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Investigation of the Pt-Al-Cr system as part of the development of the Pt-Al-Cr-Ru thermodynamic database

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APPENDICES

APPENDIX A

Publications

APPENDIX B

Thermodynamic databases for Pt-Al-Cr (in TDB format)

APPENDIX A

Publications

Conference abstracts (no proceedings)

[2004Süs2] R. Süss, L.A. Cornish and U. Glatzel, *CALPHAD XXXIII Program and Abstracts*, 34, Krakow, Poland, 30th May - 4th June 2004.

[2007Süs] R. Süss, L.A. Cornish and A. Watson, *CALPHAD XXXVI Program and Abstracts*, 146, The Pennsylvania State University, State College, Pennsylvania, 6th - 11th May 2007.

Published conference proceedings

[2003Süs3] R. Süss, L.A. Cornish and B. Joja. *Proc. 2nd International Conference of the African Materials Society*, Johannesburg, 2003. p. 138-139.

[2005Süs] R. Süss and L.A. Cornish, *Proc. Microsc. Soc. South. Afr.*, 35 (2005) 9.

[2006Cor] L.A. Cornish, R. Süss, A. Watson and S.N. Prins, Southern African Institute of Mining and Metallurgy SAIMM conference "Platinum Surges Ahead", Sun City, 8th – 12th October 2006, Symposium Series S45, 91-102.

[2006Süs2] R. Süss and L.A. Cornish, *Proc. Microsc. Soc. South. Afr.*, 36 (2006) 14.

Published journal papers

[2006Wat] A. Watson, L.A. Cornish, and R. Süss, *Rare Metals*, 25(5) (2006) 1-11.

Paper 2.3

Comparison of Experimentally Determined and CALPHAD-Determined Results of the Pt-Cr-Ru System

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Platinum alloys are being developed and characterised which have microstructures that are analogous to the γ/γ' microstructure of the nickel-based superalloys [2003Süs1]. The microstructures comprise particles of Pt_3Al in a (Pt) matrix. These Pt based superalloys, with their higher melting point and good corrosion resistance, have the potential to substitute Ni-based superalloys for high-temperature components in turbine engines. The Pt-Cr-Ru system has been studied experimentally as part of this project [2002Süs, 2003Süs2]. The system was studied in the as-cast condition, and after annealing at 600°C and 1000°C. A solidification projection and a liquidus surface were constructed, together with isothermal sections at 600°C and 1000°C. The major phases are (Ru), (Pt) and ~CrPt, with ~Cr_2Ru ($D8_b$), ~Cr_3Ru (A15) and ~Cr_3Pt (A15) being minor. Both the tetragonal ($L1_0$) and cubic (A1) forms of ~CrPt were observed. Two invariant reactions were identified in the Pt-Cr-Ru system.

The second part of the project involves building a thermodynamic database for Pt-based alloys. Previously a preliminary CALPHAD-like assessment has been done for the Pt-Cr and Cr-Ru systems, with an extrapolation into Pt-Cr-Ru [2003Gla]. The calculations were done with the Thermo-Calc™ software. The preliminary results of the CALPHAD-like assessment were compared with the experimental results. It was found that the calculated liquidus was in good agreement, considering the limited data used. Optimisation of the Pt-Cr-Ru system is to follow, as well as the calculation of isothermal sections at 600°C and 1000°C.

The financial assistance of the South African Department of Science and Technology and the Platinum Development Initiative is acknowledged.

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[2002Süs] R. Süss, L.A. Cornish, L. Glaner and D.N. Compton, 15th International Congress on Electron Microscopy, 1st - 6th September 2002, Durban, South Africa.

[2003Gla] U. Glatzel and S. Prins, CALPHAD XXXII, 25-30 May 2003, Montreal, Canada.

[2003Süs1] R. Süss, L.A. Cornish, P.J. Hill and J. Hohls, Proc. Advanced Materials and Processes for gas turbines, September 22-26 2002, Copper Mountain, Colorado, USA, TMS, 301-308.

[2003Süs2] R. Süss, U. Glatzel, S. Prins and L.A. Cornish, Proc. of the 2nd International Conference of the African Materials Research Society, University of the Witwatersrand, 8–11 December 2003, Johannesburg, 141-142.

Ongoing Development of the Thermodynamic Database for Pt-based superalloys

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The development of a database for the Pt-Al-Cr-Ru quaternary system has been ongoing since 2003 as part of a programme to develop Pt-based superalloys for high temperature and/or aggressive environments [2006Cor]. Since there are very few experimental data for these systems, and the ternary phase diagrams are unknown, experimental phase diagram work has been undertaken. Experimental work has been completed for the Al-Pt-Ru [2005Pri] and Cr-Pt-Ru [2006Süs] systems and is nearly complete for Al-Cr-Pt. This, together with calorimetric measurements to be made in the future, will be used for modelling the four component system. To date, the Al-Pt-Ru system and its constituting binaries have been assessed using Thermo-Calc [2003Pri] and Cr-Pt-Ru using Pandat [2006Wat]. Work is underway on the Al-Cr-Pt system and some of the models which were used earlier for the ordered phases in the Pt-Cr binary have been modified for the current work to ensure that the database is self consistent. Since other elements such as Co, Ni and Nb will be added to the database, a programme of experimental phase diagram study is underway [2003Cho, 2006Ndl].

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[2005Pri] S. N. Prins, L.A. Cornish and P. Boucher, *J. Alloys and Compounds*, **403** (2005) 245-257.

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[2006Süs] R. Süss, L.A. Cornish and M.J. Witcomb, *J. Alloys and Compounds*, Vol. **416** (1-2), June 2006, p. 80-92.

[2006Wat] A. Watson, L.A. Cornish, and R. Süss, *Rare Metals*, **25** (5), 1-11, (2006).

AN INVESTIGATION OF AS-CAST Pt-Al-Cr ALLOYS

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Pt-rich alloys in the Pt-Al-Cr-Ru system are being developed as the basis for two-phase alloys analogous to Ni-based superalloys for high temperature applications[1,2]. The Pt-Al-Cr system is therefore of interest. The binary phase diagrams are reasonably well-established[3], while previous work on the ternary system was limited to the Pt-rich corner[4].

The investigation was started by preparing five alloys through arc-melting the pure (at least 99.9%) elements together. The nominal compositions of these alloys are given in Table 1. The melting of the alloys was repeated several times to achieve good mixture. These as-cast samples were sectioned, mounted and ground to 1200 grit on SiC paper. The samples were polished using an oxide polishing (OP-S) system. The microstructure was examined using a JEOL JSM-840 scanning electron microscope (SEM) and the phases and overall composition of the samples were analysed using a Vantage electron dispersive X-ray spectroscopy (EDS) system. Samples were usually imaged in the backscattered electron (BSE) imaging mode. X-ray diffraction (XRD) analyses were conducted on the polished samples using a Siemens D500 diffractometer with Mo Kα radiation. Phases were confirmed by XRD.

Alloy 1 comprised dark (Cr) (W type) dendrites, with an interdendritic eutectic mixture of dark (Cr) and light $PtAl_2$ (Figure 1). This structure formed by the following reaction sequence:

$$L \rightarrow (Cr)$$
$$L \rightarrow (Cr) + PtAl_2.$$

Alloy 2 comprised dark (Cr) dendrites with a mixture of light PtAl (cubic, FeSi type) and dark (Cr) interdendritically (Figure 2). There was also a suggestion of very fine solid state precipitation. More work needs to be done.

Alloy 3 comprised dark CrPt (cubic, Cu type) dendrites with a small amount of an interdendritic eutectic-like mixture of dark CrPt and light Pt_2Al (Figure 3). It was not possible to discern whether the Pt_2Al was of the high temperature Co_2Si type, or the low temperature $GaPt_2$ type. This structure could have formed by the following reactions:

$$L \rightarrow (Pt) + Pt_3Al$$
$$Pt \rightarrow CrPt_3 \rightarrow CrPt \text{ (ordering)}$$
$$Pt_3Al \rightarrow Pt_2Al \text{ (lower temperature in the solid state).}$$

Table 1: Nominal compositions of experimental alloys (at.%)

Alloy no.	Pt	Al	Cr
1	10	30	60
2	20	20	60
3	40	10	50
4	40	50	10
5	65	5	30

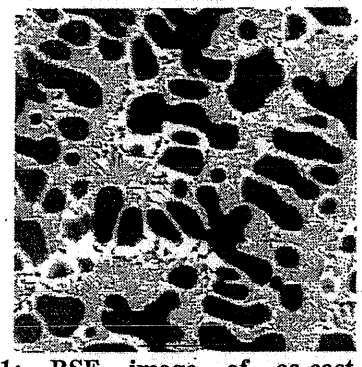


Figure 1: BSE image of as-cast nominal Pt_{10}:Al_{30}:Cr_{60}: (Cr) dark; $PtAl_2$ light.

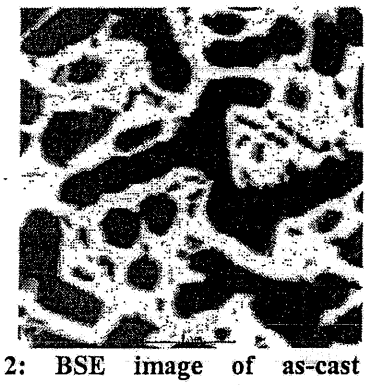


Figure 2: BSE image of as-cast nominal Pt_{20}:Al_{20}:Cr_{60}: (Cr) dark; PtAl light.

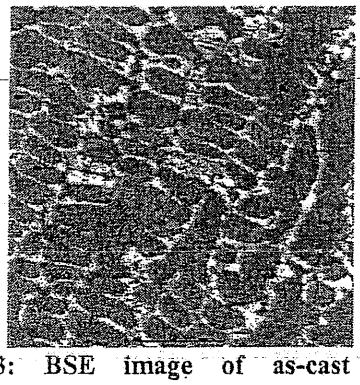


Figure 3: BSE image of as-cast nominal Pt_{40}:Al_{10}:Cr_{50}: CrPt dark; Pt_2Al light.

Alloy 4 appeared to be cored single phase (Figure 4), but XRD analysis showed that it comprised two

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phases, namely a dark Pt_2Al_3 (Al_3Ni_2 type) and lighter PtAl. These probably formed by the reaction:

$$L \rightarrow PtAl + Pt_2Al_3$$

Alloy 5 also appeared single phase (light) with a very small amount of very dark second phase particles visible (Figure 5). XRD analysis did however detect two phases, and since the very dark phase would seem to be less than 5% and therefore under the limit of reliable detection, one can assume that the two phases detected were the dark Pt_3Cr dendrites and very light Pt_3Al in-between. It was not possible to discern whether the Pt_3Al was of the $GaPt_3$ (tetragonal, DO'_C) or $AuCu_3$ (cubic, $L1_2$) type. The microstructure could have formed by:

$$L \rightarrow (Pt) + Pt_3Al$$
$$(Pt) \rightarrow Pt_3Cr$$

Plotting the compositions of the alloys and phases on a ternary diagram, a partial solidification projection for Pt-Al-Cr can be derived (Figure 6). These initial results suggest that phases like Pt_3Al and Pt_2Al may extend significantly into the ternary, with as much as ~30 at.% Cr being able to dissolve in Pt_2Al and as much as ~23 at.% Cr in Pt_3Al. Other phases that also extend into the ternary are: $PtAl_2$ (~16 at.% Cr); Pt_2Al_3 (~12 at.% Cr); PtAl (~18 at.% Cr); Pt_3Cr (~4 at.% Al); and CrPt (~7 at.% Al).

Future work will include the preparation of at least 20 more samples to determine the solidification projection and ultimately the liquidus surface for the system. Subsequent annealing of these samples at specific temperatures and their characterisation will be used to determine isothermal sections of the Pt-Al-Cr system.

This paper is published with the permission of Mintek, and we thank D&ST and the PDI for their financial support.

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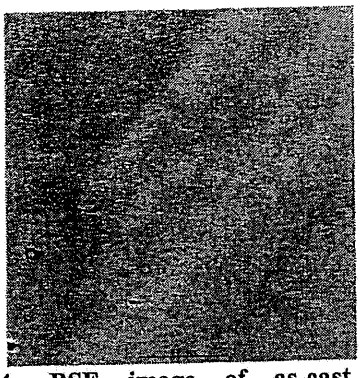


Figure 4: BSE image of as-cast nominal Pt_{40}:Al_{50}:Cr_{10}: Pt_2Al_3 dark; PtAl light.

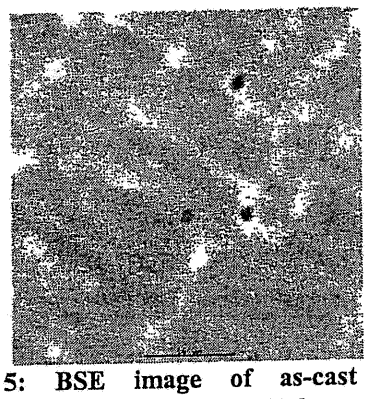


Figure 5: BSE image of as-cast nominal Pt_{65}:Al_5:Cr_{30}: Pt_3Cr dark; Pt_3Al light.

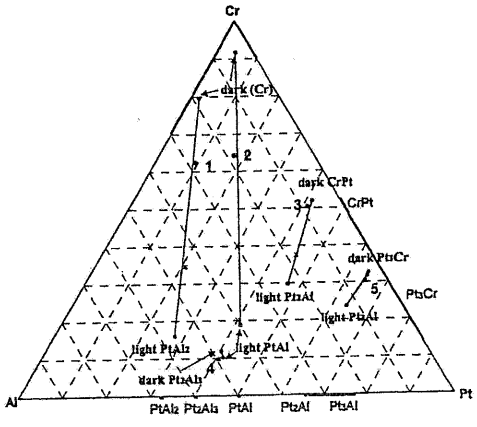


Figure 6: Partial solidification projection for the Pt-Al-Cr system.

POSSIBLE CHANGES TO THE Cr-Pt BINARY PHASE DIAGRAM

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The Pt-Cr-Ru and Pt-Al-Cr systems are of interest because Pt-rich alloys in the Pt-Al-Cr-Ru system are being developed as analogues to Ni-based superalloys for high temperature applications[1]. A multitude of ternary alloys were characterised using a JEOL JSM-840 SEM with a Vantage EDS system, and a Siemens D500 diffractometer with Mo Kα radiation for XRD analysis. The solidification projection and liquidus surface were determined for both systems.

The alloys $Pt_{10}:Cr_{80}:Ru_{10}$ and $Pt_{14}:Cr_{72}:Ru_{14}$ showed direct evidence of the invariant reaction

$$L + (Cr) \rightarrow \sim Cr_3Pt + (Pt)$$

because they had primary (Cr) (with grey Widmanstätten needles of $\sim Cr_3Pt$ within) surrounded by the $\sim Cr_3Pt$ + (Pt) eutectic (Fig. 1). In order to get the above-mentioned invariant reaction, however, the eutectic temperatures as given in the currently accepted phase diagram[2] have to be reversed. Using the accepted eutectic temperatures for Cr-Pt, one would expect either the invariant reaction

$$L + (Pt) \rightarrow \sim Cr_3Pt + (Cr),$$

or the ternary eutectic reaction

$$L \rightarrow (Cr) + \sim Cr_3Pt + (Pt),$$

neither of which was found in any of the investigated alloys[3].

In the Pt-Al-Cr system, one of the invariant reactions identified was

$$L + (Cr) + \sim Cr_3Pt \rightarrow (Pt).$$

The closest alloy to this reaction was alloy $Pt_{18}:Al_2:Cr_{80}$ which had a grey coloured layer around dark (Cr) with a white phase in between (Fig. 2). The irregular shape of the (Cr) suggested a succession of peritectic reactions. Once again, this ternary invariant reaction is not possible unless the eutectic temperatures as given in the currently accepted phase diagram are reversed. This would be consistent with a recently calculated phase diagram[4].

Two Pt-Cr alloys with the eutectic compositions as given by Massalski[2] taken as nominal compositions, were prepared and characterised as usual. The microstructure of alloy $Cr_{76}:Pt_{24}$ had an unusual appearance: dark (Cr) dendrites with ragged edges and circular inclusions, and light Cr_3Pt in between (Fig. 3). The ragged edges could be due to fast cooling, while the circular inclusions suggest a syntectic reaction (shown in older diagrams[5]) prior to a sparse eutectic reaction. The microstructure of alloy $Cr_{76}:Pt_{24}$ was more conventional, comprising light (Pt) dendrites with a dark and light Cr_3Pt + (Pt) eutectic in between (Fig. 4).

The phase compositions for both alloys were in close agreement with the phase diagram.

Therefore, there is evidence that supports the reversal of the eutectic temperatures. Considering the uncertainty regarding the eutectic reactions depicted by the dashed lines and tildes in the phase diagram given in Massalski (based on much older work[5]), it is highly plausible that the temperatures should be reversed. Differential thermal analyses should shed more light on the matter. The eutectic compositions are correct.

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Fig. 1.

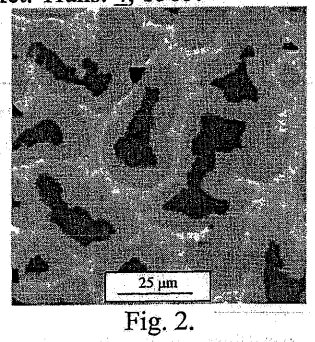


Fig. 2.

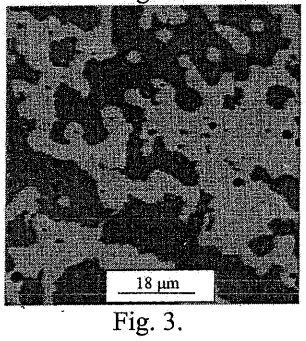


Fig. 3.

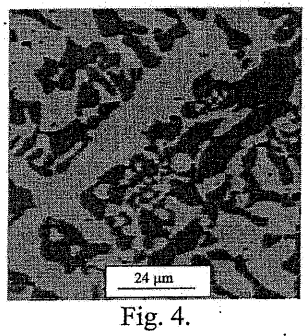


Fig. 4.

Fig. 1. BSE-SEM image of nominal $Pt_{14}:Cr_{72}:Ru_{14}$ in the as-cast condition: black (Cr); white ~CrPt; grey $\sim Cr_3Pt$.
Fig. 2. BSE-SEM image of nominal $Pt_{18}:Al_2:Cr_{80}$ in the as-cast condition: (Cr) dark; $\sim Cr_3Pt$ grey; ~CrPt white.
Fig. 3. BSE-SEM image of nominal $Cr_{87}:Pt_{13}$ in the as-cast condition: dark (Cr); light Cr_3Pt
Fig. 4. BSE-SEM image of nominal $Cr_{76}:Pt_{24}$ in the as-cast condition: dark Cr_3Pt; light (Pt).

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CORNISH, L.A., SÜSS, R., WATSON, A. and PRINS, S.A. Building a database for the prediction of phases in Pt-based superalloys. *International Platinum Conference 'Platinum Surges Ahead'*, The Southern African Institute of Mining and Metallurgy, 2006.

Building a database for the prediction of phases in Pt-based superalloys

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The work is being done using the Thermo-Calc™ software, and the database is being built up by obtaining good thermodynamic descriptions of all of the possible phases in the system. The database supplied did not cover all of the phases, and these had to be gleaned from literature, or modelled using experimental data. Similarly, not all of the experimental data were known, and where there were gaps or inconsistencies, experiments had to be undertaken. A preliminary version of the database was constructed from assessed thermodynamic data-sets for the binary systems only. The binary descriptions were combined allowing extrapolation into the ternary systems, and experimental phase equilibrium data were compared with calculated results. Very good agreement was obtained for the Pt-Al-Ru and Pt-Cr-Ru systems, which was encouraging and confirmed that the higher-order systems could be calculated from the binary systems with confidence. Since some of the phase models in databases were different, these phases had to be remodelled. However, more work is ongoing for information concerning the ternary phases present in the Al-Cr-Ru, Pt-Al-Ru (two ternary compounds in each) and Pt-Al-Cr (possibly more than three ternary compounds) systems. At later stage of the work, problems with the thermodynamic descriptions of the Cr-Ru and Pt-Cr binary systems were found. A programme of experimental work to overcome these has been devised, and is being undertaken.

Keywords: Pt-based alloys, phase diagram calculations.

Introduction

Work has been ongoing in building a thermodynamic database for the prediction of phase equilibria in Pt-based superalloys. The alloys are being developed for high temperature applications in aggressive environments. The database will aid the design of alloys by enabling the calculation of the composition and proportions of phases present in alloys of different compositions. Currently, the database contains the elements platinum, aluminium, chromium and ruthenium.

