*LN(T);
4000 N !
FUNCTION GLALIQ
298.15 +5332.653+18.23012*T-11.0188191*T*LN(T)-0.020171603*T**2
    +2.93775E-06*T**3-133541*T**(-1);
1134 Y -3942.004+171.018431*T-34.3088*T*LN(T);

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4000 N !
$
FUNCTION GHSERMN 298.15 -8115.28+130.059*T-23.4582*T*LN(T)
-0.00734768*T**2+69827*T**(-1);
1519.00 Y -28733.41+312.2648*T-48*T*LN(T)+1.656847E+30*T**(-9);
2000.00 N !
FUNCTION GMNCUB 298.15 -5800.4+135.995*T-24.8785*T*LN(T)
-0.00583359*T**2+70269*T**(-1);
1519.00 Y +442.65-0.9715*T+GHSERMN+2.310723E+30*T**(-9);
2000.00 N !
FUNCTION GMNFCC 298.15 -3439.3+131.884*T-24.5177*T*LN(T)
-0.006*T**2+69600*T**(-1);
1519.00 Y +2663.31-2.5984*T+GHSERMN+2.205113E+30*T**(-9);
2000.00 N !
FUNCTION GMNBCC 298.15 -3235.3+127.85*T-23.7*T*LN(T)
-0.00744271*T**2+60000*T**(-1);
1519.00 Y +5544.58-4.5605*T+GHSERMN-3.91695E+29*T**(-9);
2000.00 N !
FUNCTION GMNHCP 298.15 -4439.3+133.007*T-24.5177*T*LN(T)
-0.006*T**2+69600*T**(-1);
1519.00 Y +1663.31-1.4754*T+GHSERMN+2.205113E+30*T**(-9);
2000.00 N !
FUNCTION GMNLIQ 298.15 +17859.91-12.6208*T+GHSERMN-4.41929E-
21*T**7;
1519.00 Y -9993.9+299.036*T-48*T*LN(T);
2000.00 N !
$
FUNCTION GHSEROO 298.15 -3480.87-25.503038*T-11.136*T*LN(T)
-0.005098888*T**2+6.61846E-07*T**3-38365*T**(-1);
1000.00 Y -6568.763+12.65988*T-16.8138*T*LN(T)
-5.95798E-04*T**2+6.781E-09*T**3+262905*T**(-1);
3300.00 Y -13986.728+31.259625*T-18.9536*T*LN(T)
-4.25243E-04*T**2+1.0721E-08*T**3+4383200*T**(-1);
6000.00 N !
$
FUNCTION GHSESR
298.15 -7532.367+107.183879*T-23.905*T*LN(T)
-4.61225E-3*T**2-1.67477E-07*T**3-2055*T**(-1);
820 Y -13380.102+153.196104*T-30.0905432*T*LN(T)
-3.251266E-3*T**2+1.84189E-07*T**3+850134*T**(-1);
3000 N !
FUNCTION GSRBCC
298.15 -6779.234+116.583654*T-25.6708365*T*LN(T)
-3.126762E-3*T**2+2.2965E-7*T**3+27649*T**(-1);
820 Y -6970.594+122.067301*T-26.57*T*LN(T)

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-1.9493E-3*T**2-1.7895E-8*T**3+16495*T**(-1);
1050 Y +8168.357+0.423037*T-9.7788593*T*LN(T)
-9.539908E-3*T**2+5.20221E-7*T**3-2414794*T**(-1);
3000 N !
FUNCTION GSRLIQ
298.15 +2194.997-10.118994*T-5.0668978*T*LN(T)
-3.1840595E-2*T**2+4.981237E-06*T**3-265559*T**(-1);
1050 Y -10855.29+213.406219*T-39.463*T*LN(T);
3000 N !
$
FUNCTION GHSERY 100.00 -8011.09379+128.572856*T-25.6656992*T*LN(T)
-0.00175716414*T**2-4.17561786E-07*T**3+26911.509*T**(-1);
1000.00 Y -7179.74574+114.497104*T-23.4941827*T*LN(T)
-0.0038211802*T**2-8.2534534E-08*T**3;
1795.15 Y -67480.7761+382.124727*T-56.9527111*T*LN(T)
+0.00231774379*T**2-7.22513088E-08*T**3+18077162.6*T**(-1);
3700.00 N !
FUNCTION GYYBCC 100.00 -833.658863+123.667346*T-25.5832578*T*LN(T)
-0.00237175965*T**2+9.10372497E-09*T**3+27340.0687*T**(-1);
1000.00 Y -1297.79829+134.528352*T-27.3038477*T*LN(T)
-5.41757644E-04*T**2-3.05012175E-07*T**3;
1795.15 Y +15389.4975+0.981325399*T-8.88296647*T*LN(T)
-0.00904576576*T**2+4.02944768E-07*T**3-2542575.96*T**(-1);
3700.00 N !
FUNCTION GYYLIQ 100.00 +2098.50738+119.41873*T-24.6467508*T*LN(T)
-0.00347023463*T**2-8.12981167E-07*T**3+23713.7332*T**(-1);
1000.00 Y +7386.44846+19.4520171*T-9.0681627*T*LN(T)
-0.0189533369*T**2+1.7595327E-06*T**3;
1795.15 Y -12976.5957+257.400783*T-43.0952*T*LN(T);
3700.00 N !
$
FUNCTION GHSERZR 130.00 -7827.595+125.64905*T-24.1618*T*LN(T)
-0.00437791*T**2+34971*T**(-1);
2128.00 Y -26085.921+262.724183*T-42.144*T*LN(T)-1.342896E+31*T**(-9);
6000.00 N !
FUNCTION GZRBCC 130.00 -525.539+124.9457*T-25.607406*T*LN(T)
-3.40084E-04*T**2-9.729E-09*T**3+25233*T**(-1)-7.6143E-11*T**4;
2128.00 Y -4620.034+1.55998*T+GHSERZR+1.4103476E+32*T**(-9);
6000.00 N !
FUNCTION GZRLIQ 130.00 +18147.69-9.080812*T+GHSERZR+1.6275E-22*T**7;
2128.00 Y -8281.26+253.812609*T-42.144*T*LN(T);
6000.00 N !
$
FUNCTION GMN12Y 298.15 +12*GHSERMN+GHSERY-142346.62+58.97073*T;
6000.00 N !

