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**A CRITIQUE OF VARIOUS THEORIES'
ABILITY TO PREDICT THE THERMODYNAMICS OF
INORGANIC SOLUTES IN PURE LIQUID METALS**

by

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ABSTRACT

A CRITIQUE OF VARIOUS THEORIES' ABILITY TO PREDICT THE THERMODYNAMICS OF INORGANIC SOLUTES IN PURE LIQUID METALS

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Various theories exist which can be used to calculate the solubility or the activity of inorganics dissolved in liquid metal. This thesis critiques four theories by comparing theory predictions with experimental data.

Each theory contains a free parameter. Correlations were generated for the free parameters by using experimental data to back calculate the free parameters. The correlations were in turn used to predict values which were compared to the experimental data. A large amount of experimental data was gathered.

A surface tension theory of the authors (1) was found to give the best results when calculating the activity coefficient of oxygen or carbon in pure liquid transition metals. The quasi-chemical solution theory of Guggenheim (2) was found to give the best results when

calculating the activity coefficient of oxygen or carbon in pure liquid metals other than the transition metals. The quasi-chemical theory was best for calculating the activity coefficient of hydrogen and nitrogen in any pure liquid metal. The regular solution theory of Hilderbrand (3) and the interaction energy theory of Lee and Johnson (4) was found to be inadequate.

1) Tate "A Critique of Various Theories' Ability to Predict the Thermodynamics of Inorganic Solutes in Pure Liquid Metals" Masters Thesis Michigan State University, Department of Chemical Engineering 1986

2) Guggenheim "Mixtures" Oxford University Press Oxford 1952

3) Hilderbrand and Scott "The Solubility of Non-electrolytes" 3rd edition, Van Nostrand Reinhold, NY 1950

4) Lee and Johnson (I&EC Fundamentals) 1969, vol 8, page 726

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INTRODUCTION

This report derives predictive correlations for activity and solubility of carbon, hydrogen, nitrogen, and oxygen in pure liquid metals. Four theories are considered as starting points. Experimental data are then used to generate correlations relating the free parameter in each theory to physical quantities. The theory with the best predictive ability is determined by comparing predictions to experimental data.

The theories under consideration are: the interaction energy theory of Lee and Johnson (51), the regular solution theory of Hilderbrand (28), the quasi-chemical solution theory of Guggenheim (25), and a surface tension theory of the authors.

Correlations from Lee and Johnson's interaction energy theory predict the solute solubility ratio. i.e. atom fraction / pressure. Correlations from the regular solution and quasi-chemical solution theories predict the solute activity coefficient. Correlations from the surface tension theory predict the solute maximum solubility. Of course, the activity coefficient and maximum solubility are interrelated, For carbon, hydrogen, nitrogen, and oxygen in pure liquid metals the solute activity equals the reciprocal of the solute maximum solubility. Also, at these concentrations, the dissociation pressure equals that for a pure compound.

The solubility data used here represents the entire contents of the three volumes of "Constitution of Binary Phase Diagrams", the two volumes of "The Handbook of Binary Phase Diagrams", Chemical Abstracts

from 1900 through 1983, and the Metals Abstracts through 1983.

The Regular Solution Theory

The regular solution theory was developed by Hilderbrand (28). The derivation presented is based on work found in a book by Lupis (57).

The lattice energy (E) of a mixture of A and B can be modeled as the sum of binary interactions energies:

$$H1) \quad E = N_{aa}U_{aa} + N_{bb}U_{bb} + N_{ab}U_{ab}$$

Where N_{aa} , N_{bb} , and N_{ab} are the number of A-A, B-B, and A-B interactions. U_{aa} , U_{bb} , and U_{ab} are the energies of said interactions.

The total number of interactions involving an A particles is:

$$H2) \quad Z_a N_a = 2N_{aa} + N_{ab}$$

Where Z_a is the coordination number, or number of nearest neighbors, of an A particle. N_a is the number of A particles in solution. The multiplication of N_{aa} by two in equation H2 arises from A-A pairs being counted twice, once for each A particle involved.

Similarly for B particles:

$$H3) \quad ZbNb = 2Nbb + Nab$$

Combining equations H1, H2, and H3 to eliminate Naa and Nbb:

$$H4) \quad E = ZaNauaa/2 + ZbNbUbb/2 + Nab(Uab - Uaa/2 - Ubb/2)$$

The factors $ZaNauaa/2$ and $ZbNbUbb/2$ can be modeled as the energy of pure A and B. The factors are thus replaced by Ea and Eb .