Ever since the possibility of basing a new series of alloys on platinum was seen[1], work has been ongoing at Mintek, Fachhochschule Jena and Bayreuth University, Germany, with input from NIMS, Japan. Undertaking experimental work is time-consuming and very expensive in terms of equipment, materials and expertise. A number of important commercial alloy systems, such as steels, nickel-based alloys, and aluminium alloys now have thermodynamic databases which have been derived from copious experimental results published by experts. These databases can be used with appropriate software to calculate phase diagrams, phase proportion diagrams, and Pourbaix diagrams, which can be used instead of experimentation. This saves both time and money. A similar database is being derived within the project so that it will facilitate further alloy development, and also be a tool to help designers to select alloy compositions and conditions in the future. However, steels, nickel-based and aluminium alloys have been used extensively, and there are more data and accepted phase diagrams. For the Pt-based database, there are fewer commercial alloys, and experimental data, and few accepted ternary systems. Even some of the binary systems have problems. Thus, part of this work included the study of phase diagrams to address the lack of data, and to use these data to compile a thermodynamic database. Since the basis of the alloys is the Pt_{84}:Al_{11}:Ru_2:Cr_3 alloy, the thermodynamic database will be built on the Pt-Al-Cr-Ru system. The Scientific Group Thermodata Europe (SGTE) database[2] has all the elements and some of the most commonly-used phases, i.e. those that are industrially important, but contains few of the required Pt phases. Additionally, the ruthenium data have been updated to capture Ansara's modification, to obtain a better estimate of the calculated melting temperature for (hypothetical) bcc-Ru[3]. Although there is a database for precious metals[4] it is not sufficiently complete for the purposes of this investigation, and does not contain all the elements of interest to this study, or all the phases. Additionally, not all the phase descriptions necessary are present in Spencer's database. The Al-Cr system has also been independently

assessed[5], although some of the phases might ultimately be modelled a different way.

The Thermo-Calc™ programme comprises the program itself, accessed in modules through a main module, and a series of databases where the structural and thermodynamic data are stored. In these databases, each phase is described by a series of parameters. The SGTE databases cover the phases of only the most common and well-known systems and all the stable elements[2]. The intermetallic phases in the Al-Ru and Pt-Al systems are not included in the SGTE database. Providing that the elements are in the database (and all of the stable elements are in the SGTE database, or other available databases), a phase diagram can be calculated and drawn. However, if there is no description for a particular phase, then the calculated phase diagram cannot include it. The database can be modified to include new phases, or run in conjunction with another database. The aim of this project is to develop a database specifically for the Pt-rich alloys in this investigation.

Prior to building a database, it must be known which phases need descriptions. The elemental information, and any phase that is already included in the SGTE database[2], can be accessed from that database. For phases that are not represented by the SGTE database, a number of factors must be taken into consideration. Firstly, the structure of the phase has to be decided, including the number of sites for the atoms, and which particular atoms fit on the sites. Each phase is modelled with sublattices, and each sublattice usually corresponds with a type of atom position. Elements allowed in a particular sublattice are those actually found in those positions in actual crystallography. This information is usually derived from (XRD) structural information and composition ranges, and is usually made to be as simple as possible. Next, some values have to be obtained for the interaction parameters. The interaction parameters can be guessed for an initial value or set to zero, and the user can decide which parameter can be changed during optimization. In optimization, experimental data are compared against the thermodynamic description, which is adjusted to best fit the experimental data. A 'pop' file has to be created which contains the experimental data (these can include phase compositions in equilibrium with each other at known temperatures, reaction information, enthalpies, etc.) Then optimization can be conducted. Thermo-Calc™ uses the information in the pop file and, through iteration, calculates the parameters required (those that were set to be changed) to best fit the data in the pop file. The result of this process is the incorporation of new phases, which now have parameters that can be used to calculate a phase diagram that agrees with the input data.

Optimization is the iterative process in which selected expressions of the thermodynamic descriptions are allowed to change so that agreement with the experimental results is improved. The optimization was carried out with the Parrot module[6] of the Thermo-Calc software[7]. With this module, the Gibbs energy functions can be derived by fitting experimental data by a least squares method. Different types of experimental data can be used and the weights can be assigned to the data based on the uncertainties associated with the original data. Once calculated phase diagrams that agree with the experimental data are obtained and the thermodynamic descriptions have been rationalized, the base systems will be complete. Selected important binaries were optimized first, for example, Al-Ru[8] and Al-Pt[9]. More work has to be carried out on the Al-Pt system because there is no description for the two major Pt_3Al phases

Since these phases are crucial to the project, they have to be modelled satisfactorily, before incorporation into the main database. Once each binary system is modelled satisfactorily, they can be added into the ternary systems, after which each ternary system must be optimized individually. This is done using the experimental data gleaned either from literature, or, as was mostly the case, derived experimentally within the programme at the University of the Witwatersrand and Mintek (for Al-Cr-Ru[10,11]), Mintek (for Pt-Cr-Ru[12,13] and Pt-Al-Cr[14], Pt-Al-Ru[15]) or the CSIR and Mintek (for Pt-Al-Ru[16]). Only once finalised can the ternaries be combined for the Pt-Al-Cr-Ru quaternary. The Thermo-Calc™ database will then be optimized against some quaternary alloys which have already been made for the alloy development work[17,18,19]. Once this stage is complete, then the other small additions, to improve the properties (as in nickel-based superalloys), can be included in the optimization. It is envisaged that the very final stage will be focused on the optimization of only the important phases: at least the cubic and tetragonal structures of ~Pt_3Al, (Pt), ~Pt_2Al and (Ru).

The Pt-Al-Cr-Ru system is optimized in Thermo-Calc™ by studying the four component ternary systems. The reason for undertaking an optimization of whole ternaries rather than portions of them is that there are very little data available for the system, and any thermodynamic model needs to be valid over the complete range of compositions in the base system before the minor components can be added. If only a small region is to be optimized (e.g. the region between the (Ni) and Ni_3Al phases only), then it is likely that although the model would be sufficiently good locally, the fit would either be very erratic or the calculations would not be able to converge when new elements were added, or other elements added beyond their original compositions. (This phenomenon is well-known for Thermo-Calc™ and has been experienced at Mintek for copper additions in duplex stainless steels.) Thus, the ternary systems for the Pt-Al-Cr-Ru quaternary will be studied in full to provide a sound basis for the Thermo-Calc™ database. The Pt-Al-Cr-Ru system is shown schematically in Figure 1.

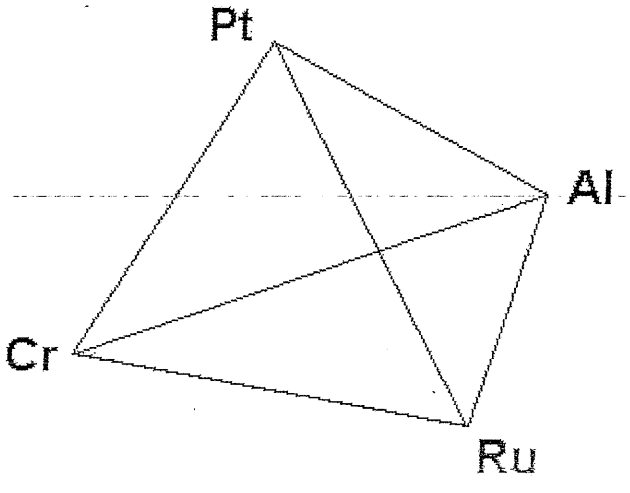


Figure 1. Schematic diagram of the Pt-Al-Cr-Ru System, showing four ternary systems and six binary systems

Building the database

Using the Compound Energy Formalism model

Introduction

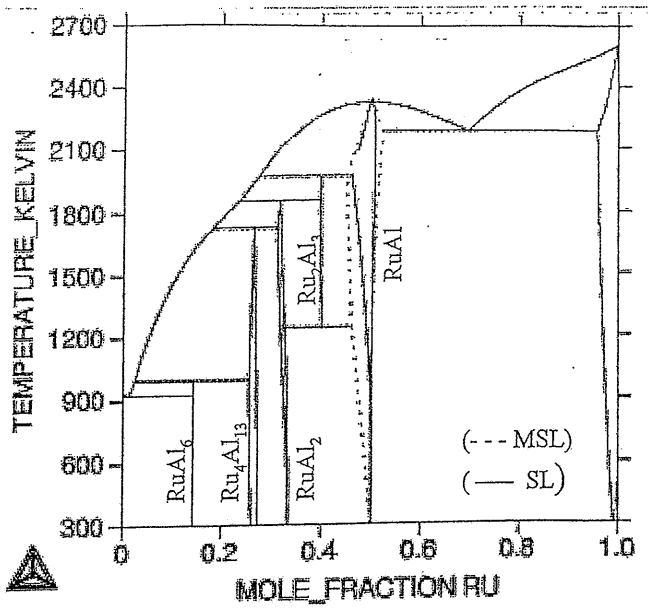
At the beginning, it was assumed that the six binary phase diagrams reported by Massalski[20] were correct, but it was realised after subsequent ternary work that this assumption was wrong. For the ternary systems, experimental work has already been completed for Al-Cr-Ru[10,11], Pt-Cr-Ru[12,13] Pt-Al-Ru[15,16], and is nearly complete for Pt-Al-Cr[14]. Some quaternary alloys have already been done[18,19], but any new alloys will probably be only within the Pt-rich corner. The aim is to input results from the phase diagram work, together with enthalpies from the single-phase or near single-phase compositions from Leeds[21], to Thermo-Calc™ for optimization. There will also be inputs from *ab initio* work from the University of Limpopo on enthalpies of formation for the Pt_3Al[22] and Cr-Ru[23] phases. Additionally, the transmission electron microscopy (TEM) results will be utilized in changes to modelling, especially of the ~Pt_3Al phase[24-26].

The Pt-Al-Cr-Ru system needed to be thoroughly researched through actual experimental work, so that the phases could be realistically described (to be as true to their crystallographic form as possible, so that any additional elements could be correctly incorporated) and then optimized using Thermo-Calc™. Only then can the other elements be added to the database descriptions. These will be the additional elements, added in smaller proportions to 'tweak' the properties. These will include at least cobalt and nickel.

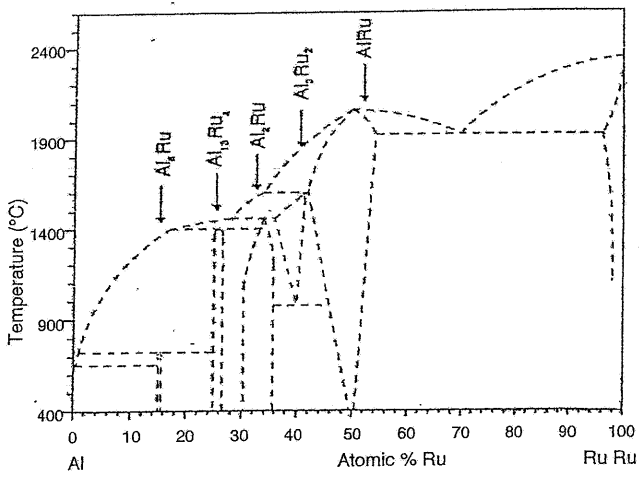
Experimental work has included the phase investigations alluded to above. Studies of as-cast alloys were done to determine the solidification reactions[10,11,12,16]. The solidification reactions and their temperatures (found by differential thermal analysis or DTA) are important inputs to Thermo-Calc™. The samples were also heat-treated at 600° and 1 000°C[13], then analysed so that the phase compositions at known temperatures could be input into Thermo-Calc™.

Ru-Al

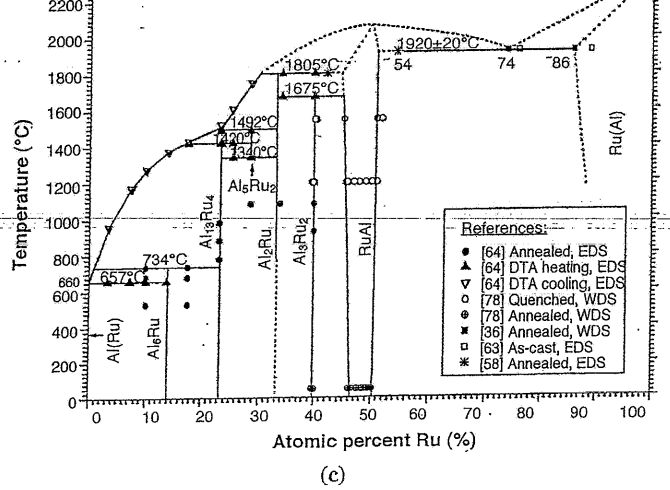
Initially, a simplified version of the four compound sublattice formalism (4CSF), a version of the compound energy formalism model[27], which models different combinations of the atoms, was used for the RuAl phase[8]. This worked very well for the Al-Ru system, as is shown in Figure 2, where the calculated diagram is compared both with that of Boniface and Cornish[31] and a phase diagram by Mücklich and Ilic[32] which was published subsequently to the calculated work. The RuAl (B2) phase was actually described by two different models: the Compound Energy Formalism (CEF), which is a simplified form of the 4CSF model, and is designated SL (for sublattice model) in Figure 2, as well as the Modified Sublattice Formalism (MSL), which describes the order-disorder transformation with one Gibbs energy function. The MSL model allowed a wider RuAl phase field (by giving more flexibility in atom positions), which is nearer to experimental findings. The $RuAl_6$ phase was described as a stoichiometric phase (i.e. 'line compound'), and the other intermetallic phases (Ru_4Al_{13}, $RuAl_2$ and Ru_2Al_3) were modelled with the sublattice model. The solubility of Ru in Al was considered negligible. The coefficients were also within



(a)



(b)



(c)

Figure 2. Comparison of the Al-Ru phase diagrams: a) Calculated[8]; b) Experimental from Boniface and Cornish[31]; c) Experimental by Mücklich and Ilic[32].

range comparable with those of other phases in other systems. It will be noticed that the two experimental phase diagrams are very similar, except for the stability of the Ru_2Al_3 phase, and the appearance of the Ru_2Al_5 phase. Boniface had observed a similar phase, but attributed it to being a ternary phase because it was found only with zirconium and silicon impurities[33]. Differences in the experimental phase diagrams are due to the use of different techniques. Boniface and Cornish[30] studied both as-cast and annealed samples, and the as-cast specimens showed that Ru_3Al_2 solidified at higher temperatures than Ru_2Al. Annealed samples[32] are less likely to show this. Since data from the experimental diagram are used to optimize the calculated phase diagram, the latter should agree with the former. Where there are differences, this is usually due to the mathematical model not allowing flexibility, or sometimes too much flexibility for complex models with limited data. In some cases, simpler models have to be used because there are insufficient data for all the parameters required by a more complex (but potentially more accurate) model.

Pt-Al

At the outset of the programme, there were two conflicting phase diagrams: those of McAlister and Kahan[34] and Oya *et al.*[35]. The major difference, which was very important to the development of the Pt-based alloys using the ~Pt3Al precipitates in a (Pt) solid solution, was the phase transformations in the ~Pt3Al (γ) phase, and the number of types of the ~Pt3Al (γ) phase. McAlister and Kahan[34] reported one transformation of the high-temperature Pt_3Al phase from $L1_2$ (γ') to a tetragonal low temperature variant (designated D0'c) (γ'_1) at ~1 280°C. However, Oya *et al.*[35] had the highest transformation $\gamma' \rightarrow \gamma'_1$ at ~340°C, and gave an additional transformation $\gamma'_1 \rightarrow \gamma'_2$ at 127°C. Previous attempts to resolve this conundrum by SEM, XRD and DTA had been unsuccessful, although Biggs found peaks at 311–337°C and 132°C for different composition samples using DTA[36]. Recent work[19] using an *in situ* heating in a TEM showed that the Oya *et al.*[35] diagram was more correct, although there is a possibility that very minor impurities are responsible, since the different workers sourced their raw material differently. The Pt-Al system had been calculated by Wu and Jin[37] using the CALPHAD method, but there was a need for re-assessment[9] because they had only one Pt_3Al phase, i.e. they did not reflect the ordering in the Pt_3Al phases. This needs to be done using a model that allows ordering to be calculated (described below). They did not include the $PtAl_2$ or β phases, owing to a lack of experimental data. A study of Pt-Al-X ternaries (where X=Ru, Ti, Cr, Ni) confirmed the presence of the Pt_2Al phase[15,36]. Experimental work on the Pt-Al-Ru ternary confirmed the presence of the β phase in the Al-Pt binary[16].

Initially, the four-compound sublattice formalism (4CSF), a version of the compound energy formalism model[27], was used. This models different combinations of four atoms of two different elements, for example: (A) (mathematically A_4), A_3B, AB (mathematically A_2B_2), AB_3, and (B) (mathematically B_4) where at least two of these appear in a system. This method was used for the (Pt)[9] and Pt_3Al[9] phases, because this model had used in the development of the nickel-based superalloy database[29,30].

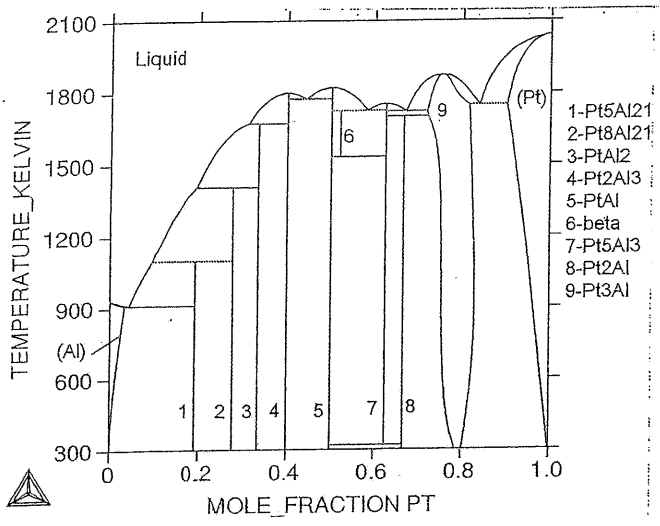
However, when the 4CSF model was applied to the Pt-Al system, the results were less successful, mainly because there were very few data, and the system was more complex. The intermetallic compounds $Pt_{21}Al_5$, $Pt_{21}Al_8$, $PtAl_2$, Pt_2Al_3, PtAl, Pt_5Al_3 and Pt_2Al were treated as stoichiometric compounds. The β phase was assumed to be stoichiometric, since very little experimental information was available, and was treated as $Pt_{52}Al_{48}$. The phase diagram shown in Figure 3 appears to agree with that of Massalski[20], which is actually from McAlister and Kahan[34], but the 4CSF model did not give the different Pt_3Al phases. The calculated compositions and temperatures for the invariant reactions of the intermetallic phases are in generally good agreement with the experimentally reported compositions and temperatures. However, there are some areas in less good agreement, in most cases because of the models being used.

The congruent formation of the Pt_3Al phase and $L \rightarrow Pt_3Al + (Pt)$ eutectic reactions are not in very good agreement with the experimental diagram, as both reactions are shifted to lower platinum compositions in the calculated system. The 4CSF model is such that the formation composition of Pt_3Al is fixed at 75 at. %, while it has been reported in the literature to form congruently at 73.2 at. %. This off-stoichiometry formation cannot be described with the model, and subsequently had an influence on the temperature as well as the enthalpy of formation for the Pt_3Al phase. The symmetry and fixed compositions of the 4CSF model also made it difficult to fix the eutectic reaction to lower Pt contents in the calculation. Furthermore, the phase area of the (Pt) solid solution is too narrow, especially at lower temperatures, although the phase area for the Pt_3Al phase is acceptable. However, the Pt_3Al phase is ordered throughout its phase area. The unstable $PtAl_3$ (L12) and Pt_2Al_2 (L10) phases, which are introduced through the 4CSF model, are not stable at any composition or temperature in the phase diagram, which is correct.

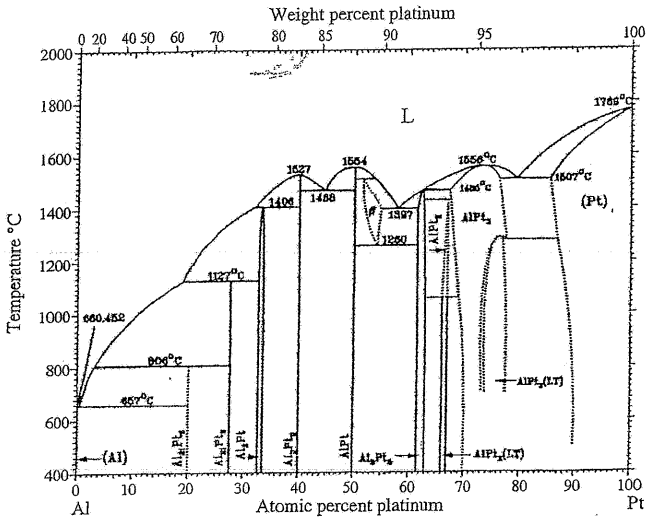
Further work on this system was postponed until more data to describe the (Pt) and Pt_3Al phases had been obtained. Currently, the Pt-Al binary is being investigated with the advent of Mintek's new Nova NANOSEM, and good results are being obtained. The data from these alloys will be used to optimize the Pt_3Al phase in the Pt-Al binary.