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FUNCTION GS4V 298.15 +GSROSOL+0.5*GCR2O3-2.5*GHSEROO; 6000 N
!
$ FUNCTION FOR NEUTRAL SRCRO3 endmember
FUNCTION GS4O 298.15 +GSROSOL+0.5*GCR2O3
+0.5*GHSEROO+30800-40*T; 6000 N !
$ FUNCTION FOR NEUTRAL ENDMEMBER SR(CR+3,VA)O3
FUNCTION GN 298.15 +GSROSOL+0.5*GCR2O3
+11.2386*T+140300-67*T; 6000 N !
FUNCTION GVCR4O 298.15 +0.5*GCR2O3+0.5*GHSEROO-279000-265*T; 6000
N !
FUNCTION GLACR4O 298.15 +0.33333*GLA2O3A+0.5*GCR2O3
+0.5*GHSEROO-200000; 6000 N !
$ FUNCTION GREFRP 298.15 +2*GSROSOL+0.5*GCR2O3+0.5*GHSEROO;
6000 N !
$
$ La-Fe-O
FUNCTION GRPRVRED 298.15 +.5*GLA2O3A+GFEO+101050-45.91*T; 6000
N !
FUNCTION GRPRV 298.15
+.5*GLA2O3A+.5*GFE2O3-65563+17.74*T-1.95*T*LN(T); 6000 N !
FUNCTION GLAFE4O 298.15
+.5*GLA2O3A+.375*GFE2O3+.375*GHSEROO-33198+26.46*T; 6000 N !
FUNCTION GVFE4O 298.15
+.333333*GLA2O3A+.5*GFE2O3+.5*GHSEROO+5000; 6000 N !
$ Sr-Fe-O
FUNCTION GSRPRV 298.15 +GSROSOL+.5*GFE2O3-44701-8.73*T; 6000 N
!
FUNCTION GSRPRVR 298.15 +GSRPRV-.5*GHSEROO+116977; 6000 N !
FUNCTION GSRPRVOX 298.15 +GSRPRV-60015+188.3*T-25.69*T*LN(T); 6000
N !
$
$ Sr2FeO4
FUNCTION GSM4_RP1 298.15 +GSRPRVOX+GSROSOL-19000; 6000 N !
$
$ Sr3Fe2O7
FUNCTION GPRV 298.15
+.5*GLA2O3A+.5*GFE2O3-65921+18.02*T-1.95*T*LN(T); 6000 N !
FUNCTION GLF3O 298.15 +GSROSOL+2*GPRV+63000-62*T; 6000 N !
FUNCTION GSR3FE2O 298.15 +2*GSRPRV+GSROSOL; 6000 N !
FUNCTION GSF4O 298.15 +2*GSRPRVOX+GSROSOL-5000-4.71*T; 6000 N
!
FUNCTION GSF3O 298.15 +GSR3FE2O+22.4772*T+GHSEROO; 6000 N !
FUNCTION GSF4V 298.15 +GSM4_RP1-6*GHSEROO; 6000 N !
$
$ Sr4Fe3O10

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FUNCTION GLS3    298.15 +.5*GLA2O3A+3*GSRPRVOX-31000-88*T;    6000 N
!
FUNCTION GLS3OV  298.15 +.5*GLA2O3A+3*GSRPRV-9943.8-26.448*T; 6000
N!
FUNCTION GSL3    298.15 +GSROSOL+3*GPRV+200000;                6000 N!
FUNCTION GSS4    298.15 +3*GSRPRVOX+GSROSOL-54000;             6000 N!
FUNCTION GSS3OV  298.15 +GSROSOL+3*GSRPRV;                     6000 N!
FUNCTION GSS3    298.15 +.5*GLS3+.5*GSS4;                      6000 N!
FUNCTION GLL3    298.15 +GSL3+GLS3-GSS3;                       6000 N!
FUNCTION GLS4    298.15 +.5*GLS3+.5*GSS4;                      6000 N!
FUNCTION GSL4    298.15 +GSS4+GSL3-GSS3;                       6000 N!
FUNCTION GLL4    298.15 +GSL4+GLS4-GSS4;                       6000 N!
$
$ Sr4Fe6O13
FUNCTION GLAYREF 298.15 +4*GSRPRV+2*GFEO+2*GHSEROO;            6000
N!
FUNCTION GLAYS   298.15 +4*GSRPRV+GFE2O3-6486-6.29*T;          6000 N!
FUNCTION GLAYRED 298.15 +4*GSRPRV+2*GFEO+43043-7.12*T;          6000 N
!
FUNCTION GLAYOX  298.15 +4*GSRPRV+GFE2O3+GHSEROO-14132+13.26*T;
6000 N!
$
$ LaSrFe12O19
FUNCTION GHEXLA  298.15
+.5*GLA2O3A+5.5*GFE2O3+GFEO-139562+22.63*T;                    6000 N!
FUNCTION G2HEX   298.15 +GSROSOL+GFEO+5.5*GFE2O3+.5*GHSEROO;
6000 N!
FUNCTION GHEX    298.15
+GSROSOL+6*GFE2O3-173012+888.77*T-115.2*T*LN(T)+5092797.5*T**(-1);
6000 N!
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$$$
$ Quaternary oxides, optimized (except perovskite functions), Povoden
$ FUNCTION GLCR3O_RP1 298.15 +GLACRO3+GSROSOL+7000-25*T;      6000
N!
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$$$
$
FUNCTION RTLNP   298.15 +8.31451*T*LN(1E-05*P);                 6000 N!
$
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$$$
$ Cr gas, from SGTE

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\$ Cr (g)