Replacing $(Uab - Uaa/2 - Ubb/2)$ with the Wab , equation H4 becomes:

$$H5) \quad E = Ea + Eb + NabWab$$

Degeneracy is the number of configurations a system can occupy at an energy level. The degeneracy of randomly positioned particles is given by Denbigh (16):

$$H6) \quad g = N! / Na!Nb!$$

Where N is the total number of particles in solution.

The probability that an arbitrary site will be occupied by an A particle is the mole fraction of A; X_a . The probability that a B particle will occupy an adjacent site is similarly X_b . The probability that both occupations will occur at the same time is $X_a X_b$. Since the molecules can be placed A-B or B-A, the probability that the two adjacent sites can be occupied by an A and B particle is $2X_a X_b$. Multiplying by the total number of pairs yields the number of A-B pairs:

$$N_{ab} = 1/2 (Z_a N_a + Z_b N_b) * 2X_a X_b$$

If the coordination numbers of A and B particles are assumed equal:

$$H7) \quad N_{ab} = Z N_a N_b / N$$

The partition function of a system is (Denbigh (16)):

$$H8) \quad Q = \frac{N_a}{q_a} \frac{N_b}{q_b} \exp (-E_i / kT)$$

Where Q is the partition function of the entire system. q_a and q_b are the partition functions of the individual A and B particles. g_i and E_i are the degeneracy and energy of the system at energy level i . k and T are Boltzmann's constant and temperature.

The summation in equation H8 is over all possible energy levels. Under the regular solution theory, the system is confined to one state, the random one. Thus it is also confined to one energy level. The summation in equation H8 can thus be removed. Combining the resulting equation H8 with equations H7, H6, and H5:

$$H9) \quad Q = (N! / N_a! N_b!) \frac{N_a}{q_a} \frac{N_b}{q_b} \exp [-(E_a + E_b + Z N_a N_b W_{ab} / N) / kT]$$

From statistical thermodynamics:

$$G = -kT \ln Q$$

Thus:

$$\text{H10)} \quad G = -kT \ln (N! / N_a! N_b!) + E_a + E_b + Z N_a N_b W_{ab} / N + N_a \ln q_a + N_b \ln q_b$$

If the terms in equation H10 which refer to the pure substances are removed, the free energy of mixing results:

$$\text{H11)} \quad G^M = -kT \ln (N! / N_a! N_b!) + Z N_a N_b W_{ab} / N + N_a \ln q_a + N_b \ln q_b$$

Using the result that $\ln X! = X \ln X - X$

$$G^M = kT (N_a \ln N_a - N_a + N_b \ln N_b - N_b - N \ln N + N) + Z N_a N_b W_{ab} / N + N_a \ln q_a + N_b \ln q_b$$

$$\text{H12)} \quad G^M = kT (N_a \ln X_a + N_b \ln X_b) + Z N_a N_b W_{ab} / N + N_a \ln q_a + N_b \ln q_b$$

Changing equation H12 to a per mole basis:

$$\text{H13)} \quad G_M^M = RT (X_a \ln X_a + X_b \ln X_b) + Z X_a X_b W_{ab} + X_a \ln q_a + X_b \ln q_b$$

If the terms in equation H13 which relate to the ideal solution are removed, the excess free energy of mixing results:

$$H14) \quad G_m^E = ZWabX_aX_b$$

Partial molar quantities can be calculated from mixture molar quantities (Denbigh (16)):

$$H15) \quad Y_a = Y_m + (1 - X_a) (dY_m / dX_a)$$

Where Y_m is a molar quantity of the mixture, and Y_a is a partial molar quantity of substance A. The partial excess molar free energy of A is:

$$H16) \quad G_a^E = G_m^E + (1 - X_a) (dG_m^E / dX_a)$$

$$= ZWabX_a (1 - X_a) + (1 - X_a) (ZWab - 2ZWabX_a)$$

$$= ZWab (1 - 2X_a + X_a^2)$$

$$H17) \quad G = ZWabX_b^2$$

Partial molar excess free energy can be related to the activity coefficient (Lupis (57)):

$$\text{H18)} \quad G_a^E = kT \ln \gamma_a$$

Where γ_a is the activity coefficient of A. Combining equations H17 and H18:

$$\text{H19)} \quad \ln \gamma_a = ZWabX_b^2 / kT$$

Calculation Scheme

Equation H19 of the derivation reads:

$$\text{H20)} \quad \ln \gamma_a = Z W_{ab} X_b^2 / kT$$

Where γ_a is the activity coefficient of the solute. Z is the coordination number or number of next nearest neighbors of the solute. X_b is the concentration of the solvent. T is temperature. k is Boltzmann's constant. W_{ab} is the change in pair wise interaction energies for the reaction:



Equation H20 can be solved for W_{ab} :

$$\text{H22)} \quad W_{ab} = RT \ln \gamma_a / X_b^2 Z$$

Note that the ideal gas law constant R , has been substituted for k in equation H22. This changes the units of W_{ab} to energy per mole.