Cr-Pt

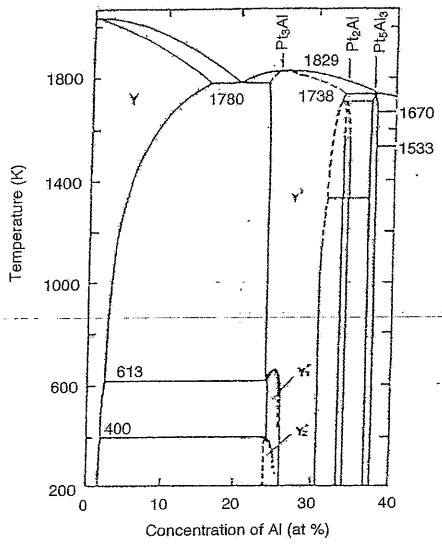
An assessment by Oikawa *et al.*[38] showed that the temperatures of the two eutectic temperatures in the Cr-Pt binary should be reversed when compared with Massalski[20]. This was initially thought to be wrong, even considering that the original data were very close (within 30±10°C). Thus, when work began on the Cr-Pt system, the work of Oikawa *et al.*[38] was ignored and the 4CSF model was used on the (Pt), Pt_3Cr and PtCr ordered phases[28]. There were many problems with using the 4CSF model, mostly because the model is complex and requires data that might be probable for the different phase types. If the phases do not exist naturally, the only way that these data can be obtained is by *ab initio* techniques. (Subsequent to this work, very good progress has been made by Preussner with the 4CSF and using the end points calculated using *ab initio* techniques[39].) The problem was that the 4CSF model needed more data than were available, and consequently the fit was very poor, as shown in Figure 4, which compares the calculated[40] and experimental phase diagrams[20]. Subsequently, experimental work on the Cr-Pt-Ru, Al-Cr-Pt and Cr-Ni-Pt ternary systems also agreed with the findings of Oikawa *et al.*[38], and those parameters are being used until subsequent experimental work indicates that a revision is necessary.



(a)

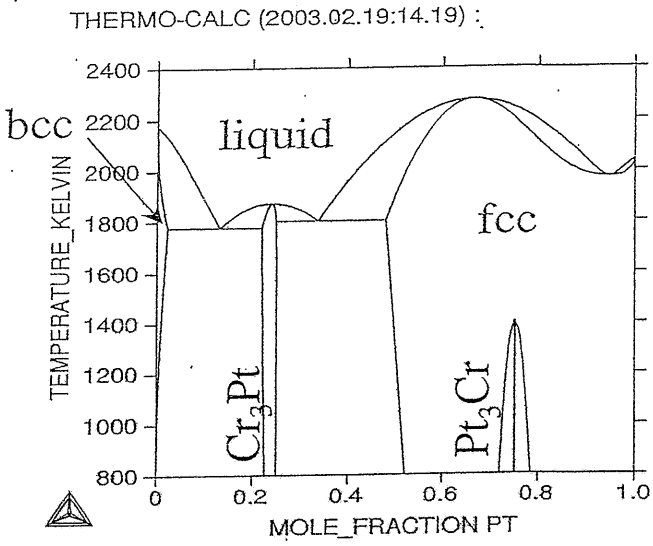


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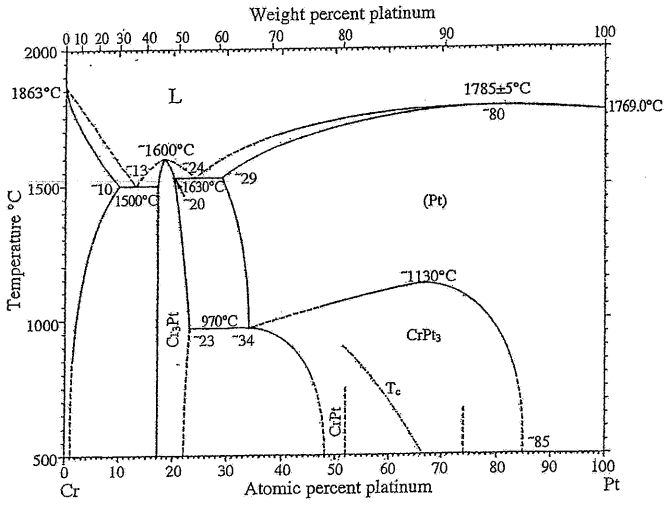


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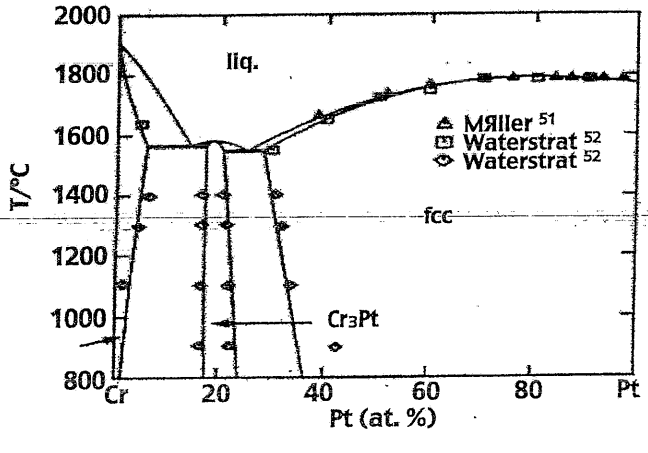
Figure 3. Comparison of Al-Pt phase diagrams: a) Calculated[9]; b) Experimental from Massalski[26] McAlister and Kahan[34]; c) Experimental from Oya *et al.*[35]



(a)



(b)



(c)

Figure 4. Comparison of Cr-Pt phase diagrams: a) Calculated initially by Glatzel and Prins[28]; b) Experimental[36]; c) Calculated by Oikawa *et al.*[38]

Cr-Ru

For the Cr-Ru system, there was no previous assessment, and the first calculation once again used the 4CSF model with poor reproducibility because the model was too complex for the data available (Figure 5). Further work and an extrapolation of the Pt-Cr, Cr-Ru and Pt-Ru binaries (the later from Spenser's database[4]) demonstrated further that the calculations were poor[40] although the fit with the ternary Pt-Cr-Ru liquidus was good[41], as shown in Figure 6. It was evident that another form of modelling was required. Subsequently, it was revealed[42] that there were problems with Massalski's[20] phase diagram, and two alloys were manufactured to study the sequence of reactions in the Cr-Ru binary. The Cr-Ru system is very difficult to study experimentally because the diffusion rates are very slow (large atoms and high melting points), and Cr oxidises easily on protracted annealing, despite precautions.

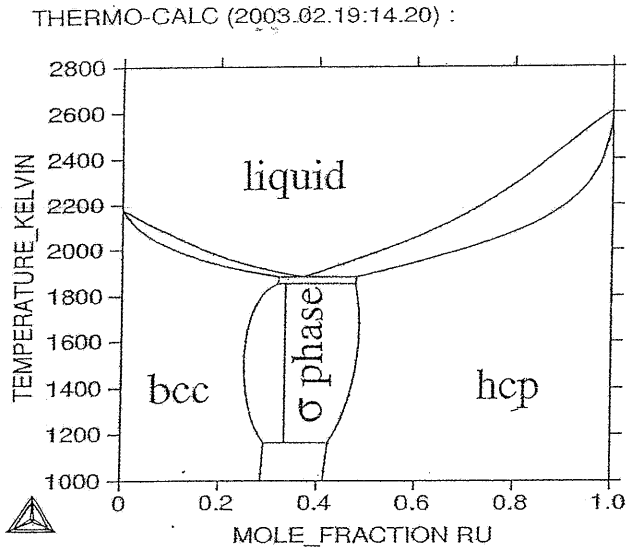
Pt-Al-Ru

The resulting database files from the Ru-Al, Pt-Al and Pt-Ru were added and the phase diagram was plotted, as an extrapolation from the binary systems, without any ternary interaction parameters or optimization with ternary data[43]. There were problems in the calculation of isothermal sections, which arose because the current models were not sufficiently robust to allow for extension into the ternary. However, the liquidus projection showed very good agreement with the experimental projection (Figure 7). Obviously, the two ~$Pt_{18}Al_{18}Ru_{64}$ and ~$Pt_{12}Al_{15}Ru_{73}$ ternary phases[16] were not calculated, because data for these were not input. The stability of the Pt_2Al phase was too high in the ternary because it solidified from the melt as a primary phase, which rendered the liquidus inaccurate for that region. This was probably because the inadequacies of modelling the phases, which allowed Pt_2Al to be too stable.

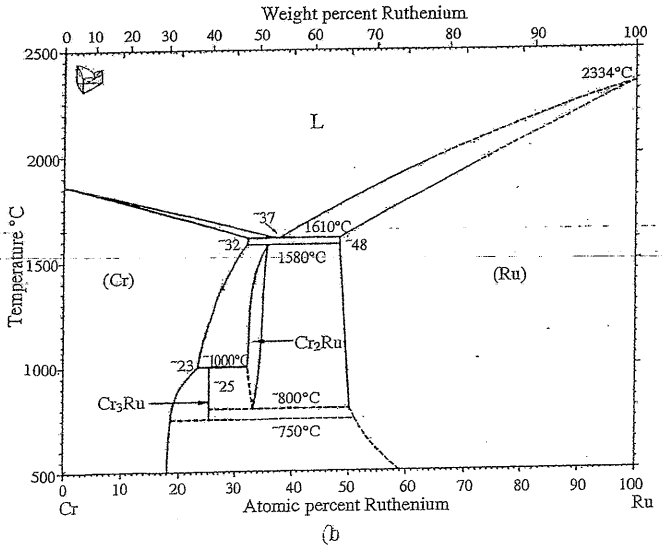
Using simpler models

General considerations

There is disagreement on which particular model should be used for (Pt) and Pt_3Al, which is similar to (Ni) and Ni_3Al. One school of thought states that as both are based on fcc,

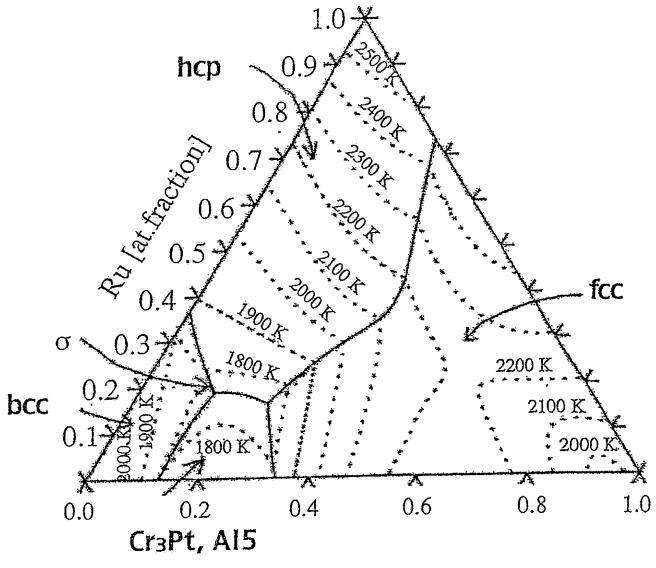


(a)

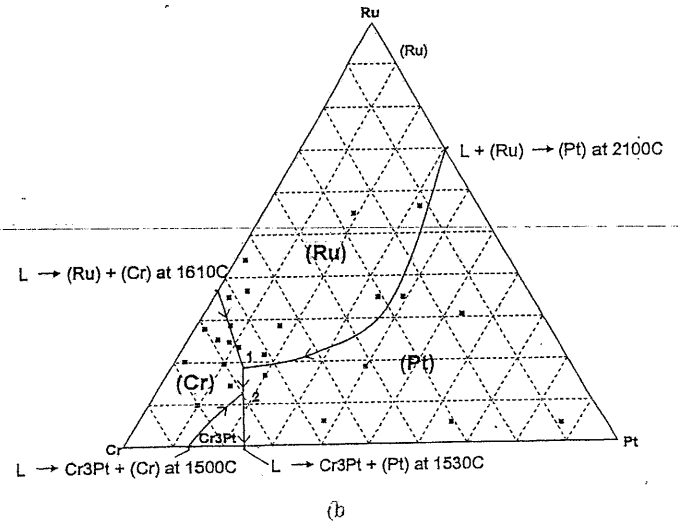


(b)

Figure 5. Comparison of Cr-Ru phase diagrams: a) Calculated by Glatzel and Prins[28]; b) Experimental from Massalski[20]



(a)

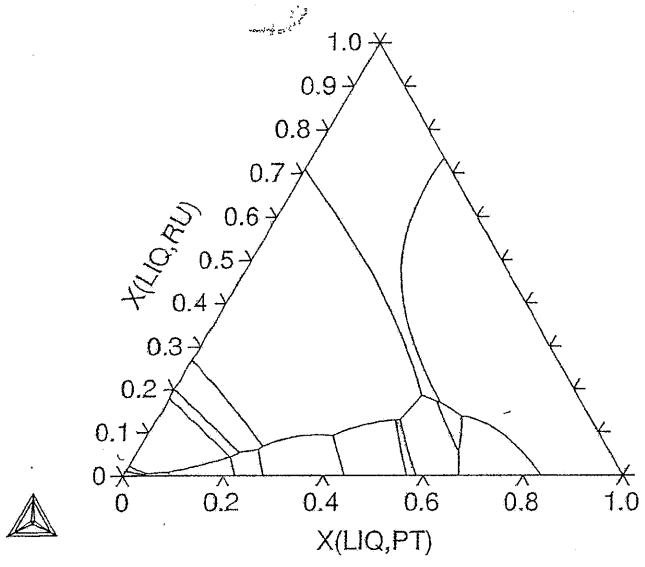


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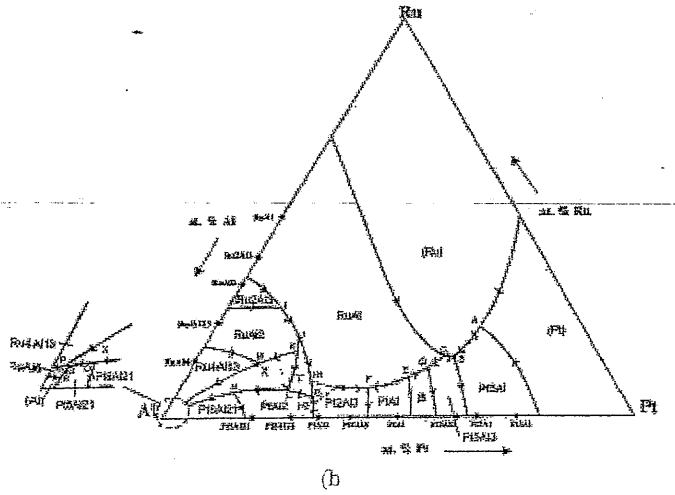
Figure 6. Comparison of liquidus surfaces of the Pt-Cr-Ru system: a) Calculated[40,41]; b) Experimental[22,41]

then Ni_3Al, which can be viewed as an ordered fcc phase, should be included as the fcc phase. On the other hand, another school of thought stipulates that, since both solidify separately, they should be modelled separately. The second school of thought would allow for Pt_3Cr and PtCr to be modelled as part of (Pt), since they form by ordering within the (Pt) phase field at lower temperatures. However, this could then cause problems in that Pt_3Al would not be incorporated in the fcc model, whereas Pt_3Cr would be. However, given that phases should be modelled the same way only if they are likely to be contiguous, this would not be a problem unless Pt_3Al is likely to be contiguous with Pt_3Cr. At the moment, this is not likely. A similar argument can be made for Pt_3Al, which just like Ni_3Al, solidifies as a separate phase from (Pt), and is not formed within.

Another source of contention is that in the current model, many parameters are needed to describe the phase. For the Ni-Al system, it could be argued that there are many data and the large number of parameters is justified. However, for Pt-Al, not only are there fewer data points, but there is also much greater uncertainty in the binary phase diagram itself regarding the reaction temperatures involving Pt_3Al and even the type of ordering. Thus, a much simpler model is prescribed for the Pt_3Al phase, both because of a dearth of data (as compared to Ni_3Al), and also because the Pt_3Al and (Pt) phases solidify separately. All the information regarding ordering needs to be gathered before any incorporation into modelling is attempted. However, it must be noted that in the Dupin database[44], the Ni_3Al phase is modelled as ordered fcc, even though it solidifies separately. The latest database from Dupin[44] was used to draw the Ni-Al phase diagram, and the γ / γ' boundary did not agree well with the experimental phase diagram, so it is questionable whether the complex modelling is really worthwhile.



(a)



(b)

Figure 7. Comparison of Pt-Al-Ru liquidus surface projections: a) Calculated by Prins *et al.*[43]; b) Experimental by Prins *et al.*[43]

In general, it is best to have the simplest models possible, because then fitting is easier and probably more meaningful. This is especially so when the data are limited. There are commercial databases available with very simple modelling, and these are very useful. One example of this is the lead-free solders database, which comprises the Ag-Cu-Sn-Ni-Au-Pd database, which was derived by modelling ternary Ag-Cu-Si, then adding Ni, Au and Pd. Here, the line compounds are used for many of the intermetallic compounds, and ordering is not considered because it is not worth the effort for the application required. Thus, the question could be asked whether the current database should be concerned with ordering. The answer could be positive, of course, because the ordered Pt_3Al phase is the basis of the alloys. However, if there are few data available, then they will be difficult to order meaningfully in any case. It would be valid to model very simply, then extend the database subsequently if there is sufficient need, and the data become available.

The sections below describe how the work was done. Most of the problems arise from lack of data, especially thermodynamic values. The computer programmes used were Winphad and Pandat, mainly because they are so much easier to use than Thermo-Calc™.

Pt-Cr

The first Pt-Cr assessment done within this work[28] built on the original assessment of Oikawa *et al.*[38], and incorporated the Compound Energy Formalism (CEF) model to the fcc phases, (Pt), Pt_3Cr and PtCr to give a worse fit[28] to the currently accepted phase diagram than the work of Oikawa *et al.*[38], and was criticised at the 2004 CALPHAD conference[40]. Part of the problem was identified as the many parameters being fitted by very few data points. In fact, in the *.pop file there were five data points for many more parameters!

A new approach was initiated. The phase diagram of Oikawa *et al.*[38] is to be recreated, and this assessment changed only when there are good experimental reasons for doing so. Until experimental results show otherwise, the assessment of Oikawa *et al.*[38] will be used, extrapolated into the ternary, and will then be re-optimized with Mintek's experimental values from the Pt-Cr-Ru system. The assessment of Oikawa *et al.*[38] is shown in Figure 4.

Pt-Ru

It was initially thought that the Spencer database[4] version of Pt-Ru would be the same as the SGTE database. However, this was not so, and the phase diagram from Spencer is a eutectic, with a maximum in (Pt) and ~10°C between the maximum and the eutectic temperature, whereas that from

SGTE is peritectic, which is consistent with available literature. Experimental work at Mintek also showed that the reaction is peritectic in nature.

When the phase diagram was initially calculated, at low temperatures the Pt solubility (i.e. the extent of the (Pt) phase field) suddenly decreased. This looked unrealistic, and could be attributed to a lack of data at low temperatures. The free energy curves were plotted, and the curve for Ru was very unusual, showing a distinct slope rather than a parabola.

The first attempt at improving the parameters through optimizing was to try and destabilise the fcc (Pt) phase by making the enthalpy interaction parameter less negative. This reduced the temperature difference between the fcc maximum and the eutectic temperature but also added a miscibility gap in fcc, which has not been reported. Next, the temperature-dependent term (entropy) was made less negative (-1.5). Eventually, this gave a peritectic reaction at 2 134°C (compared with Massalski's temperature of 2 130°C[20] which was obtained from Hutchinson[45] at 2 126°C using the experimental data). However, there was also a small miscibility gap. The two-phase regions were too Pt-rich, and the free energy curves were drawn in an attempt to ascertain why, because the phase diagram depends on the shape of these curves. The Ru curve was most likely to cause this problem, but it has to be remembered that there are few data. Part of the problem was deemed to be the unusual Ru energy curve. However, as this originated from the Ru unary data, and is set across the entire database, it would be unwise to change it because it represents a best fit value for many systems. One solution would be to add an interaction parameter, but it must be remembered that there are too few data available.

Since the solid data were reasonable, the problem seemed to be with the liquid data, so optimization was undertaken using L + hcp tie-line data extrapolated from the phase diagram[45]. This gave coefficients that were too large, although a peritectic reaction was obtained. However, since the liquidus composition was very close to the fcc values, some L + fcc tie lines (again, extrapolated from the phase diagram[45]) were input for optimization. This attempt was reasonable. The liquid free energy curve was sensible, and there is obviously a change in c_p at ~600°C. The phase diagram is shown in Figure 8. Additionally, to confirm the liquidus temperature, it was decided to run an experimental sample at ~15 at.% Ru in the DTA. The calculated peritectic temperature is 1 667°C, which should have been in the range of a 1 750°C rod. However, the DTA became unavailable.