FUNCTION F7491T

298.15 +390765.331-31.5192158*T-21.36083*T*LN(T)+7.253215E-04*T**2
-1.588679E-07*T**3+10285.15*T**(-1);

1100 Y +393886.928-44.1074654*T-19.96003*T*LN(T)+.001513089*T**2
-4.23648333E-07*T**3-722515*T**(-1);

6000 N !

\$ Cr2 (g)

FUNCTION F7763T

298.15 +598511.403+41.5353212*T-40.56798*T*LN(T)+.004961847*T**2
-1.61216717E-06*T**3+154422.85*T**(-1);

800 Y +613345.232-104.207991*T-19.7643*T*LN(T)-.007085085*T**2
-4.69883E-07*T**3-1738066.5*T**(-1);

1400 Y +642608.843-369.28626*T+17.64743*T*LN(T)-.02767321*T**2
+1.605906E-06*T**3-5831655*T**(-1);

2300 Y +553119.895+159.188555*T-52.07969*T*LN(T)-.004229401*T**2
+1.5939925E-07*T**3+14793625*T**(-1);

3900 Y +347492.34+623.137623*T-105.0428*T*LN(T)+3.9699545E-04*T**2
+1.51783483E-07*T**3+1.4843765E+08*T**(-1);

5800 Y -484185.055+2598.25559*T-334.7145*T*LN(T)+.028597625*T**2
-4.97520167E-07*T**3+7.135805E+08*T**(-1);

6000 N !

\$ CR1O1 Gas (SGTE 1998; from T.C.R.A.S Class: 5)

FUNCTION F7705T

298.15 +176483.869-31.9513659*T-30.2897*T*LN(T)-.00607059*T**2
+9.229905E-07*T**3+35263.135*T**(-1);

900 Y +170853.62+32.1684007*T-39.74749*T*LN(T)+.00119977*T**2
-1.52515733E-07*T**3+682877*T**(-1);

4000 Y +307209.502-414.237405*T+14.48744*T*LN(T)-.008463125*T**2
+1.722975E-07*T**3-64209900*T**(-1);

8400 Y -403765.708+805.224944*T-121.5329*T*LN(T)+.003139382*T**2
-1.36845867E-08*T**3+6.35563E+08*T**(-1);

10000 N !

\$ CR1O2 Gas (SGTE 1998; from T.C.R.A.S Class: 6)

FUNCTION F7713T

298.15 -121743.409-9.3513573*T-36.29523*T*LN(T)-.01993456*T**2
+3.5091E-06*T**3+193490.75*T**(-1);

700 Y -130807.622+121.470522*T-56.35306*T*LN(T)-3.3428045E-04*T**2
-6.06589333E-08*T**3+956146*T**(-1);

3400 Y -110536.941+26.3566562*T-44.22742*T*LN(T)-.003455125*T**2
+8.58097667E-08*T**3-5175510*T**(-1);

6000 N !

\$ CR1O3 Gas (SGTE 1998; from T.C.R.A.S Class: 6)

FUNCTION F7726T

298.15 -342387.72+103.718924*T-52.84504*T*LN(T)-.02759153*T**2

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+4.86524667E-06*T**3+358400*T**(-1);
700 Y -356869.109+299.291672*T-82.53502*T*LN(T)-7.979305E-05*T**2
-1.88415667E-09*T**3-2.06280000E+01*T**(-1);
4000 Y -362423.325+334.459538*T-87.10177*T*LN(T)+.001170557*T**2
-5.86174E-08*T**3+1764429*T**(-1);
6000 N !
$ CRH1 Gas (SGTE 1998; from T.C.R.A.S Class: 4)
FUNCTION F7586T
298.15 +432449.026-56.386334*T-22.37019*T*LN(T)
-.00994042*T**2+1.18913267E-06*T**3-77266.05*T**(-1);
1000 Y +421602.4+51.9865812*T-37.99681*T*LN(T)
+3.349852E-04*T**2-1.13133917E-07*T**3+1368173*T**(-1);
3500 Y +587860.713-424.36214*T+18.6022*T*LN(T)
-.007723995*T**2+7.99444833E-08*T**3-86705500*T**(-1);
5500 Y +1270342.46-2142.60191*T+219.9391*T*LN(T)
-.034109635*T**2+7.277845E-07*T**3-5.20451E+08*T**(-1);
6000 N !
$ CR1H1O1 Gas (SGTE 1998; from T.C.R.A.S Class: 6)
FUNCTION F7592T
298.15 +44188.8085+88.4113829*T-49.69831*T*LN(T)
-.002868985*T**2+8.75370667E-08*T**3+230208.6*T**(-1);
1800 Y +35801.2843+153.963612*T-58.65289*T*LN(T)
+8.80731E-04*T**2-1.82505333E-07*T**3+1371935.5*T**(-1);
4200 Y +279544.047-653.609464*T+39.55769*T*LN(T)
-.01667735*T**2+4.04557167E-07*T**3-1.120161E+08*T**(-1);
6000 N !
$ CR1H1O2 Gas (SGTE 1998; from T.C.R.A.S Class: 6)
FUNCTION F7597T
298.15 -217400.484+59.6272391*T-49.13577*T*LN(T)
-.02060312*T**2+2.88385E-06*T**3+269533.2*T**(-1);
700 Y -215609.752+68.1067877*T-51.28458*T*LN(T)
-.01359635*T**2+8.794425E-07*T**3-163278.6*T**(-1);
2400 Y -282508.308+440.738249*T-100.0948*T*LN(T)
+.002056652*T**2-5.27695667E-08*T**3+16806545*T**(-1);
6000 N !
$ CR1H1O3 Gas (SGTE 1998; from T.C.R.A.S Class: 6)
FUNCTION F7602T
298.15 -465439.226+128.026727*T-60.22963*T*LN(T)
-.034334375*T**2+5.59916833E-06*T**3+439094.1*T**(-1);
700 Y -478614.257+318.282192*T-89.43575*T*LN(T)
-.00539851*T**2+1.98466333E-07*T**3+1560648*T**(-1);
4200 Y -541570.155+535.668547*T-116.0568*T*LN(T)
-3.342993E-04*T**2+1.73310833E-08*T**3+30205210*T**(-1);
6000 N !
$ CRH2O2 Gas (SGTE 1998; from T.C.R.A.S Class: 6)

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FUNCTION F7607T

298.15 -353065.906+133.595434*T-61.52032*T*LN(T)
-.023890125*T**2+3.29953E-06*T**3+307071.7*T**(-1);
700 Y -354821.577+184.747488*T-70.00234*T*LN(T)
-.01189955*T**2+5.64119333E-07*T**3+243073.05*T**(-1);
3200 Y -449760.391+591.737803*T-121.3714*T*LN(T)
+5.40635E-04*T**2-1.78027667E-09*T**3+33616705*T**(-1);
6000 N !