γ_a , X_b , and T are available from experimental data. The reference state for the activity coefficient; γ_a , of the regular solution theory is set by equation H20. As the concentration of the solvent; X_b , goes zero, the solute activity coefficient goes to one.

The coordination number of the solute; Z , is a function of the

solvent-solute lattice structure. Data on the structure of individual solvnet-solute lattice were not analyzed. Z was assumed a constant for each solute. The coordination numbers used: oxygen six, nitrogen six, carbon four, and hydrogen one.

Discussion

System energies are modeled as due to the interaction energies of pairs (equation H1 and H5). The scheme ignores the effect of next nearest neighbors on particle interactions. This calculation scheme is lacking for liquid metal systems where electron delocalization is the rule.

The degeneracy is defined as being calculated from an assumption of randomly distributed particles (equation H6). For this assumption to hold the interaction energies of solute-solute, solute-solvent, and solvent-solvent pairs should be of the same order. Also, the solvent and solute should occupy the same lattice positions, thus they should be of the same size. The solvent and solute must also have the same coordination number (equation H7), this requirement puts more need on the solvent and solute of having the same size.

Quasi-Chemical Solution Derivation

The quasi-chemical solution theory was developed by Guggenheim (25). The derivation presented is based on work found in Lupis (57).

The quasi-chemical solution theory is similar to the regular solution theory presented in the previous sections. Both were designed for binary solutions. For a solution of A and B, equations H1 through H4 of the regular solution theory development are valid for the quasi-chemical solution development.

The developments split when defining degeneracy. The degeneracy of the regular solution is based on an assumption of randomly positioned particles. The degeneracy of the quasi-chemical solution is based on an assumption of randomly positioned pairs. The degeneracy of the quasi-chemical solution can thus be expressed:

$$G1) \quad g1 = 1/2 ZN! / (N_{aa}! N_{bb}! [(N_{ab}/2)!]^2)$$

Where N, N_{aa} , N_{bb} , and N_{ab} are the number A and B particles, A-A pairs, B-B pairs, and A-B pairs respectively. Z is the coordination number of A and B particles. The term $[(N_{ab}/2)!]$ squared arises from the distinguishability of A-B and B-A pairings.

Equation H1 over estimates the degeneracy as all pairs are not independent. If an A-A pair is adjacent to a B-B pair, two A-B pairs are necessarily produced. To account for this over counting, the factor h is introduced:

$$G2) \quad g = h g_i$$

Where h is calculated by use of the degeneracy of a random arrangement.

This is expressed by equation H6 of the regular solution derivation:

$$G3 \quad g^o = N! / N_a! N_b!$$

$$= h * 1/2 \, ZN! / (N_{aa}^o \, N_{bb}^o \, [(N_{ab}^o/2)!]^2)$$

Where the superscript o designates values predicted by regular solution model. Solving equation G3 for h , and then using this value of h in equation G2 yields:

$$G4) \quad g = \frac{N_{aa}^o! \, N_{bb}^o! \, [(N_{ab}^o/2)!]^2}{N_{aa}! \, N_{bb}! \, [(N_{ab}/2)!]^2} * \frac{N!}{N_a! \, N_b!}$$

The second group of terms on the right side of equation G4 is the regular solution theory degeneracy, which assumes a solution of

randomly positioned particles. The first factor on the right side of equation G4 can be then be thought of as a correction factor. Using equation H3 of the regular solution derivation, equation G4 trnasforms to:

$$G5) \quad q = \frac{(\frac{1}{2} Z N_a - \frac{1}{2} N_{ab}^o)! (\frac{1}{2} Z N_b - \frac{1}{2} N_{ab}^o)!}{(\frac{1}{2} Z N_a - \frac{1}{2} N_{ab})! (\frac{1}{2} Z N_b - \frac{1}{2} N_{ab})!} * \\ \frac{[(N_{ab}^o / 2)!]^2}{[(N_{ab} / 2)!]^2} * \frac{N!}{N_a! N_b!}$$