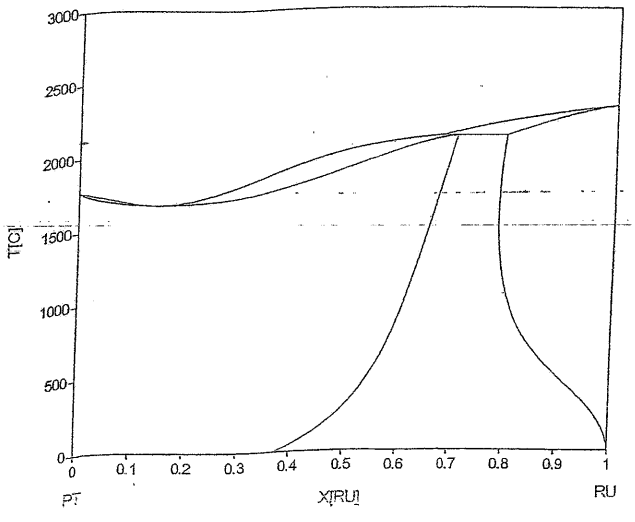


Figure 8. Best calculated Pt-Ru phase diagram to date

Cr-Ru

This system contains two intermetallic compounds: Cr_2Ru (sigma) and Cr_3Ru. The accepted models have three sublattices, so this format would be followed for the Cr-Ru system. However, especially given such limited data, it would be difficult to have mixing on all three sublattices, with many end-members needed, so it was decided that Cr only would be on one sublattice, and the remaining two would have mixing. (This is normal practice.) The current model of choice for sigma is 10:16:4 (the previous model was 8:18:4), which was in the Glatzel assessment[28], although with mixing on all three sublattices. Elements are usually mixed on many sublattices only where there is a very wide range of phase stability. In this case, there is a narrow phase stability range, so the mixing needs to be reduced.

The approach used was to build up the system with the most simple phase diagram descriptions possible: thus Cr_2Ru (sigma) and Cr_3Ru would be line compounds. The Ru and Cr unary data were derived from Kaufman[46].

The first stage was to use ideal solid solutions for the L, bcc and hcp phases: elemental data only. A eutectic was produced, but it was too near Cr. Moving away from the ideal solid solution, an L_0 enthalpy coefficient was input and optimized, using the 'real' eutectic at 1 610°C as a datum point, which improved the phase diagram. Data for tie-lines between the terminal solid solution were obtained from the best experimental diagram[20] and input for optimization. The intermetallic compounds were ignored. Then sigma formation and decomposition temperatures were added, and a value for (Cr) was invented, since Cr_3Ru was in the way.

It was noticed that the reaction temperatures for Cr_2Ru (sigma) and Cr_3Ru were suspiciously convenient: ~750, ~800 and ~1 000°C. However, with no other data available, these had to be used. It was essential that DTA was undertaken on two samples to establish these reaction temperatures. This was tried[47], but the results were inconclusive because the Ru and Cr atoms are very slow to diffuse (being large and having high melting points), and the DTA scan rate needs to be extremely slow to allow for equilibrium. Further attempts to equilibriate samples with Cr failed because the samples oxidized. The enthalpy term only for L_0 was optimized for the liquid, bcc and fcc phases, with reasonable results. Next, some tie-lines were used from the best experimental phase diagram and these were used to optimize the L_0 entropy and L_1 enthalpy, but the results were not good. In order to try to improve these results, only the L_0 enthalpy and entropy were optimized, and the results were better. Next, the sigma phase was added, together with data on the formation and dissolution, but the sigma phase did not appear on the phase diagram. The free energy curves were checked, and although sigma was present (with a small range because it was made stoichiometric), it was not stable. Only the enthalpy term was used and optimized, resulting in the phase being stable at too low temperatures. The enthalpy was consistent with the Gibbs free energy at that temperature. A slightly different approach for sigma was used: inputting and

optimising enthalpy and entropy for L_0 . The phase diagram appeared good, but it must be remembered that the values are not representative without experimental thermodynamic results.

The sigma was held constant and Cr_3Ru was added, and the L_0 enthalpy term only was input and optimized. The Cr_3Ru phase was stable below the lowest stable temperature (just as sigma was initially). An entropy term was added, and both the enthalpy and entropy terms were optimized. The phase was still stable below its temperature range, but it was now stable just below the bcc solidus, although in the right temperature range.

The next combination was to allow both the enthalpy and the entropy of Cr_2Ru but only the entropy for Cr_3Ru to vary. This gave a phase diagram which agreed with the input data, except for the decomposition of Cr_3Ru. The terminal solid solutions (bcc and hcp) were not stable enough at low temperatures and ran almost parallel to the vertical axes. Everything was now optimized, keeping all the relevant data points, and a good fit was obtained. This optimization was repeated, and became even better (the parameters were very similar to the very best subsequently obtained). The parameters for liquid, bcc and hcp were sensible, so these were fixed, and the intermetallic phase compositions were optimised. The new values were reasonable, although there was a positive heat of formation, but this could still give a compound that was stable at low temperature. The next stage was to optimize everything for the compounds, and the phase diagram gave a very good fit, as shown in Figure 9, compared with the experimental diagram shown in Figure 5.

Pt-Cr-Ru

In theory, once the binary systems were finished, the database files should have been copied into a single file, and the ternary database would be complete. However, it must be remembered that Cr_3Ru and Cr_3Pt have the same A15 structure and so these should be modelled the same, in case the phase is actually contiguous across the ternary. Currently, Cr_3Ru is a stoichiometric line compound, whereas Cr_3Pt has two sublattices, and both elements are mixed on both.

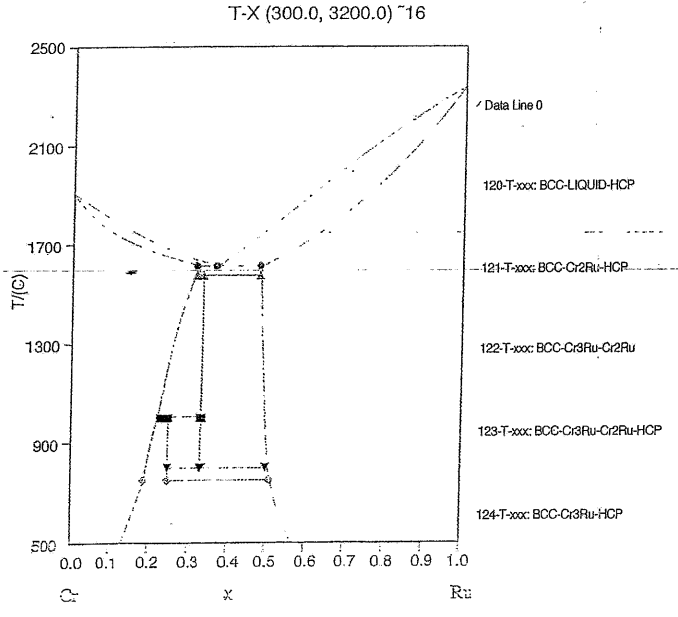


Figure 9. Best calculated Cr-Ru phase diagram to date

The experimental results of the A15 Cr_3Ru and Cr_3Pt phases are not conclusive in showing whether the phases are contiguous, despite two more samples of intermediate compositions between Cr_3Ru and Cr_3Pt being made. These samples are currently being annealed at ~850°C, because if the phases are contiguous, they should meet at this temperature for the sample compositions chosen. Depending on how the phases extend into the ternary, the sublattice on which substitution is occurring can be determined. For Cr_3Ru, if Ru is constant, then Pt substitutes for Cr; and for Cr_3Pt, if Cr is constant, Ru substitutes for Pt. However, it must be remembered that the original samples were not in equilibrium, and the latest samples were annealed for longer, to promote equilibrium. It should be noted that Waterstrat's Cr_3Pt phase[48] was more narrow (almost stoichiometric) and did not decompose at lower temperature (which is what was calculated at one stage in the present work). A likely model for this case[48] would be Cr on one sublattice and Pt + Cr on the other, but this depends on the atomic sizes. The atom sizes can be measured in different ways (to give different answers) and the most appropriate measurement should be used for how the atom will be bonded. The covalent radii show that Pt and Ru are similar, and this being so, they could sit on the same sublattice. However, it is recommended that other A15 phases are researched to see how their modelling is undertaken, especially for the composition ranges (i.e. the spread on both sides from x = 0.25). For the representation of Cr_3Pt within the ternary (and higher order phase diagrams), the model would be much simpler (and have fewer end members) if the lattices could be (Cr, Cr) (Cr, Pt, Ru).

To model the ternary system, the three binary phase diagrams were added in own database. An interaction parameter was found for hcp PtCr, and the effect of this needs to be re-checked in the boundaries. Also, the extent of coring has to be established, or interpreted, in order to add interaction parameters. The best way to check the 'full' database is to recalculate the binary phase diagrams from it, which has been successfully accomplished. In the ternary database, a ternary interaction parameter was added to increase the phase extensions into the ternary. Three had to be added to maintain the symmetry; all were –5 000, but more work was needed on these, and is under way[49]. The projected liquidus surface is shown in Figure 10. It is an improvement on the assessment by Glatzel *et al.*[28] in that it does not show primary sigma, but the invariant reactions are still incorrect, because the liquidus surfaces for (Ru) and Cr_3Pt abut, whereas those for (Cr) and (Pt) should, because of the (Pt) + (Cr) eutectic observed in the ternary samples. However, the junction between the wrong surfaces of primary solidification is smaller that was calculated previously[28], and agrees more with the experimental results. Obviously, there is more work needed on the system with interaction parameters and phase boundaries.

The isothermal section at 1 000°C is shown in Figure 11. It shows some solubility of Cr and Pt in (Ru), (Pt) and (Cr), but much less than in the experimental isothermal section. This shows that more work is needed on the interaction parameters for the (Pt) and (Cr) phases. There is a miscibility gap in (Pt), which is not seen experimentally, but is probably related to the limited extent of the calculated phase, or possibly ordering. More work is also needed here. Both intermetallic phases are present with no extension into the ternary because they were input as line

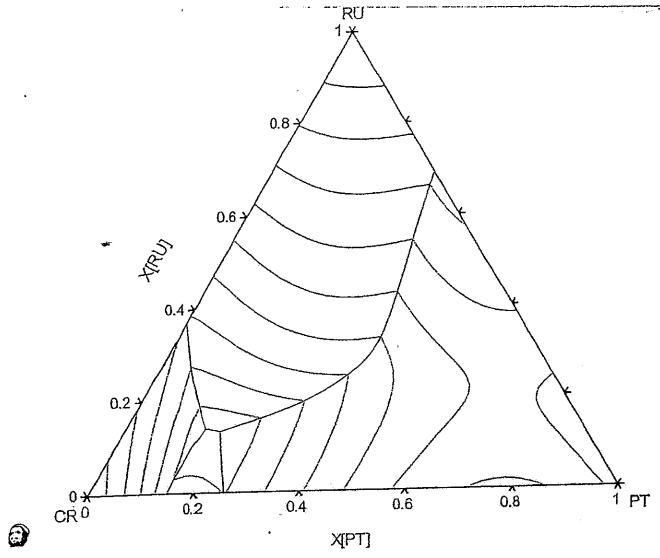
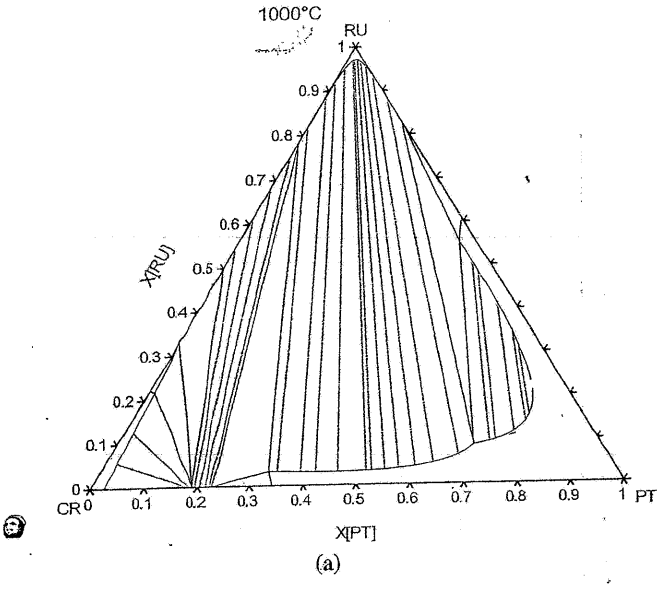
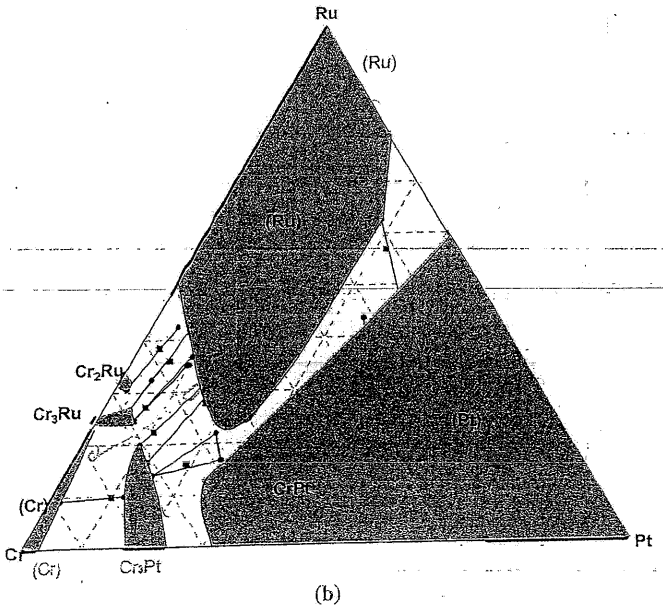


Figure 10. Best calculated liquidus surface to date for the Pt-Cr-Ru system



(a)



(b)

Figure 11. 1000°C isothermal section for the Pt-Cr-Ru system: a Calculated; b) Experimental from Süss *et al.*[13].

compounds.

The isothermal section at 600°C was similar to that in Figure 11 in that it showed a miscibility cap in (Pt), and the solubilities are much less in (Pt) and (Ru) than was observed experimentally[13]. The two intermetallic phases are absent, which is correct in the current understanding of the diagram (which might change with more experimental work).

Overall, the results for the ternary are very good, considering that they are just an extrapolation of the binaries. Once again they demonstrate the validity of the whole CALPHAD technique in calculating higher-order systems from lower-order systems. However, the match between the calculated and experimental diagrams could be improved and more work is necessary. Some of it is already under way. This work includes:

- obtaining an *ab initio* enthalpy of formation for Cr_2Ru, although, neither intermetallic phase is stable at 0K, which might pose a problem
- preparing a Cr_3Ru sample for calorimetry by mixing powders and heating to 980°C for 20 min, quenching and examining by SEM
- undertaking slow scan DTA for temperatures of formation and dissolution for the intermetallic compounds, especially in the Cr-Ru system, and for the reactions in the Cr-Pt system
- adding and optimizing interaction parameters for the (Pt) and (Ru) phases especially ((Cr) has a better fit)
- undertaking a DTA measurement of Pt_{85}:Ru_{15} for the liquidus temperature, to ascertain the possible minimum
- modelling the Cr_3Ru and Cr_3Pt phases the same way because they have the same structures and might possibly be contiguous
- verifying experimentally whether Cr_3Ru and Cr_3Pt are contiguous to see how they extend in the ternary, which will determine the mixing allowed on the individual sublattices, if they are contiguous, in which case can attempt will be made to model Pt-Ru on one sublattice only and Cr on the other sublattice, to simplify and reduce the number of end-members, i.e. coefficients
- using the sigma model for Cr_2Ru.

Although there is still much work to be done, some of which is experimental, once the Pt-Cr and Cr-Ru binary phase diagrams are confirmed more rigorously, the calculated phase diagrams can be worked on with more confidence. Currently, it would be a waste of time to optimize the database for the intermetallic phases because there are too many unknowns. This experimental work is under way. Two of the challenges are that high temperature DTA is needed for Pt-Cr, and the Cr-Ru samples are very difficult to homogenise. The probable reason that the Cr-Ru phase diagram is not confirmed must be that other workers have also experienced the same problems.

Conclusions

The Pt-Al-Cr-Ru database is progressing well, and there has been good agreement for the Pt-Cr-Ru and Pt-Al-Cr phase diagrams when they were extrapolated from the binaries, which was encouraging and confirmed that the higher order systems could be calculated from the binary systems with confidence. However, more work needs to be done on the interaction parameters of the (Pt) and (Ru) phases, as these do not extend sufficiently into the ternary, compared to the experimental results for the Pt-Cr-Ru system. The models

of the Pt_3Al and Pt_2Al phases need to be re-assessed, and if good *ab initio* data became available, it might be worthwhile to model these phases in a more complex manner. Currently, the best results have been obtained using very simple models.

There have been some problems in the binary systems, notably Pt-Al because of the modelling and the uncertainty of the Pt_3Al phase types, and Cr-Ru, which is very difficult experimentally because the diffusion rates of Cr and Ru are so slow. Annealing is also problematic because alloys with substantial Cr oxidise very easily.

There have been some hard lessons learned in the creation of the database, and these include the fact that any binary system which has uncertainties is experimentally difficult for a variety of reasons, and the most accurate data belong to systems that are commercially important. Good models can be very simple, and more complex models need many data. Many of the problems were due to insufficient good data, but work is being done within the programme to generate reliable phase data to build the thermodynamic database and hence to aid the application of high temperature alloys.

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MICROSTRUCTURAL EVOLUTION IN THE Pt-Al-Cr SYSTEM

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Pt-rich alloys in the Pt-Al-Cr-Ru system are being developed as analogues to Ni-based superalloys for high temperature applications[1], and consequently the Pt-Al-Cr system is of interest. A wide range of ternary alloy samples was manufactured by button arc-melting and subsequently heat treated at 600°C and 1000°C respectively for 1000 hours. Samples were polished using an oxide polishing (OP-S) system and characterised using a JEOL JSM-840 SEM with a Vantage EDS system, and a Siemens D500 diffractometer with Mo Kα radiation for XRD analysis.

As-cast alloy Pt_{13}:Al_4:Cr_{83} comprised three phases: dark dendrites with a suggestion of a lighter phase inside; a medium (grey) interdendritic phase; and a small white phase (Fig. 1). The white phase was too small for accurate analysis. XRD analyses confirmed the presence of (Cr) and ~CrPt. There were many unidentified XRD peaks not matched by any XRD spectra for phases in the Pt-Al, Pt-Cr and Al-Cr binaries as listed by the JCPDS database[2] or modelled using the *Crystallographica* software (available from Oxford Cryosystems) and data from Pearson's Handbook[3]. Similar peaks were found in other alloys e.g. alloy Pt_{28}:Al_{12}:Cr_{60}. This new ternary phase was designated ~$Pt_{50}Al_{32}Cr_{18}$. Taking into account the confirmed phase identities and their compositions as plotted on a ternary diagram, it was concluded that the microstructure formed by:

$L \rightarrow$ (Cr)

$L \rightarrow$ (Pt) + (Cr) + ~$Pt_{50}Al_{32}Cr_{18}$

(Pt) $\rightarrow$ ~Pt_3Cr $\rightarrow$ ~CrPt (ordering).

After annealing at 600°C, the alloy (with a slight compositional change to Pt_{15}:Al_5:Cr_{80}) was generally similar in appearance to that of its as-cast condition, except that grey Widmanstätten needles were now clearly observed inside the dark dendrites (Fig. 2). The white phase and the grey needles were too small for accurate analysis. From a ternary plot of compositions and likely extrapolation of compositions where the measured values were probably affected by the surrounding phase, the white phase was probably ternary ~$Pt_{50}Al_{32}Cr_{18}$, the dark phase (Cr), and the grey phase and needles ~Cr_3Pt (similar to samples in the Pt-Cr-Ru system[4]). Because the sample broke during removal from the mount, no XRD analyses could be performed.

After annealing at 1000°C, the alloy (suffering a slight compositional change to Pt_{14}:Al_3:Cr_{83}) showed a resemblance to its as-cast state. Higher magnification revealed that the dark dendrites were in fact a two-phase mixture of black and grey (Fig. 3). This was similar to the observation in the 600°C condition, except that the grey phase appeared rounded rather than needle-like. From a ternary plot of compositions, the black phase was (Cr), the grey phase ~Cr_3Pt and the white phase ~PtAl. Apart from (Cr), this was different to the as-cast condition. This was confirmed by XRD.

The information gleaned from samples like this was used for the derivation of solidification and liquidus projections and isothermal sections at 600°C and 1000°C for the Pt-Al-Cr system. The diagrams appear complete and are self-consistent.

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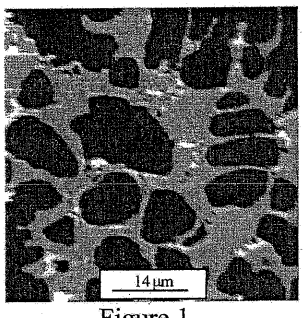


Figure 1.