\$ CRH2O3 Gas (SGTE 1998; from T.C.R.A.S Class: 7)

FUNCTION F7612T

298.15 -570546.313+175.502827*T-69.88341*T*LN(T)
-.039065985*T**2+6.00655667E-06*T**3+446219.65*T**(-1);
700 Y -586933.278+398.821738*T-103.8536*T*LN(T)
-.00710593*T**2+2.45888667E-07*T**3+1956974*T**(-1);
2400 Y -501727.308+76.5671777*T-64.22608*T*LN(T)
-.014217985*T**2+4.07615167E-07*T**3-29955760*T**(-1);
6000 N !

\$ CR1H2O4 Gas (SGTE 1998; from T.C.R.A.S Class: 7)

FUNCTION F7617T

298.15 -768780.228+269.510425*T-84.04115*T*LN(T)
-.048853265*T**2+7.72746667E-06*T**3+565029.5*T**(-1);
700 Y -788477.415+542.039678*T-125.5994*T*LN(T)
-.009186415*T**2+5.03520667E-07*T**3+2345669*T**(-1);
2700 Y -833375.93+771.207888*T-155.2922*T*LN(T)
-3.433531E-04*T**2+8.41448333E-09*T**3+15445430*T**(-1);
6000 N !

\$ CRH3O3 Gas (SGTE 1998; from T.C.R.A.S Class: 7)

FUNCTION F7622T

298.15 -671674.452+253.071378*T-83.35022*T*LN(T)
-.03938726*T**2+5.344205E-06*T**3+520808*T**(-1);
700 Y -673348.792+316.604123*T-94.09035*T*LN(T)
-.02296841*T**2+1.41863233E-06*T**3+348797.85*T**(-1);
2400 Y -782152.825+909.710197*T-171.6097*T*LN(T)
+.001612632*T**2-4.14523833E-08*T**3+29119965*T**(-1);
6000 N !

\$ CRH3O4 Gas (SGTE 1998; from T.C.R.A.S Class: 7)

FUNCTION F7627T

298.15 -829637.598+316.337347*T-92.4178*T*LN(T)
-.05478255*T**2+8.34066667E-06*T**3+664358.5*T**(-1);
700 Y -849057.973+590.287921*T-134.332*T*LN(T)
-.013946405*T**2+7.72871667E-07*T**3+2378882*T**(-1);
2500 Y -894520.802+854.389327*T-169.146*T*LN(T)
-.002253448*T**2+4.77443833E-08*T**3+13439610*T**(-1);
6000 N !

\$ CRH4O4 Gas (SGTE 1998; from T.C.R.A.S Class: 7)

```

298.15 -899273.42+364.691174*T-102.8073*T*LN(T)
      -.0590702*T**2+8.688115E-06*T**3+673521.5*T**(-1);
700 Y -919642.215+650.622024*T-146.5309*T*LN(T)
      -.016540225*T**2+7.90595833E-07*T**3+2488014*T**(-1);
2400 Y -888939.312+593.926121*T-141.1226*T*LN(T)
      -.01375828*T**2+3.98781833E-07*T**3-12550210*T**(-1);
6000 N !

```

FUNCTION F7637T

```

298.15 -920139.948+488.045944*T-117.912*T*LN(T)
      -.06790695*T**2+1.023153E-05*T**3+946231*T**(-1);
700 Y -943767.647+820.584561*T-168.7814*T*LN(T)
      -.0183363*T**2+1.0206675E-06*T**3+3042761*T**(-1);
2600 Y -1031039.87+1269.84207*T-227.0761*T*LN(T)
      -7.441575E-04*T**2+1.84764833E-08*T**3+28262585*T**(-1);
6000 N !

```

\$ Cr oxide gas, assessment Chen (2006), based on Ebbinghaus (1993)

FUNCTION GCR101G

$$\begin{aligned} & 298.15 \text{ } +173449.38-33.082803 * T-30.097 * T * \text{LN}(T)-0.006276 * T^{**} 2 \\ & \quad +31300 * T^{**}(-1)+9.556667 \text{E}-7 * T^{**} 3 ; \\ & 1000 \text{ Y } +167489.28+37.307301 * T-40.555 * T * \text{LN}(T)+0.0014795 * T^{**} 2 \\ & \quad +873600 * T^{**}(-1)+1.6916667 \text{E}-7 * T^{**} 3 ; \\ & 3000 \text{ N } ! \end{aligned}$$

FUNCTION GCR102G

298.15 -109942.78+10.590469*T-39.526*T*LN(T)-0.0155025*T**2
+245800*T**(-1)+2.4298333E-6*T**3;
1000 Y -118120.28+123.81288*T-56.696*T*LN(T)-0.0001175*T**2
+932050*T**(-1)-8.0166667E-8*T**3;
3000 N !

FUNCTION GCR103G

298.15 -341231.99+130.6074*T-57.2*T*LN(T)-.0216155*T**2
+428900*T**(-1)+3.4098333E-6*T**3;
1000 Y -354716.086+299.88954*T-82.569*T*LN(T)-0.000154*T**2
+1814700*T**(-1)+7.3333333E-9*T**3;
3000 N !