As seen in the regular solution theory the free energy of a system is given by:

$$G6) \quad G = -kT \ln(g \exp(-E/kT))$$

Where E is the energy of the system, k is Bolztmans constanst, and T is temperature. Using equation H1 of the regular solution theory developement with equation G6 yields:

$$G7) \quad G = -kT \ln \sum g \exp (-(E_a + E_b - N_{ab}W_{ab}) / kT)$$

Removing the terms in equation G7 which relate to the pure substances results in the free energy of mixing:

$$G8) \quad G^M = -kT \ln \sum g \exp (-N_{ab}W_{ab} / kT)$$

The summation in equation G8 can be replaced by the maximum term of the summation. The maximum term is found from the derivative equation:

$$G9) \quad d (g \exp (-N_{ab}W_{ab} / kT)) / d N_{ab} = 0$$

Or equivalently:

$$G10) \quad d (\ln g - N_{ab}W_{ab} / kT) / d N_{ab} = 0$$

g is defined by equation G5. In taking the derivative of g in

equation G10 only terms which are a function of N_{ab} need be retained:

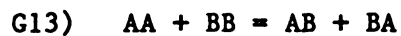
$$\begin{aligned} \text{G11)} \quad d \left(-\ln \left(\left(\frac{1}{2} Z N_a - \frac{1}{2} N_{ab} \right)! \right) - \ln \left(\left(\frac{1}{2} Z N_b - \right. \right. \right. \\ \left. \left. \left. \frac{1}{2} N_{ab} \right)! \right) - 2 \ln \left(\left(\frac{N_{ab}}{2} \right)! \right) - \frac{N_{ab} W_{ab}}{kT} \right) / d N_{ab} = 0 \end{aligned}$$

Using the result that: $d(\ln X!) = d(X \ln X - X) = \ln X \, dX$

$$\begin{aligned} \frac{1}{2} \ln \left(\frac{1}{2} Z N_a - \frac{1}{2} N_{ab} \right) + \\ \frac{1}{2} \ln \left(\frac{1}{2} Z N_b - \frac{1}{2} N_{ab} \right) - \ln \left(\frac{N_{ab}}{2} \right) - \frac{W_{ab}}{kT} = 0 \end{aligned}$$

$$\text{G12)} \quad \left(\frac{1}{2} N_{ab} \right)^2 / N_a N_b = \exp \left(-2 W_{ab} / kT \right)$$

Note that the left side of equation G12 defines the equilibrium constant for the reaction:



Thus:

$$G14) \quad (1/2Nab)^2 / NaaNbb = K = \exp (-\Delta G / RT) = \exp (-2Wab / kT)$$

Where ΔG is the free energy of the reaction in equation G13. From equation G14, Wab and ΔG can be related:

$$G15) \quad \Delta G / R = 2Wab / k$$

Equation G12 can then be written:

$$G16) \quad (1/2Nab) / ((1/2ZNa - 1/2Nab)(1/2ZNb - 1/2Nab)) = \exp (-2Wab / kT)$$

Or:

$$G17) \quad L Nab^2 + Z NabN + Z^2 NabNb = 0$$

Where $L = \exp(2Wab/kT) - 1$. Applying the quadratic formula to equation G18 yields the roots:

$$G18) \text{ Root} = ZN / 2L * (-1 + (1 + 4LXaXb)^{1/2})$$

Note only the positive root has been retained. A negative root would yield a negative value of Nab, which would have no physical meaning.

The square root function is approximated by:

$$G19) (1 + X)^{1/2} = 1 + X/2 + X^2/8 + \dots$$

Equation G18 thus becomes:

$$\text{Root} = \text{Nab} = ZN / 2L * (-1 + (1 + 4LXaXb/2 - 16L^2 Xa^2 Xb^2 / 8))$$

$$G20) \text{ Nab} = ZNaNb/N * (1 - 1XaXb)$$

Equation G20 describes the value of Nab which will yield the maximum value of the expression $g \exp(-\text{NabWab}/kT)$ in equation G8. $ZNaNb/N$ is the number of A-B pairs as predicted by the regular solution theory (equation H7 of the regular solution theory development). Equation G20 can thus be written:

$$G21) \quad N_{ab} = N_{ab}^0 (1 - L X_a X_b)$$

Where N_{ab}^0 is the number of A-B pairs as predicted by the regular solution theory.