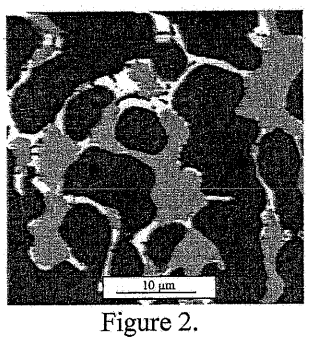


Figure 2.

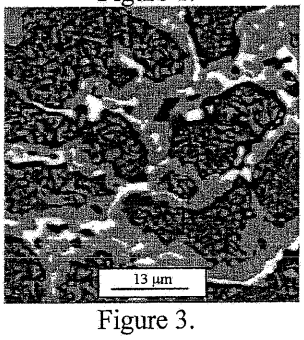


Figure 3.

Figure 1. BSE-SEM image of Pt_{13}:Al_4:Cr_{83} in the as-cast condition: (Cr) black; ~CrPt grey; ~$Pt_{50}Al_{32}Cr_{18}$ white.

Figure 2. BSE-SEM image of Pt_{15}:Al_5:Cr_{80} after annealing at 600°C: (Cr) black; ~Cr_3Pt grey; ~$Pt_{50}Al_{32}Cr_{18}$ white.

Figure 3. BSE-SEM image of Pt_{14}:Al_3:Cr_{83} after annealing at 1000°C: (Cr) black; ~Cr_3Pt grey; ~PtAl white.

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Development of a database for the prediction of phases in Pt-based Superalloys: Cr-Pt-Ru

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Abstract: Work has been ongoing in building a thermodynamic database for the prediction of phase equilibria in Pt-based superalloys. The alloys are being developed for high temperature applications in aggressive environments. The database will aid the design of alloys by enabling the calculation of the composition and proportions of phases present in alloys of different compositions. In order to extend this database, a preliminary assessment of the Cr-Pt-Ru system has been undertaken, using a combination of Pandat and *MTDATA* software. As a first step, it was necessary to provide thermodynamic models for the three associated binary systems. Owing to a lack of thermodynamic information for these systems, the binary assessments were based on phase diagrams available in the literature. Using recent experimental phase equilibria data for the ternary system, a preliminary assessment of the Cr-Pt-Ru system has been produced. In this preliminary assessment, simplified models were employed for the $L1_2$ and sigma phases with a view to extending the descriptions as new experimental information becomes available.

Key words: Cr-Pt-Rh; thermodynamics; assessment; phase diagram

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1. Introduction

Alloys based on the platinum group metals are becoming increasingly attractive for high-temperature applications, for example, as possible alternatives to nickel-based superalloys used in aerospace applications [1]. At appropriate compositions, alloys based on the Pt-Al binary system exhibit γ/γ' microstructures analogous to those of the Ni-Al system where the ordered Ni_3Al $L1_2$ intermetallic phase (γ') is precipitated in a disordered fcc matrix (γ). It is the coherent γ' phase that is the primary strengthening phase in the alloy. A close match in lattice parameter between the precipitate and the matrix (<1%) allows the γ' to precipitate homogeneously throughout the matrix. Typically, aero engines utilising nickel-based superalloys can maintain their strength at operating temperatures of up to around 1000°C, but they are susceptible to corrosion. On the other hand, using alloys based on platinum would enable a significant increase in operating temperatures (to around 1300°C) owing to their higher melting point and improved corrosion resistance over nickel-based materials. This would lead to increased efficiency, lower fuel costs and reduced emissions.

Alloy development can be expensive both in time and financially. The costs can be significantly reduced by employing computational thermodynamics where by using appropriate thermodynamic databases, multiphase multicomponent equilibria can be predicted relatively easily [2]. The present work describes a contribution to a thermodynamic database

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for development of Pt-based superalloys through a modelling of the Cr-Pt-Ru system.

2. Methodology

The basic methodology of thermodynamic database design and construction has been described in detail many times, for example in Ref. [2]. The basis for the construction of the database is the provision of reliable thermodynamic models for the unary and binary systems within the database. This relies on critical assessment of the experimental information available for each system, and by the application of appropriate models for each of the phases involved, model parameters are derived which allow the phase equilibria and thermodynamic properties of the systems to be reproduced through calculation to a reasonable degree of accuracy. It is often necessary to critically assess the higher order systems as well, typically the ternary systems and on occasion, quaternary systems should such information be available.

Unary Gibbs energy data for the elements used in the present work are taken from the SGTE unary database v4.4. These data form the basis of the critical assessment of the constituent binary systems, as for the ternary Cr-Pt-Ru system.

3. Binary systems

3.1. Cr-Pt

Of the three binary systems comprising the Cr-Pt-Ru ternary system, the Cr-Pt is the best known. Nevertheless, little experimental study of this system has taken place. The phase diagram given by Ref. [3] is based primarily on experimental investigations by Refs. [4] and [5]. The system comprises terminal solid solutions based on the components and the Cr_3Pt intermediate phase, which has the A15 crystallographic structure and is shown to melt congruently. The A15 phase, however, does not lie at its stoichiometric composition, having a maximum Pt-content of 23 at.% at 970°C. The wide (Pt) terminal solid solution exhibits both $L1_2$ ($CrPt_3$) and $L1_0$ (CrPt) ordering. Ref. [3] indicates two eutectic reactions; L ⇌ (Cr) + Cr_3Pt (at 1500°C) and L ⇌ Cr_3Pt + (Pt) (at 1530°C). A maximum in the liquidus and the fcc solidus appears at around 1785°C and ~80 at.% Pt. The phase diagram is given in Fig. 1. A thermodynamic assessment of the Cr-Pt system has been conducted [6]. However, they neglected to model the ordering of the (Pt) solid solution giving the $L1_2$ and $L1_0$ structures. Also, in their assessed phase diagram, the Cr-rich eutectic has a higher temperature than the Pt-rich. This is contrary to Ref. [3], although there is recent experimental evidence to support this. Solidification microstructures of alloys in the Cr-Pt-Ru [7], Al-Cr-Pt [8], and Cr-Ni-Pt [9] ternary systems show that the temperature order of the eutectics in the Cr-Pt system is more likely to be as given in Ref. [6] than that in Ref. [3]. The calculated phase diagram given by Ref. [6] is given in Fig. 2. Crystallographic data for the phases are given in Table 1 and invariant temperatures are given in Table 2.

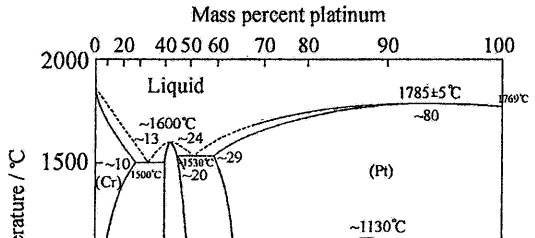


Fig. 1. Cr-Pt phase diagram [3].

3.2. Cr-Ru

The Cr-Ru system is reasonably well established, although there is some speculation regarding the intermediate phases. Fig. 3 shows the assessed phase diagram [3]. This is based on phase diagram studies conducted by Refs. [10-15]. The system comprises large terminal solid solutions of chromium and ruthenium ((Cr) & (Ru)) and associated with them is a eutectic reaction at 1610°C. Two intermediate phases are stable in the system. A sigma phase is stable over the temperature range from approximately 800°C to just below the eutectic temperature,

at 1580°C. The homogeneity range of the sigma phase field is approximately 4 at.%, centred at a Ru composition of 33 at.%. The stability range of the Cr_3Ru phase is less certain. It has a narrow homogeneity range, appearing in the phase diagram as a line compound. The phase is drawn on the phase diagram of Ref. [3], at a composition of ~32 at.% Ru, in agreement with Ref. [15]. However, it should lie at a composition of 25 at.% Ru to be consistent with the text of the article, and the fact that this region of the phase diagram is constructed with dashed lines would suggest that this part of the diagram is still uncertain. Interestingly, its crystal structure is the same as the Cr_3Pt phase, A15, suggesting the possibility of mutual solubility in the ternary Cr-Pt-Ru system. It exists over a narrow temperature range: 750-1000°C, but this is by no means certain as indicated in the published phase diagram by a dashed line. Crystallographic data and invariant temperatures are given in Tables 1 and 2, respectively.

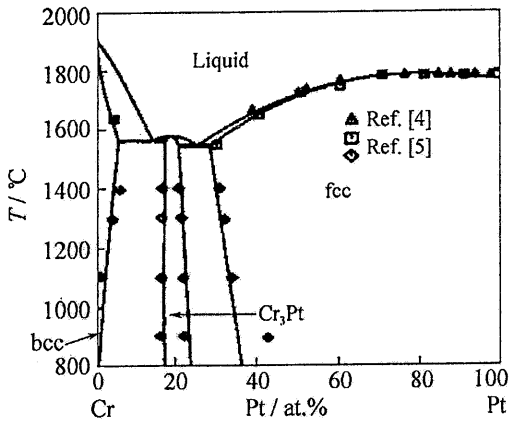


Fig. 2. Assessed Cr-Pt phase diagram [6].

Table 1. Invariant equilibria in the Cr-Pt, Cr-Ru, and Pt-Ru binary systems

System	Reaction	Composition at.% of the 2nd element			Temperature / °C	Reaction type	Reference
Cr-Pt	L ⇌ Cr		0		1863	Melting	[3]
	L ⇌ Cr_3Pt		~18			Congruent	[3]
			18.5		1582		[6]
	L ⇌ Cr_3Pt + (Cr)	~13	~17	~13	1500	Eutectic	[5]
		14	17	6	1565	Eutectic	[6]
	L ⇌ Cr_3Pt + (Pt)	~24	~20	~29	1530	Eutectic	[5]
		25	20.5	28	1548	Eutectic	[6]
	(Pt) ⇌ Cr_3Pt		~67		~1130	Congruent	[3]
	(Pt) ⇌ Cr_3Pt + $CrPt_3$	~34	~23	-	970	Eutectoid	[3]
	L ⇌ (Pt)		~80		1785	Congruent	[3]
Cr-Ru	L ⇌ (Cr) + (Ru)	~37	~32	~48	1610	Eutectic	[3]
		37.2	32.9	48.5	1611	Eutectic	This work
	(Cr) + (Ru) ⇌ Cr_2Ru	~32	~48	~33	1580	Peritectoid	[3]
		32.4	48.4	33.3	1578	Peritectoid	This work
	(Cr) + Cr_2Ru ⇌ Cr_3Ru	~23	~33	~32*	~1000	Peritectoid	[3]
		22.1	33.3	26	985.9	Peritectoid	This work
	Cr_2Ru ⇌ Cr_3Ru + (Ru)	~33	~32*	~50	~800	Eutectoid	[3]
		33.3	25.7	50.6	803.7	Eutectoid	This work
	Cr_3Ru ⇌ (Cr) + (Ru)	~32*	~18	~51	~750	Eutectoid	[3]
		25.6	19	51.2	751	Eutectoid	This work
Pt-Ru	L ⇌ (Pt) + (Ru)	73.5	72.6	80.9	2127.6	Eutectic	This work
	L⇌(Pt)		~69.5		~2129.4	Congruent	This work

Note: * Incorrectly marked on the diagram—see above.

Table 2. Crystallographic data of the phases [3]

Phase	Composition	Pearson symbol	Space group	Strukturbericht designation	Prototype
(Cr) – bcc	0-10 at.% Pt 0-32 at.% Ru	*cI*2	*Im*-3*m*	A2	W
Cr_3Pt	17-~23 at.% Pt	*cP*8	*Pm*-3*n*	A15	Cr_3Si
CrPt	~48-~52 at.% Pt	*tP*2	*P*4/*mmm*	$L1_0$	AuCu
$CrPt_3$	~34-85 at.% Pt	*cP*4	*Pm*-3*m*	$L1_2$	$AuCu_3$
(Pt) – fcc	0-~71 at.% Cr 0-~70 at.% Ru	*cF*4	*Fm*-3*m*	A1	Cu
Cr_3Ru	~25 at.% Ru	*cP*8	*Pm*-3*n*	A15	Cr_3Si
Cr_2Ru	32-36 at.% Ru	*tP*30	$P4_2/mnm$	$D8_b$	σCrFe
(Ru) – hcp	0-52 at.% Cr	*hP*2	$P6_3/mmc$	A3	Mg

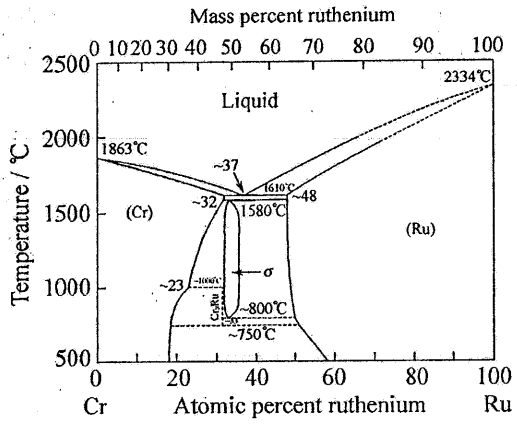


Fig. 3. Cr-Ru phase diagram [3].

3.3. Pt-Ru

Little experimental data exist for this system. The assessed diagram from Ref. [3] is given in Fig. 4. The phase diagram comprises two terminal solid solutions, (Pt) and (Ru), associated with a peritectic reaction, although this is uncertain as indicated by the dashed lines in the phase diagram.

4. Cr-Pt-Ru ternary phase diagram

Only two investigations of the ternary system have been conducted. Zhao [16] presents a comprehensive isothermal section for 1200°C. Diffusion multiples were prepared and underwent a HIPping treatment at 1200°C for 40 h. Studies incorporating EPMA and EBSD analysis were employed to locate the fcc, hcp, bcc, and A15 phase boundaries. The results indicate quite a large extension of the Cr_3Pt phase into the ternary system at this temperature. It does not meet the Cr-Ru binary, of course, as the A15 phase is not stable in the Cr-Ru system at this temperature. Interestingly, the direction of this extension is towards compositions richer in Ru than the Cr_3Ru stoichiometry at the Cr-Ru binary edge which would tend to agree with the findings of Ref. [15]. The isothermal section given by Ref. [16] is reproduced in Fig. 5. Isothermal sections for 1000 and 600°C have been presented [17]. Phase boundaries were determined by annealing alloys of different compositions for 1000 h or 600 h before examination using SEM/EDX.

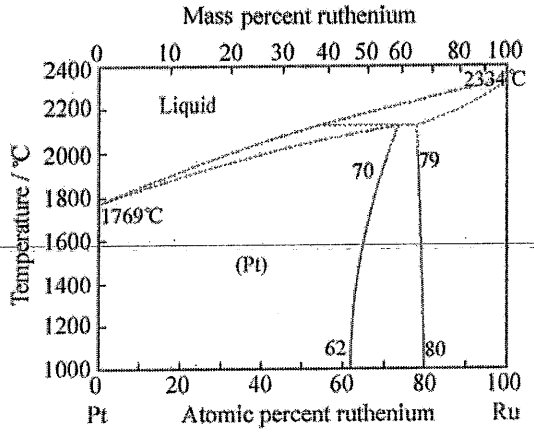


Fig. 4. Pt-Ru phase diagram [3]

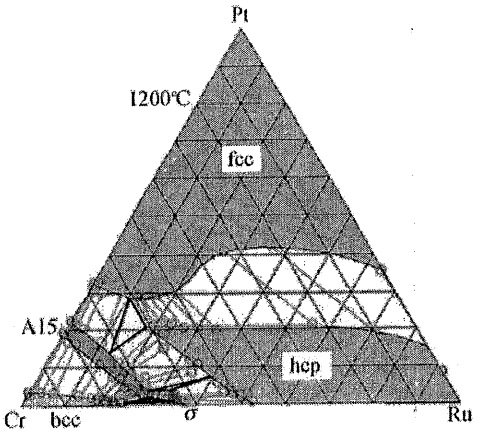


Fig. 5. Experimental isothermal section for 1200°C [16].

5. Optimisation

In the optimisation process, the parameters to the Gibbs energy expressions for each of the phases are adjusted in order that they can be used to calculate phase equilibria, which agree with the experimental information used. This is achieved by using appropriate software that performs a least squares analysis of the calculated and experimental data. The software then adjusts the parameters in order to minimise the sum of the squares of the errors between the calculated and experimental data. The software used in this work was WinPhad, Pandat [18] and *MTDATA* [19].

5.1. Choice of Models

The temperature dependence of the Gibbs energy was described by:

$$G(T) = A + BT + CT\ln T + \sum DT^n \qquad (1)$$

where *A-D* are adjustable parameters. The compositional dependence of a binary substitutional solution phase (for example, the liquid phase) ϕ, of components *i* and *j* is given by:

$$G_m^{\phi} = x_i G_i^{\Theta,\phi} + x_j G_j^{\Theta,\phi} + RT(x_i \ln x_i + x_j \ln x_j) + G_m^E \qquad (2)$$

where the G^{Θ} terms are the 'so-called' lattice stability terms and the G^E term is the excess Gibbs energy of mixing. The excess Gibbs energy is described by the 'Redlich-Kister' polynomial [20]:

$$G_m^E = x_i x_j \sum_{n=0} {}^nL(x_i - x_j)^n \qquad (3)$$

where ${}^nL$ are adjustable parameters. Extrapolation of the binary Gibbs energies into the ternary system was carried out using the method of Muggianu [21].

Owing to the general lack of experimental information available regarding the $L1_2$ and $L1_0$ phases in the ternary system, it was decided that the ordering would not be modelled on this occasion. This makes the modelling of the ternary system considerably easier and also means that the optimisation of the Cr-Pt system given by Ref. [6] could be used directly without any modification. Another simplification was introduced by treating the Cr_2Ru sigma phase as stoichiometric, as from the experimental information available, its extension into the ternary systems seems to be small. On the other hand, the Cr_3Ru A15 phase was treated in the same manner as the Cr_3Pt A15 phase to enable the phase to extend well across the ternary system from the Cr-Pt binary edge. The model used for this phase was the compound energy model incorporating two sublattices with components mixing on each sublattice. The compositional dependence in such a model is given by:

$$G_m = \sum_i \sum_j y_i^1 y_j^2 G_{ij}^{\Theta} + RT \sum_s a^s \sum_i y_i^s \ln y_i^s + G_m^E \qquad (4)$$

where *a* is the stoichiometry of each sublattice *s* and the *y* terms are site fractions. The G_{ij}^{Θ} terms are the Gibbs energies of formation of the 'virtual' compounds associated with the phase, where each sublattice is occupied completely by a single component. The excess Gibbs energy related to mixing on the different sublattices is given by:

$$G_m^E = \sum_{i_1} \sum_{i_2} \sum_j y_{i_1}^1 y_{i_2}^1 y_j^2 L_{i_1,i_2:j} + \sum_i \sum_{j_1} \sum_{j_2} y_i^1 y_{j_1}^2 y_{j_2}^2 L_{i:j_1,j_2} + \sum_{i_1} \sum_{i_2} \sum_{j_1} \sum_{j_2} y_{i_1}^1 y_{i_2}^1 y_{j_1}^2 y_{j_2}^2 L_{i_1,i_2:j_1,j_2} \qquad (5)$$

Details of the modelling used for each of the individual phases are given in Table 3.