FUNCTION GCRH101G

298.15 +68260.3035915366+52.8748592066681*T-46.257*T*LN(T)

$-0.0022405 \cdot T^{**2} + 185600 \cdot T^{**(-1)} - 1.5083333333333333E-7 \cdot T^{**3};$
 1000 Y $+56683.83692487 + 136.528447327492 \cdot T - 57.551 \cdot T \cdot \ln(T)$
 $+0.0017905 \cdot T^{**2} + 2218000 \cdot T^{**(-1)} - 2.75166666666667E-7 \cdot T^{**3};$
 3000 N !
 \$ CRO(OH)1 Gas REASSESSED BY MING CHEN (2006) BASED ON EBBINGHAUS (1993)
 FUNCTION GCRH1O2G
 298.15 $-274384.318854868 + 190.515744152316 \cdot T - 74.175 \cdot T \cdot \ln(T)$
 $+0.003057 \cdot T^{**2} + 266750 \cdot T^{**(-1)} - 9.135E-7 \cdot T^{**3};$
 1000 Y $-276268.518854868 + 180.696587450316 \cdot T - 72.053 \cdot T \cdot \ln(T)$
 $-0.001535 \cdot T^{**2} + 938850 \cdot T^{**(-1)} + 5.15E-8 \cdot T^{**3};$
 3000 N !
 \$ CRO2(OH) Gas, assessment Cgen 2006, based on Ebbinghaus 1993
 FUNCTION GCRH1O3G
 298.15 $-465014.792765063 + 261.78538072314 \cdot T - 83.724 \cdot T \cdot \ln(T)$
 $-0.014623 \cdot T^{**2} + 715900 \cdot T^{**(-1)} + 2.39E-6 \cdot T^{**3};$
 1000 Y $-471251.426098397 + 347.947179789566 \cdot T - 96.902 \cdot T \cdot \ln(T)$
 $-0.0018435 \cdot T^{**2} + 1338300 \cdot T^{**(-1)} + 9.33333333333334E-8 \cdot T^{**3};$
 3000 N !
 \$ CR(OH)2 Gas, assessment Cgen 2006, based on Ebbinghaus 1995
 FUNCTION GCRH2O2G
 298.15 $-351288.381040966 + 195.861187758742 \cdot T - 75.927 \cdot T \cdot \ln(T)$
 $-0.000745 \cdot T^{**2} + 243850 \cdot T^{**(-1)} - 9.2E-7 \cdot T^{**3};$
 1000 Y $-359644.247707633 + 228.973348382991 \cdot T - 79.455 \cdot T \cdot \ln(T)$
 $-0.004093 \cdot T^{**2} + 2094950 \cdot T^{**(-1)} + 1.91166666666667E-7 \cdot T^{**3};$
 3000 N !
 \$ CRO(OH)2 Gas, assessment Chen 2006, based on Ebbinghaus 1995
 FUNCTION GCRH2O3G
 298.15 $-578683.368076208 + 391.200887831716 \cdot T - 109.525 \cdot T \cdot \ln(T)$
 $-0.000562 \cdot T^{**2} + 663150 \cdot T^{**(-1)} - 5.678333333333333E-07 \cdot T^{**3};$
 1000 Y $-582354.368076208 + 394.600755129996 \cdot T - 109.25 \cdot T \cdot \ln(T)$
 $-0.003973 \cdot T^{**2} + 1.89666666666667E-07 \cdot T^{**3} + 1688150 \cdot T^{**(-1)};$
 3000 N !
 \$ CRO2(OH)2 Gas, assessment Chen 2006, based on Ebbinghaus 1993
 FUNCTION GCRH2O4G
 298.15 $-774253.262922295 + 381.407986877701 \cdot T - 107.819 \cdot T \cdot \ln(T)$
 $-0.0191755 \cdot T^{**2} + 513600 \cdot T^{**(-1)} + 1.995833333333333E-06 \cdot T^{**3};$
 1000 Y $-792715.129588962 + 547.844356162281 \cdot T - 131.457 \cdot T \cdot \ln(T)$
 $-0.004921 \cdot T^{**2} + 3311450 \cdot T^{**(-1)} + 2.545E-7 \cdot T^{**3};$
 3000 N !
 \$ CR(OH)3 Gas, assessment Chen 2006, based on Ebbinghaus 1995
 FUNCTION GCRH3O3G
 298.15 $-650064.71221395 + 464.373635257849 \cdot T - 125.498 \cdot T \cdot \ln(T)$
 $+0.005874 \cdot T^{**2} + 498450 \cdot T^{**(-1)} - 2.3775E-6 \cdot T^{**3};$
 1000 Y $-656537.878880616 + 448.299516123462 \cdot T - 121.163 \cdot T \cdot \ln(T)$