From equation G21 it is seen that if L is positive N_{ab} is greater than N_{ab}^0 . For L to be positive, W_{ab} and in turn ΔG , must be positive. Thus if the reaction to form A-B pairs from A-A pairs and B-B pairs is exothermic, the number of A-B pairs predicted by the quasi-chemical theory is greater than the number predicted by the regular solution theory.

Equation G20 can be substituted in equation G4 to obtain a new expression for g . After long calculations, the excess free energy results:

$$G22) \quad G^E / kT = 1/2 Z X_b \ln (1 + L) + 1/2 Z L X_b^2 \\ + 1/2 Z L^2 X_b^2 - Z L^2 (1/4 + 5/3 L) X_b^4$$

Using equation H14 of the regular solution theory:

$$G23) \quad G_a^E = G_m^E + (1 - X_a) dG_m^E / dX_a$$

Since $d(X_a) = d(1-X_b) = -d(X_b)$ equation G23 transform to:

$$G24) \quad G_a^E = G_m^E - X_b \, dG_m^E / dX_b$$

Equation G22) thus yeilds:

$$G25) \quad \ln \gamma_a = G_a^E / RT = \\ 1/2 ZL X_b^2 - ZL^2 X_b^3 + 3/4 ZL^2 X_b^4 (1 + 20/3L)$$

Calculation Scheme

Equation G25 of the derivation reads:

$$G26) \quad \ln \gamma_a = 1/2 ZL X_b^2 - ZL^2 X_b^3 + 3/4 ZL^2 X_b^4 (1 + 20/3L)$$

Where γ_a is the activity coefficient of the solute. X_b is the solvent concentration. Z is the solute coordination number. L is defined:

$$\text{G27)} \quad L = \exp (2W_{ab} / kT) - 1$$

Where k is Boltzmann's constant. T is temperature. W_{ab} is defined in the same manner as for the regular solution theory. k can be replaced with the ideal gas law constant. This will make the units of W_{ab} energy per mole.

Equation G26 can be written:

$$\text{G28)} \quad 5ZX_b^4 L^3 + (3/4ZX_b^4 - ZX_b^3)L^2 + 1/2ZX_b^2 L - \ln \gamma_a = 0$$

X_b and γ_a can be obtained from experimental data. Z is assumed constant (see regular solution theory calculation scheme). Equation G28 can be solved for L by using synthetic division. L can be used in equation G27 to calculate W_{ab} .

The reference state for the activity coefficient for the quasi-chemical theory is defined by equation G26. As the concentration of the solvent goes to zero the activity coefficient of the solute goes to one.

Discussion

As in the regular solution theory, the quasi-chemical solution theory models system energies as due to first order interaction energies (equations H1 and H5 of the regular solution derivation). The effect of next nearest neighbors on interaction energies is ignored.

The degeneracy of the quasi-chemical solution is defined as being calculated from the assumption of a solution of randomly distributed pairs (equation G1). This scheme allows for preferred pairs. The interaction energies of the solute-solute, solute-solvent, and solvent-solvent do not have to be of the same order.

But the solvent and solute should be of the same size. Equation G1 requires that the solvent and solute have the same coordination number.

Lee and Johnson Theory Development

The following is based on work found in Lee (51).

The chemical potential of a solute particle is given by (Fowler (22)):

$$L1) \quad \mu_s^l = -\psi_s - kT \ln \phi_s + kT \ln (N_s/V)$$

Where μ_s^l , ψ_s , and ϕ_s are the chemical potential, potential energy, and total partition function of the solute. Note that ψ_s has a reference value of zero in the gas state. V is the volume of solution; N_s is the number of solute particles; k is the boltzman constant; and T is the absolute temperature. Note that:

$$L2) \quad N_s / V = \# \text{ of solute molecules} / \text{volume of solution}$$

$$N_s / V = \# \text{ of solute molecules} / \# \text{ solution molecules}$$

$$* \text{ average molecular volume of solution molecules}$$

$$N_s / V = X_s / \bar{v} \text{ ave soln}$$

Assuming that the average molecular volume of all solution molecules is equal to the molecular volume of solvent molecules ($\bar{v}_1$):

$$L3) \quad N_s / V = X_s / \bar{v}_1$$

The chemical potential can be modeled:

$$L4) \quad \psi_s = E_d + W(r) + g$$

Where E_d is the work of discharging the interaction energies of the solute molecule when removed from the gas phase. $W(r)$ is the energy required to create a hole in the pure solvent. g is the energy required to put the solute in the hole. The solute and solvent are modeled as not interacting; g is zero.