Table 3. Models and optimised parameters

Component Unary Data

Cr

G(LIQUID,Cr;0) = 15483.015+146.059775*T-26.908*Tln(T)+1.89435E-3*T^2-1.47721E-6*T^3+139250/T+
237.615E-23*T^7
(298.15<T<2180K)
-16459.984+335.616316*T-50*Tln(T)
(2180<T<6000K)

G(BCC,Cr:Va;0) = -8856.94+157.48*T-26.908*Tln(T) +1.89435E-3*T^2 -1.47721E-6*T^3 +139250/T
(298.15<T<2180K)
-34869.344+344.18*T-50*Tln(T)-2885.26E29/T^9
(2180<T<6000K)
TC(BCC,Cr:Va;0) = -311.5, BMAGN(BCC_A2,CR:VA;0) = -0.008
(298.15<T<6000K)

G(FCC,Cr:Va;0) = -1572.94+157.643*T-26.908*Tln(T) +1.89435E-3*T^2-1.47721E-6*T^3 +139250/T
(298.15<T<2180K)
-27585.344+344.343*T-50*Tln(T)-2885.26E29/T^9
(2180<T<6000K)
TC(FCC,Cr:Va;0) = -1109, BMAGN(FCC_A1,CR:VA;0) -2.46,
(298.15<T<6000K)

G(HCP,Cr:Va;0) = -4418.94+157.48*T-26.908*Tln(T) +1.89435E-3*T^2-1.47721E-6*T^3 +139250/T
(298.15<T<2180K)
-30431.344+344.18*T-50*Tln(T)-2885.26E29/T^9
(2180<T<6000K)
TC(HCP,Cr:Va;0) = -1109, BMAGN(HCP_A3,CR:VA;0) = -2.46
(298.15<T<6000K)

Pt

G(LIQUID,Pt;0) = 12518.385+115.113092*T-24.5526*Tln(T) -2.48297E-3*T^2-0.020138E-6*T^3 +7974/T
(298.15<T<600K)
19023.491+32.94182*T-12.3403769*Tln(T)-11.551507E-3*T^2+0.931516E-6*T^3 -601426/T
(600<T<2041.5K)
1404.468+205.858962*T-36.5*Tln(T)
(2041.5<T<4000K)

G(BCC,Pt:Va;0) = 7404.369+121.988275*T-24.5526*Tln(T) -2.48297E-3*T^2 -0.020138E-6*T^3 +7974/T
(298.15<T<1300K)
5746.826+159.129615*T-30.2527*Tln(T)+2.321665E-3*T^2-0.656946E-6*T^3 -272106/T
(298.15<T<2041.5K)
-207048.216+1016.95892*T-136.192996*Tln(T)+20.454938E-3*T^2 -0.759259E-6*T^3+7153902/T
(2041.5<T<4000K)

G(FCC,Pt:Va;0) = -7595.631+124.388275*T-24.5526*Tln(T) -2.48297E-3*T^2-0.020138E-6*T^3 +7974/T
(298.15<T<1300K)
-9253.174+161.529615*T-30.2527*Tln(T)+2.321665E-3*T^2-0.656946E-6*T^3 -272106/T

(1300<K<2041.5K)
-222048.216+1019.35892**T*-136.192996**T*ln(*T*)+20.454938E-3**T*^{2} -0.759259E-6**T*^{3}+71539020/*T*
(2041.5<*T*<4000K)

G(HCP,Pt:Va;0) = -5095.631+124.488275**T*-24.5526**T*ln(*T*) -2.48297E-3**T*^{2}-0.020138E-6**T*^{3} +7974/*T*
(298.15<*T*<1300K)
-6753.174+161.629615**T*-30.2527**T*ln(*T*)+2.321665E-3**T*^{2}-0.656946E-6**T*^{3} -272106/*T*
(1300<*T*<2041.5K)
-219548.216+1019.45892**T*-136.192996**T*ln(*T*)+20.454938E-3**T*^{2} -0.759259E-6**T*^{3}+71539020/*T*
(2041.5<*T*<4000K)

Ru

G(LIQUID,Ru;0) = 19918.743+119.467485**T*-22.9143287**T*ln(*T*) -4.062566E-3**T*^{2}+0.17641E-6**T*^{3} +56377/*T*
(298.15<*T*<800K)
50827.232-179.818561**T*+19.539341**T*ln(*T*)-26.524167E-3**T*^{2}+1.667839E-6**T*^{3} -3861125/*T*
(800<*T*<2607K)
-17161.807+349.673561**T*-51.8816**T*ln(*T*)
(2607<*T*<4500)

G(BCC,Ru:Va;0) = 18938.127+121.666233**T* -22.9143287**T*ln(*T*)-4.062566E-3**T*^{2}+0.17641E-6**T*^{3}+56377/*T*
(298.15<*T*<1500K)
-32948.103+483.316214**T*-72.3241219**T*ln(*T*)+18.726245E-3**T*^{2}-1.952433E-6**T*^{3} +11063885/*T*
(1500<*T*<2607K)
-38562273+168604.317**T*-21329.705**T*ln(*T*)+5221.639E-3**T*^{2}-240.245985E-6**T*^{3} +130.829926E8/*T*
(2607<*T*<2740K)
-29268.304+358.282314**T*-51.8816**T*ln(*T*)
(2740<*T*<4500K)

G(FCC,Ru:Va;0) = 4938.127+125.466233**T* -22.9143287**T*ln(*T*)-4.062566E-3**T*^{2}+0.17641E-6**T*^{3} +56377/*T*
(298.15<*T*<1500K)
-46948.103+487.116214**T*-72.3241219**T*ln(*T*)+18.726245E-3**T*^{2}-1.952433E-6**T*^{3} +11063885/*T*
(1500<*T*<2607K)
-38576273+168608.117**T*-21329.705**T*ln(*T*)+5221.639E-3**T*^{2}-240.245985E-6**T*^{3} +130.829926E8/*T*
(2607<*T*<2740K)
-43268.304+362.082314**T*-51.8816**T*ln(*T*)
(2740<*T*<4500K)

G(HCP,Ru:Va;0) = -7561.873+127.866233**T* -22.9143287**T*ln(*T*)-4.062566E-3**T*^{2}+0.17641E-6**T*^{3} +56377/*T*
(298.15<*T*<1500K)
-59448.103+489.516214**T*-72.3241219**T*ln(*T*)+18.726245E-3**T*^{2}-1.952433E-6**T*^{3} +11063885/*T*
(1500<*T*<2607K)
-38588773+168610.517**T*-21329.705**T*ln(*T*)+5221.639E-3**T*^{2}-240.245985E-6**T*^{3} +130.829926E8/*T*
(2607<*T*<2740K)
-55768.304+364.482314**T*-51.8816**T*ln(*T*)
(2740<*T*<4500K)

(continued Table 3)

Phase	Constitution	Parameter	Value	Source
Liquid	(Cr,Pt,Ru)	${}^0L$(Cr,Pt)	−135800	[6]
		${}^1L$(Cr,Pt)	5500	[6]
		${}^0L$(Cr,Ru)	−17386.332	This work
		${}^0L$(Pt,Ru)	−28071.046 − 11.515654T	This work
		${}^1L$(Pt,Ru)	−11369.048	This work
bcc	(Cr,Pt,Ru):(Va)$_3$	${}^0L$(Cr,Pt)	−105000	[6]
		${}^0L$(Cr,Ru)	−22426.461 + 1.950073T	This work
		${}^1L$(Cr,Ru)	8866.523	This work
fcc	(Cr,Pt,Ru):(Va)	${}^0L$(Cr,Pt)	−146232.35	[6]
		${}^1L$(Cr,Pt)	3437.65	[6]
		${}^0L$(Cr,Ru)	1988.662 − 2.83672T	This work
		${}^1L$(Cr,Ru)	390.321	This work
		${}^0L$(Pt,Ru)	−67966.086 + 0.455942T	This work
		${}^1L$(Pt,Ru)	−13113.006 + 7.827195T	This work
hcp	(Cr,Pt,Ru):(Va)$_{0.5}$	${}^0L$(Cr,Pt)	−137981 − 0.058413T	[6]
		${}^1L$(Cr,Pt)	9551.99 − 0.001652T	[6]
		${}^0L$(Cr,Ru)	1988.662 − 2.83672T	This work
		${}^1L$(Cr,Ru)	390.321	This work
		${}^0L$(Pt,Ru)	−28869.113 − 7.889606T	This work
		${}^1L$(Pt,Ru)	−7333.888 + 0.682843T	This work
$A15$	(Cr,Pt,Ru)$_{0.75}$:(Cr,Pt,Ru)$_{0.25}$	G(A15,Cr:Cr)	15000 + G(bcc,Cr;0)	[6]
		G(A15,Pt:Pt)	10000 + G(fcc,Pt;0)	[6]
		G(A15,Ru:Ru)	25000 + G(hcp,Ru;0)	This work
		G(A15,Cr:Pt)	−28500 + 0.75G(bcc,Cr;0) + 0.25G(fcc,Pt;0)	[6]
		G(A15,Pt:Cr)	10000 + 0.75G(fcc,Pt;0) + 0.25G(bcc,Cr;0)	[6]
		G(A15,Cr,Ru)	2556.077 − 5.24126T + 0.75G(bcc,Cr;0) + 0.25G(hcp,Ru;0)	This work
		G(A15,Ru:Cr)	37443.92 + 5.24126T + 0.75G(hcp,Ru;0) + 0.25G(bcc,Cr;0)	This work
		L(A15,Cr,Pt:Cr)	1250	[6]
		L(A15,Cr,Pt:Pt)	1250	[6]
		L(A15,Cr:Cr:Pt)	−25250	[6]
		L(A15,Pt:Cr:Pt)	1250	[6]
		L(A15,Cr:Pt,Ru)	−1.709 + 0.00479T	This work
		L(A15,Pt:Cr,Ru)	5450.82 + 6.65232T	This work

5.2. Cr-Pt

As indicated in the previous section, the optimisation by Ref. [6] was accepted in this work. The optimised phase diagram is given in Fig. 2 and the Gibbs energy parameters are given in Table 3. However, it was necessary to derive Gibbs energy parameters for the metastable hcp phase in the bi-

nary system. This was initially set to the same set of values as for the fcc phase but the parameters were later optimised using the ternary data (see below).

5.3. Cr-Ru

Gibbs energy parameters for the bcc, hcp, sigma, and A15 phases were optimised using WinPhad together with the invariant temperatures and compositions given in Table 1, taken from Ref. [3]. The phase diagram calculated using Pandat is given in Fig. 6. The fit of the calculated phase diagram to the experimental invariants is very good, with only slight deviation occurring for the A15 phase. This is acceptable in this case as the experimental data for the stability of this phase have a degree of uncertainty. But more importantly, the model used is compatible with that used for the Cr_3Pt A15 phase.

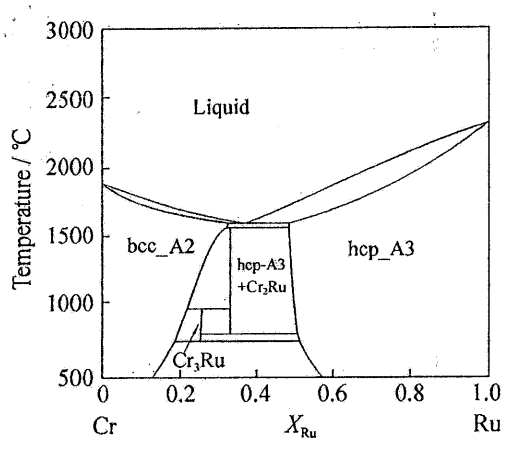


Fig. 6. Assessed Cr-Ru phase diagram.

5.4. Pt-Ru

Optimisation of this system was particularly difficult in that there are very few experimental data. The equilibria involving the liquid phase are unknown and the nature of the invariant reaction is uncertain. Massalski [3] assumes a peritectic reaction takes place in this system, using experimental data from Ref. [22]. But, it was found that the most reasonable fit to the phase boundaries of the (Pt) + (Ru) two-phase field, where a few compositions had been measured, resulted in the appearance of a very shallow eutectic reaction. The phase diagram, optimised using WinPhad and calculated using Pandat, is given in Fig. 7. The optimised parameters are given in Table 3.

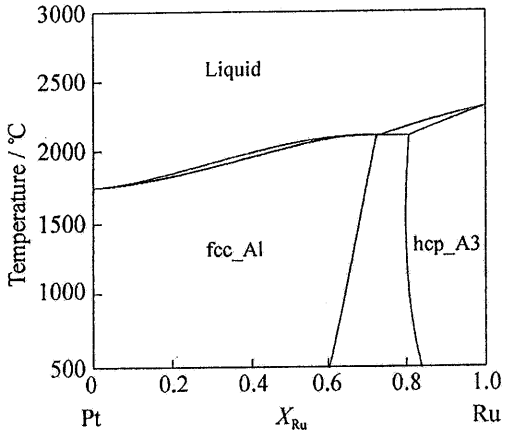


Fig. 7. Assessed Pt-Ru phase diagram.

5.5. Cr-Pt-Ru ternary system

The thermodynamic description of the ternary system was optimised using the experimental data of Ref. [16] as this set of data seemed to be more complete and self-consistent. The assessment module of *MTDATA* was used to perform the optimisation. During the optimisation process it was found that it was necessary to adjust only the Gibbs energy description of the metastable hcp phase in the Cr-Pt binary in order to get a reasonable fit to the experimental phase diagram data for the fcc and hcp phase boundaries. No ternary interactions were required for these phases.

The experimental data for the A15 phase fitted reasonably well although this was a little improved by allowing the optimisation to give a Gibbs energy description for the metastable Pt_3Ru A15 phase. The A15 phase extends from the Cr-Pt edge as required but too far into the ternary. Also, the A15 phase field is not wide enough as it extends into the ternary, which is probably due to the fact the phase is modelled with a very narrow homogeneity range in the Cr-Ru system. Improvement to the modelling of this phase in the binary system would undoubtedly improve the overall modelling of this phase, but this would require further experimental study of its stability range. The fit to the experimental bcc phase diagram data, however, is very good. The calculated

phase diagram for 1200°C, along with the experimental data is given in Fig. 8. The fit of the experimental data from Ref. [17] is not so good, particularly with respect to the hcp phase boundary. Again, this could be improved by a better description of the A15 phase. The calculated diagram for 1000°C is given in Fig. 9.

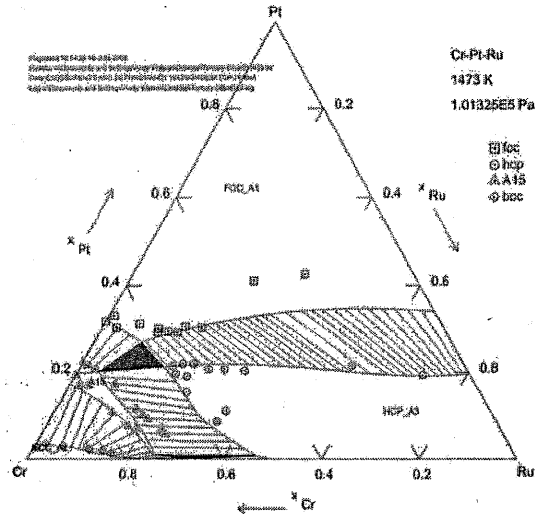


Fig. 8. Calculated isothermal section for the Cr-Pt-Ru system for 1200°C with experimental data from Ref. [16].

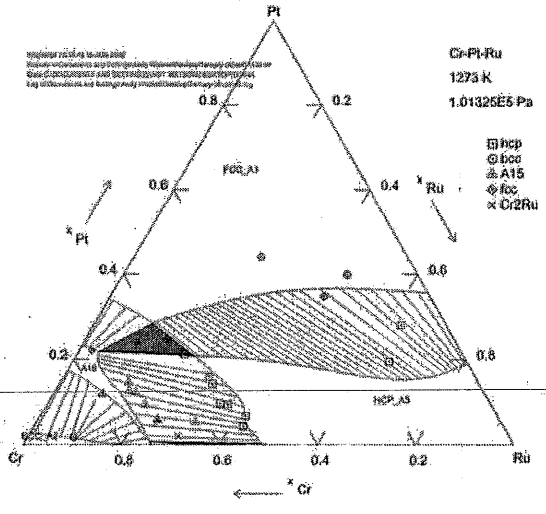


Fig. 9. Calculated isothermal section for the Cr-Pt-Ru system for 1000°C with experimental data from Ref. [17].

6. Discussion

It is interesting that a good fit to the fcc and hcp experimental data for 1200°C can be achieved just by adjusting the metastable hcp interactions in the Cr-Pt binary system. Only two fcc data points at this temperature do not fit the calculated phase boundary. Introducing a ternary interaction parameter for both the fcc and hcp phases can improve the fit to these data points, but bearing in mind that this applies to only two experimental data points, it is probably better to have a simpler description for the system as a whole. Most improvement to the calculated diagram would be achieved by improvement to the description of the A15 phase. Destabilising the Cr_3Ru A15 phase in the Cr-Ru binary would have the effect of reducing the extension of the A15 phase into the ternary, which is desirable, but this would of course, have implications with respect to the Cr-Ru phase diagram. In any case, the Cr-Ru binary system in the stability region of the Cr_3Ru A15 phase is still uncertain and should be investigated further in order that the binary system could be better described.

7. Conclusions

The Cr-Ru and Pt-Ru systems have been modelled using experimental phase diagram data available in the literature. The descriptions for these binary systems have been combined with that for the Cr-Pt system from Ref. [6] to calculate isothermal sections of the ternary system. It was found that a reasonable fit to the ternary experimental data available in the literature could be achieved by producing a suitable description for the metastable binary Cr-Pt hcp phase. Further work is required to improve the fit of experimental phase diagram data for the A15 phase.