$+3.14618667E-07*T**3-1280036*T**(-1);$
 2100 Y $-18840.1663+92.3120249*T-32.05082*T*LN(T)-0.0010728235*T**2$
 $+1.14281783E-08*T**3+3561002.5*T**(-1);$
 6000 N !
 \$ H Gas (JANAF 1982, assessment dated 3/77 from SGTE)
 FUNCTION HGAS
 298.15 $+211801.621+24.4989821*T-20.78611*T*LN(T);$
 6000 N !
 \$ H2O1 Gas (SGTE 1998; from T.C.R.A.S Class: 4)
 FUNCTION F10963T
 298.15 $-250423.434+4.45470312*T-28.40916*T*LN(T)$
 $-0.00623741*T**2-6.01526167E-08*T**3-64163.45*T**(-1);$
 1100 Y $-256145.879+30.1894682*T-31.43044*T*LN(T)$
 $-0.007055445*T**2+3.05535833E-07*T**3+1246309.5*T**(-1);$
 2800 Y $-268423.418+116.690197*T-42.96842*T*LN(T)$
 $-0.003069987*T**2+6.97594167E-08*T**3+2458230.5*T**(-1);$
 8400 Y $-489068.882+553.259882*T-92.4077*T*LN(T)$
 $+0.0016703495*T**2-1.32333233E-08*T**3+1.765625E+08*T**(-1);$
 18000 Y $-165728.771+239.645643*T-59.77872*T*LN(T)$
 $+2.213599E-04*T**2-1.2921095E-09*T**3-4.1931655E+08*T**(-1);$
 20000 N !
 \$ H1O1 Gas (SGTE 1998; from T.C.R.A.S Class: 1)
 FUNCTION F10666T
 298.15 $+30698.6898+15.9096451*T-29.97699*T*LN(T)$
 $+0.001713168*T**2-6.799205E-07*T**3-25503.82*T**(-1);$
 1000 Y $+31735.5127-12.686636*T-25.42186*T*LN(T)$
 $-0.003149545*T**2+1.34404917E-07*T**3+116618.65*T**(-1);$
 3000 Y $+41016.0783-20.7343256*T-24.94216*T*LN(T)$
 $-0.0023107985*T**2+5.91863E-08*T**3-6415210*T**(-1);$
 8600 Y $-154907.953+370.326117*T-69.24542*T*LN(T)$
 $+0.0019361405*T**2-1.47539017E-08*T**3+1.4391015E+08*T**(-1);$
 18000 Y $+326722.277-65.0792741*T-24.2768*T*LN(T)$
 $+6.42189E-05*T**2-1.30298483E-10*T**3-8.292415E+08*T**(-1);$
 20000 N !
 \$ H1O2 Gas (SGTE 1998; from T.C.R.A.S Class: 4)
 FUNCTION F10729T
 298.15 $+1075.64106-55.242048*T-24.45435*T*LN(T)$
 $-0.018507875*T**2+2.36297E-06*T**3-29469.05*T**(-1);$
 800 Y $-7932.99164+54.2016233*T-40.775*T*LN(T)$
 $-0.00501027*T**2+2.122915E-07*T**3+925845*T**(-1);$
 3600 Y $-67875.8961+275.406716*T-68.1173*T*LN(T)$
 $+6.12331E-04*T**2-6.573855E-09*T**3+26048030*T**(-1);$
 6000 N !
 \$ H2O2 Gas (JANAF SECOND EDIT SGTE)
 FUNCTION F10983T

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298.15 -147258.971-37.1497212*T-26.10636*T*LN(T)
      -.036948065*T**2+6.659505E-06*T**3+65357.65*T*(-1);
700 Y -156470.505+120.191295*T-50.94271*T*LN(T)
      -.007931945*T**2+4.29733833E-07*T**3+684985.5*T*(-1);
1500 N !
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$$$
$ La(g)
FUNCTION F12026T
298.15 +422273.955-30.3347881*T-22.06299*T*LN(T)-0.005444405*T**2
      +4.71447833E-07*T**3+102710.1*T*(-1);
600 Y +426628.905-85.4786162*T-13.83676*T*LN(T)-0.011938995*T**2
      +1.33826017E-06*T**3-312130.2*T*(-1);
1300 Y +404460.17+114.016725*T-42.00406*T*LN(T)+0.0037094435*T**2
      -2.70261E-07*T**3+2891891*T*(-1);
3200 Y +497751.747-246.085237*T+2.791973*T*LN(T)-0.006002155*T**2
      +1.30043383E-07*T**3-34158815*T*(-1);
8200 Y -92343.0441+773.338363*T-111.0188*T*LN(T)+0.0037862445*T**2
      -2.82257667E-08*T**3+5.418475E+08*T*(-1);
10000 N !
$ LaO(g)
FUNCTION F12049T
298.15 -131496.968-24.5469483*T-31.53764*T*LN(T)-0.0051956*T**2
      +7.60442333E-07*T**3+103677.85*T*(-1);
900 Y -133112.849+7.93847638*T-36.65559*T*LN(T)+2.4937065E-04*T**2
      -2.05688333E-07*T**3+108868.35*T*(-1);
2500 Y -137735.323-23.9414477*T-31.58251*T*LN(T)-0.003177688*T**2
      +6.84986667E-08*T**3+5676870*T*(-1);
5400 Y -39118.6731-213.786313*T-10.21743*T*LN(T)-0.005021225*T**2
      +9.162985E-08*T**3-74562000*T*(-1);
10000 N !
$ La2O(g)
FUNCTION F12085T
298.15 -69316.3279+46.9195461*T-51.12563*T*LN(T)-0.005701935*T**2
      +8.637425E-07*T**3+212452.95*T*(-1);
1000 Y -73167.5826+93.9280358*T-58.13034*T*LN(T)-1.332372E-05*T**2
      +4.41584333E-10*T**3+616730*T*(-1);
6000 N !
$ La2O2(g)
FUNCTION F12089T
298.15 -642532.065+54.8487791*T-51.72813*T*LN(T)-0.028452875*T**2
      +4.99643833E-06*T**3+271002.95*T*(-1);
700 Y -657497.385+256.452173*T-82.32033*T*LN(T)-1.8245965E-04*T**2
      +6.891315E-09*T**3+1664162*T*(-1);
5100 Y -672122.137+293.83814*T-86.72291*T*LN(T)+4.319301E-04*T**2