E_d is modeled:

$$L5) \quad E_d = E_i + p \, \text{del}V$$

Where E_i is the reversible work of discharging the interaction energies of the solute molecule in the gas phase. $p \, \text{del}V$ is the work required

to change the volume of the solute molecule on going from gas state to a liquid state.

E_1 is modeled using the dispersive portion of the Lennard-Jones (6-12) potential energy function:

$$L6) \quad E_1 = 4 \epsilon_s a_s^6 \sum (1/r)^6$$

Where ϵ_s is the maximum energy of dispersion between gas molecules. a_s is the collision diameter of the solute gas molecule. r is the radial distance between molecules. Summing over all molecules, equation L6 becomes:

$$L7) \quad E_1 = 4 \epsilon_s a_s^6 \int_{a_s}^{\infty} (-4\pi \rho_s r^2 dr / r^6)$$

Where ρ_s is the density of the solute in the gas phase. Integration yields:

$$L8) \quad E_1 = -(16/3)\pi \epsilon_s a_s^6 \rho_s$$

The second factor on the right side of equation L5 is given by:

$$L9) \quad p \, dV = p \left(4\pi a s^6 / 3 - \sqrt{s} \right)$$

Where $\sqrt{s}$ is the molecular volume of the solute molecule in the gas phase.

Combining equations L9, L8, and L5:

$$L10) \quad E_d = (-16/3)\pi \epsilon_s a s^2 \rho_s + p \left(4\pi a s^3 / 3 - \sqrt{s} \right)$$

Using the ideal gas law to transform equation L10:

$$L11) \quad E_d = -16\pi \epsilon_s a s^2 p / (3kT) + 4\pi a s^3 p / 3 - kT$$

Riess (90) models $W(r)$ of equation L4:

$$L12) \quad d(W(r)) = p 4\pi r^2 dr + \sigma 8\pi dr$$

Where p is pressure, r is the radius of the cavity created, and σ is the surface tension of the solvent. The first term on the right side of equation L12 is the work of expanding the cavity. The second term on the right is the work done in overcoming the surface tension of the solvent in creating the cavity. Integrating:

$$L13) \quad W(r) = (4/3)\pi r^3 p + 4\pi r^2 \sigma$$

To account for curvature on surface tension, a film thickness parameter (δ) must be added to L13:

$$L14) \quad W(r) = (4/3)\pi r^3 p + 4\pi r^2 \sigma (1 - (2\delta/r))$$

Film thickness parameters are difficult to measure or model. This reduces the usefulness of equation L14 for this work. The film thickness parameter will not be used in this work. Reiss (90) references development of the film thickness parameter.

Reiss (92) in another work states that the probability of creating a cavity of radius L ; which does not contain the center of a

solvent molecule, is related to work required to create the cavity:

$$L15) \quad \text{RHO}(L) = \exp (-W(L) / kT)$$

Where $\text{RHO}(L)$ is the probability of creating the cavity and $W(L)$ is the work required to create the cavity. For cavities of radius less than or equal to of the radius of the solvent molecule, the pobability that said cavity will contain the center of a solvent molecule is $(4/3)\pi L^3 \rho$. . Where L is the radius of the cavity and ρ is the number density of the solvent. It follows that the probability the cavity does not contain the center of a solvent molecule is:

$$L16) \quad \text{RHO}(L) = 1 - (4/3)\pi L^3 \rho$$

Combining equation L15 and L16:

$$L17) \quad W(L) = -kT \ln (1 - (4/3)\pi r^3 \rho)$$

Equation L17 thus discribes the work required to create a cavity of radius less than or equal to the radius of the solvent molecule. This reduces the usefulness of equation L17.

Reiss (90) in another work models the factor $W(r)$ by a polynomial expansion:

$$\text{L18)} \quad W(r) = K_3 r^3 + K_2 r^2 + K_1 r + K_0$$

Comparison of equation L18 and L14 yeilds:

$$\text{L19)} \quad K_3 = (4/3) \pi p$$

Reiss then calculates the remaining constants of equation L18 by comparing equations L17 and L18 and their derivatives at the point where the radius of the cavity equal the radius of the solvent. Comparing equations L17 and L18:

$$\text{L20)} \quad K_0 + K_1 a_1 + K_2 a_1^2 + K_3 a_1^3 = -kT \ln (1 - 4\pi a_1^3 \rho / 3)$$