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APPENDIX B

Thermodynamic databases for Pt-Al-Cr (in TDB format)

```
$ Database file written 2007-2-23 by R.Süss

 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 AL   FCC_A1                      2.6982E+01  4.5773E+03
2.8322E+01!
 ELEMENT CR   BCC_A2                      5.1996E+01  4.0500E+03
2.3560E+01!
 ELEMENT PT   FCC_A1                      1.9508E+02  5.7237E+03
4.1631E+01!

 FUNCTION ZERO       298.15 0.0; 6000.00  N !
 FUNCTION UN_ASS     298.15 0.0; 6000.00  N !


 FUNCTION GHSERCR    2.98150E+02  -8856.94+157.48*T-26.908*T*LN(T)
     +.00189435*T**2-1.47721E-06*T**3+139250*T**(-1);  2.18000E+03  Y
      -34869.344+344.18*T-50*T*LN(T)-2.88526E+32*T**(-9);  6.00000E+
03  N !
 FUNCTION GHSERAL    298.15  -7976.15+137.071542*T-24.3671976*T*LN(T)
     -.001884662*T**2-8.77664E-07*T**3+74092*T**(-1);  7.00000E+02  Y
      -11276.24+223.02695*T-38.5844296*T*LN(T)+.018531982*T**2
     -5.764227E-06*T**3+74092*T**(-1);  9.33600E+02  Y
      -11277.683+188.661987*T-31.748192*T*LN(T)-1.234264E+28*T**(-9);
     2.90000E+03  N !
 FUNCTION GHCPAL     298.15  +5481-1.799*T+GHSERAL#;   6000   N !
 FUNCTION GALBCC     298.15  +10083-4.813*T+GHSERAL#;   6000   N
     !
 FUNCTION GHSERPT    298.15  -7595.631+124.388276*T-24.5526*T*LN(T)
     -.00248297*T**2-2.0138E-08*T**3+7974*T**(-1);  1.30000E+03  Y
      -9253.174+161.529616*T-30.2527*T*LN(T)+.002321665*T**2
     -6.56947E-07*T**3-272106*T**(-1);  2.04210E+03  Y
      -222518.973+1021.21087*T-136.422689*T*LN(T)+.020501692*T**2
     -7.60985E-07*T**3+71709819*T**(-1);  4.00000E+03  N !


$******************************************

 FUNCTION APL0FCC    298.15  -110531-22.9*T;   6000 N !
 FUNCTION APL1FCC    298.15  -25094;   6000 N !
 FUNCTION APL2FCC    298.15  21475;   6000 N !

 FUNCTION GAL3PT1  298.15 +3*UAP#; 6000 N !
 FUNCTION GAL2PT2  298.15 +4*UAP#; 6000 N !
 FUNCTION GAL1PT3  298.15 +3*UAP#-3913; 6000 N !

 FUNCTION ALPTG0     2.98150E+02  +GAL3PT1#+1.5*GAL2PT2#+GAL1PT3#;
     6.00000E+03   N !
 FUNCTION ALPTG1     2.98150E+02  +2*GAL3PT1#-2*GAL1PT3#;   6.00000E+
03   N !
 FUNCTION ALPTG2     2.98150E+02  +GAL3PT1#-1.5*GAL2PT2#+GAL1PT3#;
     6.00000E+03   N !

 FUNCTION UL0 298.15  +1412.8+5.7*T;   6000   N !
 FUNCTION UAP 298.15  -13595+8.3*T;   6000   N !
 FUNCTION REC  298.15 UAP#; 6000 N !


$******************************************

 FUNCTION GCR3PT1    2.98150E+02  3.1206240E+03;   3.00000E+03   N !
 FUNCTION GCR2PT2    2.98150E+02  -8.5417081E+03;   3.00000E+03   N !
 FUNCTION GCR1PT3    2.98150E+02  -4.6100000E+03;   3.00000E+03   N !
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 FUNCTION REC2          2.98150E+02  1.0002000E+03;    3.00000E+03   N !

$*****************************************

 FUNCTION L04ALCR     2.98150E+02  0;    3.00000E+03   N !
 FUNCTION ALCR2PT     2.98150E+02  +83650-55*T;    3.00000E+03   N !
 FUNCTION ALCRPT2     2.98150E+02  +83650-55*T;    3.00000E+03   N !
 FUNCTION AL2CRPT     2.98150E+02  +83650-55*T;    3.00000E+03   N !
 FUNCTION GALCR3     2.98150E+02  0;    3.00000E+03   N !
 FUNCTION GAL2CR2     2.98150E+02  0;    3.00000E+03   N !
 FUNCTION GAL3CR     2.98150E+02  0;    3.00000E+03   N !

$*****************************************


 TYPE_DEFINITION % SEQ *!
 DEFINE_SYSTEM_DEFAULT ELEMENT 2 !
 DEFAULT_COMMAND DEF_SYS_ELEMENT VA /- !


 PHASE LIQUID:L % 1 1.0 !
    CONSTITUENT LIQUID:L :AL,CR,PT :  !

   PARAMETER G(LIQUID,AL;0)  2.98150E+02  +3028.879+125.251171*T
  -24.3671976*T*LN(T)-.001884662*T**2-8.77664E-07*T**3+74092*T**(-1)
  +7.9337E-20*T**7;  7.00000E+02  Y
   -271.21+211.206579*T-38.5844296*T*LN(T)+.018531982*T**2-5.764227E-
06*T**3
  +74092*T**(-1)+7.9337E-20*T**7;  9.33470E+02  Y
   -795.996+177.430178*T-31.748192*T*LN(T);  2.90000E+03  N REF0 !
   PARAMETER G(LIQUID,CR;0)  2.98150E+02  +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;  2.18000E+03  Y
   -16459.984+335.616316*T-50*T*LN(T);  6.00000E+03  N REF0 !
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  -24.5526*T*LN(T)-.00248297*T**2-2.0138E-08*T**3+7974*T**(-1);
6.00000E+02
   Y
   +19019.913+33.017485*T-12.351404*T*LN(T)-.011543133*T**2+9.30579E-
07*T**3
  -600885*T**(-1);  2.04210E+03  Y
   +1404.968+205.861909*T-36.5*T*LN(T);  4.00000E+03  N REF0 !
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N REF0 !
   PARAMETER G(LIQUID,AL,CR;1)  2.98150E+02  -11000;    6.00000E+03
N REF0 !

   PARAMETER G(LIQUID,AL,PT;0)  298.15  -352536+114.8*T;    6.00E+03
N
  REF0 !
   PARAMETER G(LIQUID,AL,PT;1)  298.15  +68566-53*T;    6.00E+03   N
  REF0 !
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N REF0 !

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  -321.855174*T*LN(T)-.016942582*T**2-1.2608724E-05*T**3+1093512*T**
(-1);
  7.00000E+02  Y
   -317252.52+2794.29791*T-478.244726*T*LN(T)+.207640502*T**2
```

```
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  -2.95442E-06*T**3+278500*T**(-1)-1.353577E+29*T**(-9);  2.18000E+03
Y
   -369300.846+2789.69068*T-449.230112*T*LN(T)-5.771876E+32*T**(-9);
  2.90000E+03  N REF0 !


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(-1);
  7.00000E+02  Y
   -338710+3236.7898*T-555.413585*T*LN(T)+.244704466*T**2-7.7889371E-
05*T**3
  +1241696*T**(-1);  9.33470E+02  Y
   -338737.794+2790.05399*T-466.542496*T*LN(T)+.0037887*T**2
  -2.95442E-06*T**3+278500*T**(-1)-1.599682E+29*T**(-9);  2.18000E+03
Y
   -390762.602+3163.45399*T-512.726496*T*LN(T)-5.772122E+32*T**(-9);
  2.90000E+03  N REF0 !


 PHASE AL4CR  %  2 4   1 !
    CONSTITUENT AL4CR  :AL : CR :  !

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1);
  7.00000E+02  Y
   -142986.9+1068.72378*T-181.245718*T*LN(T)+.076022278*T**2
  -2.4534118E-05*T**3+435618*T**(-1);  9.33470E+02  Y
   -142995.452+931.266612*T-153.900768*T*LN(T)+.00189435*T**2
  -1.47721E-06*T**3+139250*T**(-1)-4.9221E+28*T**(-9);  2.18000E+03
Y
   -169007.856+1117.96661*T-176.992768*T*LN(T)-2.885753E+32*T**(-9);
  2.90000E+03  N REF0 !


 PHASE AL8CR5_H  %  2 8   5 !
    CONSTITUENT AL8CR5_H  :AL : CR :  !

   PARAMETER G(AL8CR5_H,AL:CR;0)  2.98150E+02  -255825.9+1825.6443*T
  -329.477581*T*LN(T)-.005605546*T**2-1.4407362E-05*T**3+1288986*T**
(-1);
  7.00000E+02  Y
   -282226.62+2513.28757*T-443.215437*T*LN(T)+.157727606*T**2
  -5.3499866E-05*T**3+1288986*T**(-1);  9.33470E+02  Y
   -282243.724+2238.37322*T-388.525536*T*LN(T)+.00947175*T**2
  -7.38605E-06*T**3+696250*T**(-1)-9.8442E+28*T**(-9);  2.18000E+03
Y
   -412305.744+3171.87322*T-503.985536*T*LN(T)-1.442729E+33*T**(-9);
  2.90000E+03  N REF0 !


 PHASE AL8CR5_L  %  2 8   5 !
    CONSTITUENT AL8CR5_L  :AL : CR :  !

   PARAMETER G(AL8CR5_L,AL:CR;0)  2.98150E+02  -337608.9+1884.1443*T
  -329.477581*T*LN(T)-.005605546*T**2-1.4407362E-05*T**3+1288986*T**
(-1);
  7.00000E+02  Y
   -364009.62+2571.78757*T-443.215437*T*LN(T)+.157727606*T**2
  -5.3499866E-05*T**3+1288986*T**(-1);  9.33470E+02  Y
```

```
   -364026.724+2296.87322*T-388.525536*T*LN(T)+.00947175*T**2
  -7.38605E-06*T**3+696250*T**(-1)-9.8442E+28*T**(-9);  2.18000E+03
Y
   -494088.744+3230.37322*T-503.985536*T*LN(T)-1.442729E+33*T**(-9);
  2.90000E+03  N REF0 !


 PHASE AL9CR4_H  %  2 9   4 !
    CONSTITUENT AL9CR4_H  :AL : CR :  !

   PARAMETER G(AL9CR4_H,AL:CR;0)  2.98150E+02  -241646.11+1807.59734
*T
  -326.936778*T*LN(T)-.009384558*T**2-1.3807816E-05*T**3+1223828*T**
(-1);
  7.00000E+02  Y
   -271346.92+2581.19601*T-454.891866*T*LN(T)+.174365238*T**2
  -5.7786883E-05*T**3+1223828*T**(-1);  9.33470E+02  Y
   -271366.162+2271.91738*T-393.365728*T*LN(T)+.0075774*T**2
  -5.90884E-06*T**3+557000*T**(-1)-1.107472E+29*T**(-9);  2.18000E+03
Y
   -375415.778+3018.71738*T-485.733728*T*LN(T)-1.154215E+33*T**(-9);
  2.90000E+03  N REF0 !


 PHASE AL9CR4_L  %  2 9   4 !
    CONSTITUENT AL9CR4_L  :AL : CR :  !

   PARAMETER G(AL9CR4_L,AL:CR;0)  2.98150E+02  -337963.11+1879.85134
*T
  -326.936778*T*LN(T)-.009384558*T**2-1.3807816E-05*T**3+1223828*T**
(-1);
  7.00000E+02  Y
   -367663.92+2653.45001*T-454.891866*T*LN(T)+.174365238*T**2
  -5.7786883E-05*T**3+1223828*T**(-1);  9.33470E+02  Y
   -367683.162+2344.17138*T-393.365728*T*LN(T)+.0075774*T**2
  -5.90884E-06*T**3+557000*T**(-1)-1.107472E+29*T**(-9);  2.18000E+03
Y
   -471732.778+3090.97138*T-485.733728*T*LN(T)-1.154215E+33*T**(-9);
  2.90000E+03  N REF0 !


 PHASE ALCR2  %  2 1   2 !
    CONSTITUENT ALCR2  :AL : CR :  !

   PARAMETER G(ALCR2,AL:CR;0)  2.98150E+02  -58390.03+443.263038*T
  -78.1831976*T*LN(T)+.001904038*T**2-3.832084E-06*T**3+352592*T**(-
1);
  7.00000E+02  Y
   -61690.12+529.218446*T-92.4004296*T*LN(T)+.022320682*T**2
  -8.718647E-06*T**3+352592*T**(-1);  9.33470E+02  Y
   -61692.258+494.854153*T-85.564192*T*LN(T)+.0037887*T**2-2.95442E-
06*T**3
  +278500*T**(-1)-1.230524E+28*T**(-9);  2.18000E+03  Y
   -113717.066+868.254153*T-131.748192*T*LN(T)-5.770646E+32*T**(-9);
  2.90000E+03  N REF0 !


$ TYPE_DEFINITION & GES A_P_D BCC_A2 MAGNETIC  -1.0    4.00000E-01 !
 PHASE BCC_A2  %  2 1   3 !
    CONSTITUENT BCC_A2  :AL,CR,PT : VA :  !

   PARAMETER G(BCC_A2,AL:VA;0)  2.98150E+02  +2106.85+132.280038*T
  -24.3671976*T*LN(T)-.001884662*T**2-8.77664E-07*T**3+74092*T**(-1);
  7.00000E+02  Y
   -1193.24+218.235446*T-38.5844296*T*LN(T)+.018531982*T**2
  -5.764227E-06*T**3+74092*T**(-1);  9.33470E+02  Y
```

```
   -1195.378+183.871153*T-31.748192*T*LN(T)-1.230524E+28*T**(-9);
  2.90000E+03  N REF0 !
   PARAMETER G(BCC_A2,CR:VA;0)  2.98150E+02  -8856.94+157.48*T
  -26.908*T*LN(T)+.00189435*T**2-1.47721E-06*T**3+139250*T**(-1);
  2.18000E+03  Y
   -34869.344+344.18*T-50*T*LN(T)-2.885261E+32*T**(-9);  6.00000E+03
N REF0 !
   PARAMETER TC(BCC_A2,CR:VA;0)  2.98150E+02  -311.5;  6.00000E+03
N REF0 !
   PARAMETER BMAGN(BCC_A2,CR:VA;0)  2.98150E+02  -.008;  6.00000E+03
N
  REF0 !
   PARAMETER G(BCC_A2,AL,CR:VA;0)  2.98150E+02  -54900+10*T;
6.00000E+03
  N REF0 !
   PARAMETER G(BCC_A2,PT:VA;0)  2.98150E+02  +15000-2.4*T+GHSERPT#;
  4.00000E+03  N REF0 !
   PARAMETER G(BCC_A2,CR,PT:VA;0)  2.98150E+02  -105000;  6.00000E+
03   N
  REF0 !


$ TYPE_DEFINITION ' GES A_P_D FCC_A1 MAGNETIC  -3.0    2.80000E-01 !
 PHASE FCC_A1  %  2 1   1 !
    CONSTITUENT FCC_A1  :AL,CR,PT : VA :  !

   PARAMETER G(FCC_A1,AL:VA;0)  2.98150E+02  -7976.15+137.093038*T
  -24.3671976*T*LN(T)-.001884662*T**2-8.77664E-07*T**3+74092*T**(-1);
  7.00000E+02  Y
   -11276.24+223.048446*T-38.5844296*T*LN(T)+.018531982*T**2
  -5.764227E-06*T**3+74092*T**(-1);  9.33470E+02  Y
   -11278.378+188.684153*T-31.748192*T*LN(T)-1.230524E+28*T**(-9);
  2.90000E+03  N REF0 !
   PARAMETER G(FCC_A1,CR:VA;0)  2.98150E+02  -1572.94+157.643*T
  -26.908*T*LN(T)+.00189435*T**2-1.47721E-06*T**3+139250*T**(-1);
  2.18000E+03  Y
   -27585.344+344.343*T-50*T*LN(T)-2.885261E+32*T**(-9);  6.00000E+03
N
  REF0 !
   PARAMETER TC(FCC_A1,CR:VA;0)  2.98150E+02  -1109;  6.00000E+03
N REF0 !
   PARAMETER BMAGN(FCC_A1,CR:VA;0)  2.98150E+02  -2.46;  6.00000E+03
N
  REF0 !
   PARAMETER G(FCC_A1,AL,CR:VA;0)  2.98150E+02  -45900+6*T;
6.00000E+03
  N REF0 !
   PARAMETER G(FCC_A1,AL,PT:VA;0)  298.15  +APL0FCC#+ALPTG0#+1.5
*REC#;
  6000   N REF0 !
   PARAMETER G(FCC_A1,AL,PT:VA;1)  298.15  +APL1FCC#+ALPTG1#;  6000
N
  REF0 !
   PARAMETER G(FCC_A1,AL,PT:VA;2)  298.15  +APL2FCC#+ALPTG2#-1.5
*REC#;
  6000   N REF0 !
   PARAMETER G(FCC_A1,PT:VA;0)  2.98150E+02  GHSERPT#;  4.00000E+03
N REF0 !
   PARAMETER G(FCC_A1,CR,PT:VA;0)  2.98150E+02  -1.4623245E+05;
6.00E+03   N
 REF0 !
   PARAMETER G(FCC_A1,CR,PT:VA;1)  2.98150E+02  3.4383376E+03;
6.00E+03   N
  REF0 !
```

```
 PHASE PT2AL  %  2 .334   .666 !
    CONSTITUENT PT2AL  :AL,CR : PT,CR :  !
 PARAMETER G(PT2AL,AL:CR;0)  298.15  10000+0.334*GHSERAL#+0.666
*GHSERCR#;
   3000   N REF0 !
PARAMETER G(PT2AL,CR:PT;0)  298.15  20000+0.334*GHSERCR#+.666
*GHSERPT#;
   3000   N REF0 !
PARAMETER G(PT2AL,CR:CR;0)  298.15  150000+GHSERCR#;   3000   N REF0
!

   PARAMETER G(PT2AL,AL:PT;0)  298.15  -84989+24.9*T+.334*GHSERAL#
  +.666*GHSERPT#;   3000   N REF0 !
PARAMETER G(PT2AL,AL,CR:PT;0)  298.15  -118000+19.9*T;   3000   N
REF0 !
PARAMETER G(PT2AL,AL:PT,CR;0)  298.15  -178000+44.7*T;   3000   N
REF0 !
PARAMETER G(PT2AL,AL,CR:CR;0)  298.15  -118000+19.9*T;   3000   N
REF0 !
PARAMETER G(PT2AL,CR:PT,CR;0)  298.15  -178000+44.7*T;   3000   N
REF0 !

 PHASE PTAL  %  2 .5   .5 !
    CONSTITUENT PTAL  :AL,CR : PT,CR :  !

   PARAMETER G(PTAL,AL:PT;0)  298.15  -94071+24.1*T+.5*GHSERAL#
  +.5*GHSERPT#;   3000   N REF0 !
  PARAMETER G(PTAL,AL:CR;0)  298.15  20000+0.5*GHSERAL#+0.5*GHSERCR#;
3000   N REF0 !
PARAMETER G(PTAL,CR:PT;0)  298.15  35000+0.5*GHSERCR#+0.5*GHSERPT#;
3000   N REF0 !
PARAMETER G(PTAL,CR:CR;0)  298.15 200000+GHSERCR#;   3000   N REF0 !
PARAMETER G(PTAL,AL,CR:CR;0)  298.15  -187060+65.9*T;   3000   N REF0
!
PARAMETER G(PTAL,CR:PT,CR;0)  298.15  -234908+81.6*T;   3000   N REF0
!
PARAMETER G(PTAL,AL,CR:PT;0)  298.15  -187060+65.9*T;   3000   N REF0
!
PARAMETER G(PTAL,AL:PT,CR;0)  298.15  -234908+81.6*T;   3000   N REF0
!


 PHASE PTAL2  %  2 .666   .334 !
    CONSTITUENT PTAL2  :AL,CR : PT,CR :  !

   PARAMETER G(PTAL2,AL:PT;0)  298.15  -87898+23.3*T+.666*GHSERAL#
  +.334*GHSERPT#;   3000   N REF0 !
 PARAMETER G(PTAL2,AL:CR;0)  298.15  +20000+0.666*GHSERAL#+0.334
*GHSERCR#;
3000   N REF0 !
PARAMETER G(PTAL2,CR:PT;0)  298.15  -39562.5+62.5*T+0.666*GHSERCR#+
0.334*GHSERPT#;
3000   N REF0 !
PARAMETER G(PTAL2,CR:CR;0)  298.15  +170000+GHSERCR#;   3000   N REF0
!
PARAMETER G(PTAL2,AL,CR:CR;0)  298.15  -108000+19.9*T;   3000   N
REF0 !
PARAMETER G(PTAL2,CR:PT,CR;0)  298.15  -168000+44.7*T;   3000   N
REF0 !
PARAMETER G(PTAL2,AL,CR:PT;0)  298.15  -108000+19.9*T;   3000   N
REF0 !
PARAMETER G(PTAL2,AL:PT,CR;0)  298.15  -168000+44.7*T;   3000   N
REF0 !


 PHASE PT2AL3  %  2 .6   .4 !
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```
    CONSTITUENT PT2AL3  :AL : PT :  !

   PARAMETER G(PT2AL3,AL:PT;0)  298.15  -8.9885E+04+21.5*T+.6
*GHSERAL#
  +.4*GHSERPT#;   3000   N REF0 !


 PHASE PT5AL21  %  2 .8077   .1923 !
    CONSTITUENT PT5AL21  :AL : PT :  !

   PARAMETER G(PT5AL21,AL:PT;0)  298.15  -56873+14.8*T+.8077*GHSERAL#
  +.1923*GHSERPT#;   3000   N REF0 !


 PHASE PT5AL3  %  2 .375   .625 !
    CONSTITUENT PT5AL3  :AL : PT :  !

   PARAMETER G(PT5AL3,AL:PT;0)  298.15  -87260+24*T+.375*GHSERAL#
  +.625*GHSERPT#;   3000   N REF0 !


 PHASE PT8AL21  %  2 .7242   .2759 !
    CONSTITUENT PT8AL21  :AL : PT :  !

   PARAMETER G(PT8AL21,AL:PT;0)  298.15  -82342+23.7*T+.7242*GHSERAL#
  +.2759*GHSERPT#;   3000   N REF0 !


   PHASE BETA  %  2 .48   .52 !
    CONSTITUENT BETA  :AL : PT :  !

   PARAMETER G(BETA,AL:PT;0)  2.98150E+02  -92723+23.88*T+.48
*GHSERAL#
  +.52*GHSERPT#;   6000   N REF0 !

  PHASE CR3PT_A15  %  2 3   1 !
    CONSTITUENT CR3PT_A15  :CR,PT : CR,PT :  !

   PARAMETER G(CR3PT_A15,CR:CR;0)  2.98150E+02  +60000+4*GHSERCR#;
  6.00000E+03   N REF0 !
   PARAMETER G(CR3PT_A15,PT:CR;0)  2.98150E+02  +40000+GHSERCR#+3
*GHSERPT#;
   6.00000E+03   N REF0 !
   PARAMETER G(CR3PT_A15,CR:PT;0)  2.98150E+02  -114000+3
*GHSERCR#+GHSERPT#;
    6.00000E+03   N REF0 !
   PARAMETER G(CR3PT_A15,PT:PT;0)  2.98150E+02  +40000+4*GHSERPT#;
  6.00000E+03   N REF0 !
   PARAMETER G(CR3PT_A15,CR,PT:CR;0)  2.98150E+02  5000;   6.00000E+
03   N
  REF0 !
   PARAMETER G(CR3PT_A15,CR:CR,PT;0)  2.98150E+02  -101000;
6.00000E+03
  N REF0 !
   PARAMETER G(CR3PT_A15,PT:CR,PT;0)  2.98150E+02  5000;   6.00000E+
03   N
  REF0 !
   PARAMETER G(CR3PT_A15,CR,PT:PT;0)  2.98150E+02  5000;   6.00000E+
03   N
  REF0 !

TYPE_DEFINITION ) GES AMEND_PHASE_DESCRIPTION L12 DIS_PART FCC_A1,,,!
$ THIS PHASE HAS A DISORDERED CONTRIBUPTON FROM FCC_A1
TYPE_DEFINITION & GES AMEND_PHASE_DESCRIPTION L12 MAJ 1
PT:PT:PT:PT:VA:!
TYPE_DEFINITION ( GES AMEND_PHASE_DESCRIPTION L12 C-S ,,
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PT:PT:PT:AL:VA:!
TYPE_DEFINITION ( GES AMEND_PHASE_DESCRIPTION L12 C-S ,,
PT:PT:PT:CR:VA:!
TYPE_DEFINITION ( GES AMEND_PHASE_DESCRIPTION L12 C-S ,,
CR:CR:PT:PT:VA:!

PHASE L12  %)&( 5 .25   .25  .25   .25  1 !
CONSTITUENT L12 :AL,CR,PT%:AL,CR,PT%:AL,CR,PT%:AL%,CR,PT:VA:  !


PARAMETER G(L12,AL:AL:AL:AL:VA;0) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:CR:CR:VA;0) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:PT:PT:VA;0) 298.15 0; 6000 N !

PARAMETER G(L12,PT:PT:PT:AL:VA;0) 298.15 GAL1PT3; 6000 N !
PARAMETER G(L12,PT:PT:AL:PT:VA;0) 298.15 GAL1PT3; 6000 N !
PARAMETER G(L12,PT:AL:PT:PT:VA;0) 298.15 GAL1PT3; 6000 N !
PARAMETER G(L12,AL:PT:PT:PT:VA;0) 298.15 GAL1PT3; 6000 N !
PARAMETER G(L12,AL:AL:AL:PT:VA;0) 298.15 GAL3PT1; 6000 N !
PARAMETER G(L12,AL:AL:PT:AL:VA;0) 298.15 GAL3PT1; 6000 N !
PARAMETER G(L12,AL:PT:AL:AL:VA;0) 298.15 GAL3PT1; 6000 N !
PARAMETER G(L12,PT:AL:AL:AL:VA;0) 298.15 GAL3PT1; 6000 N !
PARAMETER G(L12,AL:AL:PT:PT:VA;0) 298.15 GAL2PT2; 6000 N !
PARAMETER G(L12,AL:PT:PT:AL:VA;0) 298.15 GAL2PT2; 6000 N !
PARAMETER G(L12,PT:AL:PT:AL:VA;0) 298.15 GAL2PT2; 6000 N !
PARAMETER G(L12,AL:PT:AL:PT:VA;0) 298.15 GAL2PT2; 6000 N !
PARAMETER G(L12,PT:AL:AL:PT:VA;0) 298.15 GAL2PT2; 6000 N !
PARAMETER G(L12,PT:PT:AL:AL:VA;0) 298.15 GAL2PT2; 6000 N !
PARAMETER G(L12,AL,PT:AL:AL:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:AL:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:AL:AL:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:AL:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:AL:AL:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:AL:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:AL:PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:AL:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:AL:PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:AL:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:PT:AL:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:PT:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:PT:AL:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:PT:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:PT:PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:PT:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:PT:PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:PT:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,PT:AL:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL,PT:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,PT:AL:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL,PT:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,PT:PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL,PT:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,PT:PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL,PT:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL,PT:AL:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL,PT:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL,PT:AL:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL,PT:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL,PT:PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL,PT:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL,PT:PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL,PT:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:AL,PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL:AL,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:AL,PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL:AL,PT:PT:VA;1) 298.15 0; 6000 N !
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```
PARAMETER G(L12,AL:AL:AL:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL:AL:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:PT:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL:PT:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:AL:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:PT:AL:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:PT:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:PT:PT:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:AL,PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:PT:AL,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:AL,PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:PT:AL,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:AL:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL:AL:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:PT:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL:PT:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:AL:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:PT:AL:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:PT:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:PT:PT:AL,PT:VA;1) 298.15 0; 6000 N !

PARAMETER G(L12,CR:CR:CR:AL:VA;0) 298.15 GALCR3; 6000 N !
PARAMETER G(L12,CR:CR:AL:CR:VA;0) 298.15 GALCR3; 6000 N !
PARAMETER G(L12,CR:AL:CR:CR:VA;0) 298.15 GALCR3; 6000 N !
PARAMETER G(L12,AL:CR:CR:CR:VA;0) 298.15 GALCR3; 6000 N !
PARAMETER G(L12,AL:AL:AL:CR:VA;0) 298.15 GAL3CR; 6000 N !
PARAMETER G(L12,AL:AL:CR:AL:VA;0) 298.15 GAL3CR; 6000 N !
PARAMETER G(L12,AL:CR:AL:AL:VA;0) 298.15 GAL3CR; 6000 N !
PARAMETER G(L12,CR:AL:AL:AL:VA;0) 298.15 GAL3CR; 6000 N !
PARAMETER G(L12,AL:AL:CR:CR:VA;0) 298.15 GAL2CR2; 6000 N !
PARAMETER G(L12,AL:CR:CR:AL:VA;0) 298.15 GAL2CR2; 6000 N !
PARAMETER G(L12,CR:AL:CR:AL:VA;0) 298.15 GAL2CR2; 6000 N !
PARAMETER G(L12,AL:CR:AL:CR:VA;0) 298.15 GAL2CR2; 6000 N !
PARAMETER G(L12,CR:AL:AL:CR:VA;0) 298.15 GAL2CR2; 6000 N !
PARAMETER G(L12,CR:CR:AL:AL:VA;0) 298.15 GAL2CR2; 6000 N !
PARAMETER G(L12,AL,CR:AL:AL:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:AL:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:AL:AL:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:AL:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:AL:CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:AL:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:AL:CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:AL:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:CR:AL:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:CR:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:CR:AL:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:CR:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:CR:CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:CR:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:CR:CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:CR:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,CR:AL:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:AL,CR:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,CR:AL:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:AL,CR:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,CR:AL:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:AL,CR:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,CR:AL:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:AL,CR:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,CR:CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:AL,CR:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,CR:CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:AL,CR:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,CR:CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:AL,CR:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,CR:CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
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PARAMETER G(L12,CR:AL,CR:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:AL,CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:AL:AL,CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:AL,CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:AL:AL,CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:AL,CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:CR:AL,CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:AL,CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:CR:AL,CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:AL,CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:AL:AL,CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:AL,CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:AL:AL,CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:AL,CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:CR:AL,CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:AL,CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:CR:AL,CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:AL:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:AL:AL:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:CR:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:AL:CR:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:AL:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:CR:AL:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:CR:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:CR:CR:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:AL:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:AL:AL:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:CR:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:AL:CR:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:AL:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:CR:AL:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:CR:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:CR:CR:AL,CR:VA;1) 298.15 0; 6000 N !

PARAMETER G(L12,PT:PT:PT:CR:VA;0) 298.15 GCR1PT3; 6000 N !
PARAMETER G(L12,PT:PT:CR:PT:VA;0) 298.15 GCR1PT3; 6000 N !
PARAMETER G(L12,PT:CR:PT:PT:VA;0) 298.15 GCR1PT3; 6000 N !
PARAMETER G(L12,CR:PT:PT:PT:VA;0) 298.15 GCR1PT3; 6000 N !
PARAMETER G(L12,CR:CR:CR:PT:VA;0) 298.15 GCR3PT1; 6000 N !
PARAMETER G(L12,CR:CR:PT:CR:VA;0) 298.15 GCR3PT1; 6000 N !
PARAMETER G(L12,CR:PT:CR:CR:VA;0) 298.15 GCR3PT1; 6000 N !
PARAMETER G(L12,PT:CR:CR:CR:VA;0) 298.15 GCR3PT1; 6000 N !
PARAMETER G(L12,CR:CR:PT:PT:VA;0) 298.15 GCR2PT2; 6000 N !
PARAMETER G(L12,CR:PT:PT:CR:VA;0) 298.15 GCR2PT2; 6000 N !
PARAMETER G(L12,PT:CR:PT:CR:VA;0) 298.15 GCR2PT2; 6000 N !
PARAMETER G(L12,CR:PT:CR:PT:VA;0) 298.15 GCR2PT2; 6000 N !
PARAMETER G(L12,PT:CR:CR:PT:VA;0) 298.15 GCR2PT2; 6000 N !
PARAMETER G(L12,PT:PT:CR:CR:VA;0) 298.15 GCR2PT2; 6000 N !
PARAMETER G(L12,CR,PT:CR:CR:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:CR:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:CR:CR:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:CR:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:CR:PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:CR:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:CR:PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:CR:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:PT:CR:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:PT:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:PT:CR:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:PT:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:PT:PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:PT:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:PT:PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:PT:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR,PT:CR:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR,PT:CR:CR:VA;1) 298.15 0; 6000 N !
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PARAMETER G(L12,CR:CR,PT:CR:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR,PT:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR,PT:PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR,PT:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR,PT:PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR,PT:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR,PT:CR:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR,PT:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR,PT:CR:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR,PT:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR,PT:PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR,PT:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR,PT:PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR,PT:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:CR,PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR:CR,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:CR,PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR:CR,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:CR,PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:PT:CR,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:CR,PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:PT:CR,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:CR,PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR:CR,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:CR,PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR:CR,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:CR,PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:PT:CR,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:CR,PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:PT:CR,PT:PT:VA;1) 298.15 0; 6000 N !