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-9.75906E-09*T**3+11187120*T**(-1);
6000 N !
$ Sr(g) :
FUNCTION F14450T
298.15 +154227.522-24.1431703*T-20.98549*T*LN(T)
+1.951298E-04*T**2-3.09095833E-08*T**3+4675.2365*T**(-1);
1800 Y +111247.483+242.365806*T-56.52776*T*LN(T)
+0.0133862*T**2-9.57800833E-07*T**3+9843260*T**(-1);
3300 Y +770872.513-2114.76782*T+233.253*T*LN(T)
-0.04337796*T**2+1.134592E-06*T**3-2.7250735E+08*T**(-1);
4900 Y -196742.694+263.327068*T-44.45892*T*LN(T)
-0.008078665*T**2+2.96671167E-07*T**3+3.57637E+08*T**(-1);
6200 Y -949056.902+1952.13337*T-239.3059*T*LN(T)
+0.01421437*T**2-1.79062E-07*T**3+8.9842E+08*T**(-1);
9600 Y +34305.7758+474.957384*T-77.25547*T*LN(T)
+0.00232914*T**2-1.54504333E-08*T**3-2.2245325E+08*T**(-1);
10000 N !
$ Sr2(g) :
FUNCTION F14465T
298.15 +295010.66+61.845039*T-54.13634*T*LN(T)
+0.040485225*T**2-9.264165E-06*T**3-70453.75*T**(-1);
500 Y +307156.188-147.411671*T-20.95926*T*LN(T)
+1.012636E-04*T**2-8.03856667E-09*T**3-905190.5*T**(-1);
3000 N !
$ SrO(g) :
FUNCTION F12810T
298.15 -25476.9742+3.04351985*T-34.37623*T*LN(T)
-0.0026980695*T**2+3.78874167E-07*T**3+120146.05*T**(-1);
900 Y -44602.142+205.651627*T-63.83687*T*LN(T)
+0.017645965*T**2-2.284235E-06*T**3+2463047*T**(-1);
1800 Y +243278.077-1500.21201*T+161.9497*T*LN(T)
-0.0612273*T**2+2.896125E-06*T**3-66468000*T**(-1);
2900 Y -571113.316+1685.71589*T-234.6556*T*LN(T)
+0.024571595*T**2-5.82819833E-07*T**3+2.468897E+08*T**(-1);
4500 Y -14433.8514+256.066959*T-66.76292*T*LN(T)
+0.002226246*T**2-2.98498E-08*T**3-97083400*T**(-1);
8800 Y +52967.3441+134.904343*T-53.17021*T*LN(T)
+0.001008387*T**2-9.46948833E-09*T**3-1.6008755E+08*T**(-1);
10000 N !
$ Mn(g)
FUNCTION F12439T 298.15 +276164.054-34.4987547*T-20.786*T*LN(T);
1575.00 Y +275547.585-29.2480566*T-21.52064*T*LN(T)
+3.819474E-04*T**2-3.66030333E-08*T**3+95180.95*T**(-1);
2100.00 Y +274521.741-16.3844926*T-23.35302*T*LN(T)
+0.0013469965*T**2-1.18903067E-07*T**3;

```

2400.00 N !

\$ MnO(g)

FUNCTION F12454T 298.15 +151356.092-24.1662496*T-31.02229*T*LN(T)
-0.005519525*T**2+8.47063667E-07*T**3+97921.9*T**(-1);
900.00 Y +146503.882+29.4389965*T-38.90434*T*LN(T)
+4.8722855E-04*T**2-5.46958333E-08*T**3+687003.5*T**(-1);
4100.00 Y +163891.797+1.24225715*T-35.94693*T*LN(T)
+6.220655E-04*T**2-7.949125E-08*T**3-12461235*T**(-1);
6000.00 N !

\$ MnO2(g)

FUNCTION F12461T 298.15 +9095.11807-9.18675027*T-36.92694*T*LN(T)
-0.01944391*T**2+3.43552E-06*T**3+201368.45*T**(-1);
700.00 Y -4061.05468+167.414546*T-63.68895*T*LN(T)
+0.004964408*T**2-7.80481667E-07*T**3+1423101*T**(-1);
2000.00 Y +74138.9718-312.782575*T+1.646534*T*LN(T)
-0.01801756*T**2+7.59669E-07*T**3-16355180*T**(-1);
3900.00 Y -269662.307+860.503282*T-143.1466*T*LN(T)
+0.008591745*T**2-1.67854167E-07*T**3+1.388169E+08*T**(-1);
6000.00 N !

\$ O(g) :

FUNCTION F7397T 298.15 +243206.529-42897.0876*T**(-1)-20.7513421*T
-21.0155542*T*LN(T)+1.26870532E-04*T**2-1.23131285E-08*T**3;
2950.00 Y +252301.473-3973170.33*T**(-1)-51.974853*T
-17.2118798*T*LN(T)-5.41356254E-04*T**2+7.64520703E-09*T**3;
6000.00 N !

\$ O3(g) :

FUNCTION F7683T 298.15 +133772.042-11328.9959*T**(-1)-84.8602165*T
-19.8314069*T*LN(T)-0.0392015696*T**2+7.90727187E-06*T**3;
600.00 Y +120765.524+997137.156*T**(-1)+120.113376*T
-51.8410152*T*LN(T)-0.00353983136*T**2+3.20640143E-07*T**3;
1500.00 Y +115412.196+1878139.02*T**(-1)+164.679664*T
-58.069736*T*LN(T)-2.84399032E-04*T**2+5.95650279E-10*T**3;
6000.00 N !

\$ Y(g):

FUNCTION F14722T 298.15 +413926.156+43.942359*T-34.19791*T*LN(T)
+0.0122297*T**2-2.14534333E-06*T**3+97071.5*T**(-1);
700.00 Y +417505.307-13.2762864*T-25.29082*T*LN(T)
+0.002768476*T**2-3.169895E-07*T**3-157006.6*T**(-1);
2000.00 Y +439627.78-100.082079*T-14.64876*T*LN(T)
+0.001182233*T**2-3.39037833E-07*T**3-7693105*T**(-1);
3300.00 Y +656873.926-957.210194*T+92.15071*T*LN(T)
-0.022050485*T**2+6.04918167E-07*T**3-90137500*T**(-1);
5500.00 Y -81672.0087+877.446829*T-122.4532*T*LN(T)
+0.005666115*T**2-6.61492667E-08*T**3+3.865857E+08*T**(-1);
10000.00 N !

\$ Y2O(g):

```
FUNCTION F12945T 298.15 -18834.6011+47.2728187*T-49.14357*T*LN(T)
-0.007582635*T**2+1.2067E-06*T**3+211591.55*T**(-1);
900.00 Y -23590.8983+106.946886*T-58.08361*T*LN(T)
-2.2921245E-05*T**2+7.790445E-10*T**3+695520*T**(-1);
6000.00 N !
```

\$ YO(g):