Where a_1 is the radius of the solvent molecule. Taking derivatives:

$$\text{L21)} \quad K1 + 2K2a1 + 3K3a1^2 =$$

$$kT (1 / (1 - (4/3)\pi\rho a1^3)) * 4\pi\rho a1^2$$

$$\text{L22)} \quad 2K2 + 6K3a1 =$$

$$kT \{ (1 / (1 - (4/3)\pi\rho a1^3))^2 * 16\pi^2\rho a1^4 +$$

$$8\pi\rho a1 * (1 / (1 - (4/3)\pi\rho a1^3)) \}$$

With the simplifications:

$$\text{L23A)} \quad K3 = 4\pi\rho / 3$$

$$\text{L23B)} \quad y = 4\pi\rho a1^3 / 3$$

Equation L23 transforms to:

$$\text{L24)} \quad K2 = (kT / 2a1^2) * \{ 9(y / (1 - y))^2 + 6y / (1 - y) \} -$$

$$4\pi\rho a1$$

Combining equations L21 and L23 with the aforementioned

simplifications:

$$\text{L25) } K1 = (-kT / a1) * \{ 9(y / (1 - y))^2 + 3y / (1 - y) \} + 4\pi p a1^3$$

Similarly, equation L20 yields:

$$\text{L26) } K0 = -kT \ln (1 - y) + kT (4.5 (y / (1 - y))^2) - 4\pi p a1^3 / 3$$

Combining equations L18, L24, L25, and L26:

$$\begin{aligned} \text{L27) } W(r) = & -kT \ln (1 - y) + kT (4.5 (y / (1 - y))^2) - 4\pi p a1^3 / 3 \\ & - (r / a1) kT \{ 9(y / (1 - y))^2 + 3y / (1 - y) \} \\ & - (r / a1)^2 kT \{ 4.5(y / (1 - y))^2 + 3y / (1 - y) \} \\ & + 4\pi p a1^2 r - 4\pi p a1 r^2 + (4/3) \pi p r^3 \end{aligned}$$

The radial measure terms (r and a) in equation L27 are of order E-8. Thus the pressure (p) terms in equation L27 are of order E-20. y is defined by equation L23B. The number density factor (ρ) is of order E23. Thus y is of order E-1. The pressure terms in equation L27 can thus be eliminated to yield:

$$\begin{aligned}
W(r) = & -kT \ln (1 - y) + 4.5kT (y / (1 - y))^2 \\
& -(r / a1) kT (9 (y / (1 - y))^2 + 3y / (1 - y)) \\
& +(r / a1)^2 kT (4.5 (y / (1 - y))^2 + 3y / (1 - y))
\end{aligned}$$

Combining this short form of equation L27 with equations L1, L3, L4, and L11 yields:

$$\begin{aligned}
L28) \quad \mu_s^f = & -kT \ln (1 - y) + 4.5kT (y / (1 - y))^2 \\
& -(r / a1) kT (9 (y / (1 - y))^2 + 3y / (1 - y)) \\
& +(r / a1)^2 kT (4.5 (y / (1 - y))^2 + 3y / (1 - y)) \\
& + 16\pi\epsilon_s a s^2 p / (3kT) + 4\pi a s^3 p / 3 - kT \\
& + kT \ln \phi_s + kT \ln (X_s / \sqrt{1})
\end{aligned}$$

As in equation L27, the pressure terms in equation L28 can be removed by unit analysis. Note that this simplification effectively reduces equation L11 to:

$$L29) \quad E_d = -kT$$

The chemical potential of a ideal gas molecule is given by
(Fowler (22)):

$$\text{L30)} \quad \mu_s^g = -kT \ln \phi_s + kT \ln (P_s / kT)$$

Where ϕ_s is the partition function of a lone solute gas molecule. Note that the term ϕ_s is the same in equations L1, L29, and L30. P_s is the partial pressure of the solute.