PARAMETER G(L12,CR:CR:AL:PT:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,CR:CR:PT:AL:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,CR:PT:CR:AL:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,CR:AL:CR:PT:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,CR:AL:PT:CR:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,CR:PT:AL:CR:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,AL:PT:CR:CR:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,PT:AL:CR:CR:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,AL:CR:CR:PT:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,PT:CR:CR:AL:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,AL:CR:PT:CR:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,PT:CR:AL:CR:VA;0) 298.15 ALCR2PT; 6000 N !
PARAMETER G(L12,PT:PT:AL:CR:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,PT:PT:CR:AL:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,PT:CR:PT:AL:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,PT:AL:PT:CR:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,PT:AL:CR:PT:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,PT:CR:AL:PT:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,AL:CR:PT:PT:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,CR:AL:PT:PT:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,AL:PT:PT:CR:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,CR:PT:PT:AL:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,AL:PT:CR:PT:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,CR:PT:AL:PT:VA;0) 298.15 ALCRPT2; 6000 N !
PARAMETER G(L12,AL:AL:CR:PT:VA;0) 298.15 AL2CRPT; 6000 N !
PARAMETER G(L12,AL:AL:PT:CR:VA;0) 298.15 AL2CRPT; 6000 N !
PARAMETER G(L12,AL:PT:AL:CR:VA;0) 298.15 AL2CRPT; 6000 N !
PARAMETER G(L12,AL:CR:AL:PT:VA;0) 298.15 AL2CRPT; 6000 N !
PARAMETER G(L12,AL:CR:PT:AL:VA;0) 298.15 AL2CRPT; 6000 N !
PARAMETER G(L12,AL:PT:CR:AL:VA;0) 298.15 AL2CRPT; 6000 N !
PARAMETER G(L12,CR:PT:AL:AL:VA;0) 298.15 AL2CRPT; 6000 N !
PARAMETER G(L12,PT:CR:AL:AL:VA;0) 298.15 AL2CRPT; 6000 N !
PARAMETER G(L12,CR:AL:AL:PT:VA;0) 298.15 AL2CRPT; 6000 N !
PARAMETER G(L12,PT:AL:AL:CR:VA;0) 298.15 AL2CRPT; 6000 N !
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PARAMETER G(L12,CR:AL:PT:AL:VA;0) 298.15 AL2CRPT; 6000 N !
PARAMETER G(L12,PT:AL:CR:AL:VA;0) 298.15 AL2CRPT; 6000 N !

PARAMETER G(L12,AL,PT:AL:CR:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:AL:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:AL:CR:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:AL:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:AL:CR:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:AL:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:AL:PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:AL:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:CR:AL:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:CR:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:CR:AL:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:CR:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:CR:AL:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:CR:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:CR:CR:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:CR:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:CR:PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:CR:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:CR:CR:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:CR:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:CR:CR:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:CR:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:CR:PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:CR:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:CR:PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:CR:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:PT:CR:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:PT:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:PT:CR:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:PT:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:PT:AL:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:PT:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:PT:CR:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:PT:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,PT:PT:PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL,PT:PT:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,PT:AL:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL,PT:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,PT:CR:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL,PT:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,PT:CR:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL,PT:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,PT:CR:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL,PT:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL,PT:PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL,PT:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,PT:AL:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL,PT:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,PT:AL:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL,PT:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,PT:AL:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL,PT:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,PT:CR:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL,PT:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,PT:CR:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL,PT:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,PT:CR:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL,PT:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,PT:PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL,PT:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,PT:PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL,PT:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL,PT:PT:PT:VA;0) 298.15 UL0; 6000 N !
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PARAMETER G(L12,CR:AL,PT:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:AL,PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL:AL,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:AL,PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL:AL,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:AL,PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:PT:AL,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:AL,PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:PT:AL,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL,PT:AL:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL,PT:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL,PT:CR:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL,PT:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL,PT:CR:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL,PT:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL,PT:CR:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL,PT:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL,PT:PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL,PT:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:AL,PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL:AL,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:AL,PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:CR:AL,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:AL,PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:CR:AL,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:AL,PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:CR:AL,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:AL,PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:PT:AL,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:AL,PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL:AL,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:AL,PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL:AL,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:AL,PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL:AL,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:AL,PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:CR:AL,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:AL,PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:CR:AL,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:AL,PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:CR:AL,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:AL,PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:PT:AL,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:AL,PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:PT:AL,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:AL,PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:PT:AL,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:AL,PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL:AL,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:AL,PT:AL:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:CR:AL,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:AL,PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:CR:AL,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:AL,PT:PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:CR:AL,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:AL,PT:CR:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:PT:AL,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:CR:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:AL:CR:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:AL:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:CR:AL:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:CR:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:CR:CR:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:PT:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,AL:CR:PT:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:CR:AL,PT:VA;0) 298.15 UL0; 6000 N !
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PARAMETER G(L12,AL:PT:CR:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:AL:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL:AL:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:CR:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL:CR:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:PT:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:AL:PT:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:AL:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:CR:AL:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:CR:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:CR:CR:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:PT:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:CR:PT:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:AL:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:PT:AL:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:CR:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:PT:CR:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:PT:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,CR:PT:PT:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:CR:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:AL:CR:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:AL:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:CR:AL:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:CR:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:CR:CR:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:PT:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:CR:PT:AL,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:CR:AL,PT:VA;0) 298.15 UL0; 6000 N !
PARAMETER G(L12,PT:PT:CR:AL,PT:VA;1) 298.15 0; 6000 N !

PARAMETER G(L12,AL,CR:AL:AL:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:AL:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:AL:CR:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:AL:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:AL:PT:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:AL:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:AL:PT:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:AL:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:AL:PT:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:AL:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:CR:AL:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:CR:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:CR:CR:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:CR:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:CR:PT:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:CR:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:CR:PT:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:CR:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:CR:PT:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:CR:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:PT:AL:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:PT:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:PT:AL:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:PT:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:PT:AL:PT:VA;0) 298.15 L04ALCR; 6000 N !
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PARAMETER G(L12,AL,CR:PT:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:PT:CR:PT:VA;0) 298.15 L04ALCR; 6000 N !
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PARAMETER G(L12,AL,CR:PT:PT:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:PT:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL,CR:PT:PT:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:PT:PT:CR:VA;1) 298.15 0; 6000 N !
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PARAMETER G(L12,AL,CR:PT:PT:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL,CR:PT:PT:PT:VA;1) 298.15 0; 6000 N !
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PARAMETER G(L12,AL:PT:AL,CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:PT:AL,CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:AL,CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:PT:AL,CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:AL,CR:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,AL:PT:AL,CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:AL,CR:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:AL:AL,CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:AL,CR:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:CR:AL,CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:AL,CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:PT:AL,CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:AL,CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:PT:AL,CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:AL,CR:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:PT:AL,CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:AL,CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:AL:AL,CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:AL,CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:AL:AL,CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:AL,CR:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:AL:AL,CR:PT:VA;1) 298.15 0; 6000 N !
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PARAMETER G(L12,PT:CR:AL,CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:CR:AL,CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:AL,CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:CR:AL,CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:AL,CR:PT:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:CR:AL,CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:AL,CR:AL:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:PT:AL,CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:AL,CR:CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:PT:AL,CR:CR:VA;1) 298.15 0; 6000 N !
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PARAMETER G(L12,AL:CR:PT:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
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PARAMETER G(L12,AL:PT:AL:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
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PARAMETER G(L12,AL:PT:CR:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
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PARAMETER G(L12,CR:AL:PT:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:AL:PT:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:PT:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:CR:PT:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:AL:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:PT:AL:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:CR:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:PT:CR:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:PT:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,CR:PT:PT:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:AL:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:AL:AL:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:CR:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:AL:CR:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:PT:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:AL:PT:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:AL:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:CR:AL:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:CR:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:CR:CR:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:PT:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:CR:PT:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:AL:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:PT:AL:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:CR:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:PT:CR:AL,CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:PT:AL,CR:VA;0) 298.15 L04ALCR; 6000 N !
PARAMETER G(L12,PT:PT:PT:AL,CR:VA;1) 298.15 0; 6000 N !

PARAMETER G(L12,CR,PT:AL:AL:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:AL:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:AL:AL:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:AL:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:AL:AL:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:AL:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:AL:CR:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:AL:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:AL:CR:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:AL:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:AL:CR:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:AL:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:AL:PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:AL:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:AL:PT:CR:VA;0) 298.15 UL1; 6000 N !
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PARAMETER G(L12,CR,PT:AL:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:AL:PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:AL:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:CR:AL:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:CR:AL:AL:VA;1) 298.15 0; 6000 N !
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PARAMETER G(L12,CR,PT:CR:AL:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:CR:AL:PT:VA;1) 298.15 0; 6000 N !
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PARAMETER G(L12,CR,PT:CR:PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:CR:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:PT:AL:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:PT:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:PT:AL:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:PT:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:PT:AL:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:PT:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:PT:CR:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:PT:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR,PT:PT:PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR,PT:PT:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR,PT:AL:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR,PT:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR,PT:AL:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR,PT:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR,PT:AL:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR,PT:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR,PT:CR:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR,PT:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR,PT:CR:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR,PT:CR:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR,PT:CR:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR,PT:CR:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR,PT:PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR,PT:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR,PT:PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR,PT:PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR,PT:PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR,PT:PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR,PT:AL:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR,PT:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR,PT:AL:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR,PT:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR,PT:AL:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR,PT:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR,PT:CR:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR,PT:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR,PT:PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR,PT:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR,PT:AL:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR,PT:AL:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR,PT:AL:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR,PT:AL:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR,PT:AL:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR,PT:AL:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR,PT:CR:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR,PT:CR:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR,PT:PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR,PT:PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:CR,PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:AL:CR,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:CR,PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:AL:CR,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:CR,PT:PT:VA;0) 298.15 UL1; 6000 N !
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PARAMETER G(L12,AL:AL:CR,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:CR,PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR:CR,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:CR,PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR:CR,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:CR,PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR:CR,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:CR,PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:PT:CR,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:CR,PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:PT:CR,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:CR,PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:PT:CR,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:CR,PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:AL:CR,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:CR,PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:AL:CR,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:CR,PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:AL:CR,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:CR,PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR:CR,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:CR,PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:PT:CR,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:CR,PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:AL:CR,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:CR,PT:CR:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:AL:CR,PT:CR:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:CR,PT:PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:AL:CR,PT:PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:CR,PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR:CR,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:CR,PT:AL:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:PT:CR,PT:AL:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:AL:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:AL:AL:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:CR:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:AL:CR:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:AL:PT:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:AL:PT:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:AL:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR:AL:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:CR:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR:CR:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:CR:PT:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:CR:PT:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:AL:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:PT:AL:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:CR:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:PT:CR:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,AL:PT:PT:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,AL:PT:PT:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:AL:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:AL:AL:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:CR:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:AL:CR:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:AL:PT:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:AL:PT:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:AL:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR:AL:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:CR:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR:CR:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:CR:PT:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:CR:PT:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:AL:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:PT:AL:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:CR:CR,PT:VA;0) 298.15 UL1; 6000 N !
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PARAMETER G(L12,CR:PT:CR:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,CR:PT:PT:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,CR:PT:PT:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:AL:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:AL:AL:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:CR:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:AL:CR:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:AL:PT:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:AL:PT:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:AL:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR:AL:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:CR:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR:CR:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:CR:PT:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:CR:PT:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:AL:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:PT:AL:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:CR:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:PT:CR:CR,PT:VA;1) 298.15 0; 6000 N !
PARAMETER G(L12,PT:PT:PT:CR,PT:VA;0) 298.15 UL1; 6000 N !
PARAMETER G(L12,PT:PT:PT:CR,PT:VA;1) 298.15 0; 6000 N !
   PARAMETER G(L12,AL,PT:AL,PT:*:*:VA;0)  298.15  +REC#;  3000  N
  REF0 !
   PARAMETER G(L12,AL,PT:*:AL,PT:*:VA;0)  298.15  +REC#;  3000  N
  REF0 !
   PARAMETER G(L12,AL,PT:*:*:AL,PT:VA;0)  298.15  +REC#;  3000  N
  REF0 !
   PARAMETER G(L12,*:AL,PT:AL,PT:*:VA;0)  298.15  +REC#;  3000  N
  REF0 !
   PARAMETER G(L12,*:AL,PT:*:AL,PT:VA;0)  298.15  +REC#;  3000  N
  REF0 !
   PARAMETER G(L12,*:*:AL,PT:AL,PT:VA;0)  298.15  +REC#;  3000  N
  REF0 !
   PARAMETER G(L12,CR,PT:CR,PT:*:*:VA;0)  2.98150E+02  +REC2#;
  3.00000E+03  N REF0 !
   PARAMETER G(L12,CR,PT:*:CR,PT:*:VA;0)  2.98150E+02  +REC2#;
  3.00000E+03  N REF0 !
   PARAMETER G(L12,CR,PT:*:*:CR,PT:VA;0)  2.98150E+02  +REC2#;
  3.00000E+03  N REF0 !
   PARAMETER G(L12,*:CR,PT:CR,PT:*:VA;0)  2.98150E+02  +REC2#;
  3.00000E+03  N REF0 !
   PARAMETER G(L12,*:CR,PT:*:CR,PT:VA;0)  2.98150E+02  +REC2#;
  3.00000E+03  N REF0 !
   PARAMETER G(L12,*:*:CR,PT:CR,PT:VA;0)  2.98150E+02  +REC2#;
  3.00000E+03  N REF0 !

 PHASE TAO_1  %  3 .5  .3  .2  !
    CONSTITUENT TAO_1  :PT : AL : CR : !

PARAMETER G(TAO_1,PT:AL:CR;0)  298.15  -130000+40.28*T+.5*GHSERPT+
.3*GHSERAL+.2*GHSERCR; 3000 N REF0 !

 LIST_OF_REFERENCES
 NUMBER  SOURCE
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