```
FUNCTION F12929T 298.15 -55980.1334-24.7804591*T-30.58571*T*LN(T)
-0.005797885*T**2+9.044075E-07*T**3+92955.75*T**(-1);
900.00 Y -62402.7508+43.7949244*T-40.60318*T*LN(T)
+0.0014897095*T**2-1.41268333E-07*T**3+896318.5*T**(-1);
3100.00 Y +22970.3078-236.507016*T-6.632106*T*LN(T)
-0.004295709*T**2+3.30261667E-08*T**3-38281150*T**(-1);
5900.00 Y +78439.9263-450.3653*T+19.37683*T*LN(T)
-0.00859432*T**2+1.53217517E-07*T**3-45013010*T**(-1);
9600.00 Y -949291.433+1103.17067*T-151.1803*T*LN(T)
+0.004000447*T**2-2.13031E-08*T**3+1.118062E+09*T**(-1);
10000.00 N !
```

\$ Y2O2(g):

```
FUNCTION F13270T 298.15 -575737.712+51.4042333*T-49.55549*T*LN(T)
-0.030210885*T**2+5.27799667E-06*T**3+255509.3*T**(-1);
700.00 Y -591679.029+265.724012*T-82.06371*T*LN(T)
-2.6169375E-04*T**2+1.0952625E-08*T**3+1742125.5*T**(-1);
4500.00 Y -594803.763+277.512452*T-83.52789*T*LN(T)
+4.9195245E-05*T**2-1.17628333E-09*T**3+3139224*T**(-1);
6000.00 N !
```

\$ YO2(g):

```
FUNCTION F13266T 298.15 -453353.172+38.0172466*T-44.87379*T*LN(T)
-0.011836705*T**2+2.00650833E-06*T**3+281931.45*T**(-1);
800.00 Y -459941.788+124.969156*T-58.0167*T*LN(T)
-3.724498E-05*T**2+1.29613517E-09*T**3+910973.5*T**(-1);
6000.00 N !
```

\$ Gas Zr

```
FUNCTION GZRGAS 298.15 +586876.841+74.4171195*T-38.69111*T*LN(T)
+0.01152846*T**2-1.693255E-06*T**3+270638.8*T**(-1);
700.00 Y +595990.293-26.0530509*T-24.06106*T*LN(T)
+0.001743641*T**2-5.94312333E-07*T**3-748947.5*T**(-1);
1300.00 Y +593841.673-46.0204551*T-20.46361*T*LN(T)
-0.002961084*T**2+1.08391433E-07*T**3+526352.5*T**(-1);
2700.00 Y +630745.052-161.965371*T-6.647343*T*LN(T)
-0.0046738955*T**2+1.06833583E-07*T**3-15872340*T**(-1);
6600.00 Y +504260.272+131.813821*T-40.68801*T*LN(T)
-6.38357E-04*T**2+1.79125333E-08*T**3+71496950*T**(-1);
10000.00 N !
```

\$ Gas Zr2 (ssub)

FUNCTION F15702T 298.15 +892794.963-14.4120751*T-37.13672*T*LN(T)
 -3.2039655E-04*T**2-4.30605167E-09*T**3+85422.15*T**(-1);
 3600.00 Y +874148.858+9.34917918*T-39.33356*T*LN(T)
 -0.001019669*T**2+6.09799667E-08*T**3+14065805*T**(-1);
 6000.00 N !

\$ Gas ZrO (ssub)

FUNCTION F12964T 298.15 +84650.2479-322.816859*T+21.98592*T*LN(T)
 -0.10713165*T**2+2.81704E-05*T**3-333363.35*T**(-1);
 500.00 Y +42648.3264+404.464721*T-93.37933*T*LN(T)
 +0.03332466*T**2-3.80849833E-06*T**3+2526299*T**(-1);
 1100.00 Y +84838.707+11.527709*T-37.46259*T*LN(T)
 +9.16682E-05*T**2-7.005105E-08*T**3-3491878*T**(-1);
 4100.00 Y +106867.647-98.6658671*T-23.49987*T*LN(T)
 -0.00315689*T**2+5.93994E-08*T**3-6661880*T**(-1);
 9600.00 Y +255442.536-262.961955*T-6.281221*T*LN(T)
 -0.0038787795*T**2+6.18786667E-08*T**3-2.2466925E+08*T**(-1);
 10000.00 N !

\$ Gas ZrO2 (ssub)

FUNCTION F13281T 298.15 -332610.845+3.22325893*T-38.10718*T*LN(T)
 -0.01852473*T**2+3.29626E-06*T**3+218721.05*T**(-1);
 700.00 Y -342836.09+140.579945*T-58.93983*T*LN(T)
 +6.65405E-04*T**2-8.11812167E-08*T**3+1173742*T**(-1);
 2600.00 Y -272800.105-96.5265444*T-30.24766*T*LN(T)
 -0.0038011495*T**2-1.83201667E-11*T**3-28436635*T**(-1);
 4900.00 Y -36436.1523-803.246487*T+54.45089*T*LN(T)
 -0.017172935*T**2+3.92562833E-07*T**3-1.509956E+08*T**(-1);
 6000.00 N !

\$ Gas Ar (ssub5)

FUNCTION F877 298.15 -6197.3787-15.6250179*T-20.78611*T*LN(T);
 6000 N !

\$

FUNCTION RV71 298.15 +300000; 6000.00 N !
 FUNCTION RV72 298.15 0; 6000.00 N !
 FUNCTION RV73 298.15 +62427; 6000.00 N !
 FUNCTION RV74 298.15 0; 6000.00 N !
 FUNCTION RV75 298.15 +63158; 6000.00 N !
 FUNCTION RV76 298.15 0; 6000.00 N !

VITA

SHADI DARVISH

Born Tehran, Iran

2008- 2012	B. Sc. in Materials Science and Engineering, Sharif University of Technology, Tehran, Iran.
2014-2016	M. Sc. in Materials Science and Engineering, Florida International University (FIU), Miami, Florida
2014-2018	Ph. D. in Materials Science and Engineering, Florida International University (FIU), Miami, Florida

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