At equilibrium:

$$\text{L31)} \quad \mu_s^l = \mu_s^g$$

Equations L30 and L28 combine to yield:

$$\begin{aligned} \text{L32)} \quad \ln (P_s / X_s) = & -\ln (1 - y) + 4.5 (y / (1 - y))^2 - 1 \\ & + \ln (kT / \sqrt{1}) \\ & - (r / a_1) (9 (y / (1 - y))^2 + 3y / (1 - y)) \\ & + (r / a_1)^2 (4.5 (y / (1 - y))^2 + 3y / (1 - y)) \end{aligned}$$

Where a_1 , v_1 are the radius and molecular volume of the solvent molecule

P_s , X_s are the partial pressure and mole fraction of the solute

r is the sum of the solute and solvent radii

y is defined by equation L23B

Calculation Scheme

In equation L32 P_s and X_s are the solute partial pressure and concentration in the liquid solution. The term P_s/X_s has units of pressure over atom fraction. Most experimentally measured solubility data is in units of pressure to the 0.5 power over atom fraction. When the pressure equals one, the numerical values of the ratios P_s/X_s and square root $(P_s) / X_s$ are equal. It will be assumed that experimentally measured solubility ratios used are valid at one atmosphere pressure. In actuality, most experimental data was given at one atmosphere.

With the following substitutions:

$$KH = X_s / P_s = X_s / (\text{square root } P_s) \quad @ P_s = 1 \text{ atmosphere}$$

$$D = y / (1 - y)$$

equation L31 transforms to:

$$\begin{aligned} \text{L32)} \quad 0 = & \ln (KH \, kT / ((1 - y) \sqrt{1})) + 4.5D^2 - 1 \\ & - (r / a_1) (9D^2 + 3D) + (r / a_1)^2 (4.5D^2 + 3D) \end{aligned}$$

Equation L32 can be written:

$$\text{L33)} \quad 0 = Ar^2 + Br + C$$

$$\text{where } A = (4.5D^2 + 3D) / a_1^2$$

$$B = - (9D^2 + 3D) / a_1$$

$$C = \ln (KH \, kT / (1 - y) \sqrt{1})) + 4.5D^2 - 1$$

Equation L33 can be solved for r by using the quadratic equation:

$$\text{L34)} \quad r = a_1 + a_2 = (-B \pm \sqrt{B^2 - 4AC}) / 2A$$

If the expression determinate in equation L34 is negative the roots are imaginary. Since the roots represent r, which is a radial distance, the determinate must be greater than or equal to zero:

$$\text{L35)} \quad B^2 - 4AC \geq 0$$

$$\text{Or:} \quad C \leq B^2 / 4AC$$

$$\begin{aligned} \text{Or:} \quad \ln (KH \, kT / (1 - y) \sqrt{1})) + 4.5D^2 - 1 \leq \\ \{ (9D^2 + 3D)^2 / a_1^2 \} / \{ 4 (4.5D^2 + 3D) / a_1^2 \} \end{aligned}$$

$$\begin{aligned} \ln (KH \, T) \leq (81D^4 + 54D^3 + 9D^2) / (18D^2 + 12D) \\ - 4.5D^2 + 1 + \ln ((1 - y) \sqrt{1} / k) \end{aligned}$$

$$\text{L36)} \quad \ln (KH \, T) \leq (9D + 4) / (6D + 4) + \ln ((1 - y) \sqrt{1} / k)$$

D in equation L36 is defined:

$$\text{L37)} \quad D = y / (1 - y)$$

$$\text{L38)} \quad y = (4/3)\pi\rho a_1^3$$

a_1 and ρ are the radius and the number density of the solvent. If the solvent atoms are assumed spherical, the radius of the solvent can be calculated from number density data:

$$\text{L39)} \quad a_1 = (3 / (4\pi\rho))^{1/3}$$

Combining equations L39 and L38 yields a value of y of one. This is unacceptable; if y equals one, equation L38 predicts a value of D of one over zero. To avoid this problem a packing fraction parameter is added to equation L39:

$$\text{L40)} \quad a_1 = (3PF / (4\pi\rho))^{1/3}$$

Where PF is the fraction of space that the solvent atoms occupy in the solvent lattice. Combining equations L40 and L38 shows that y equals the packing fraction PF. Equation L36 modifies to:

$$\text{L41)} \quad \ln (KH T) \leq (5PF + 4) / (2PF + 4) + \ln ((1 - PF) \sqrt{1/k})$$

The factor $\sqrt{1/k}$, the solvent molecular volume divided by Boltzmann's constant, is equal to V_m/R , the molar volume divided by the ideal gas law constant. This substitution modifies equation L41 to:

$$\text{L42)} \quad \ln (KH T) \leq (5PF + 4) / (2PF + 4) + \ln ((1 - PF) V_m / 82.05)$$

Note that the units of V_m in the equation above is necessarily cubic centimeters per gram mole, due to the value of the ideal gas constant, R , used.

The molar volume of liquid metals is between 1 and 200.

Substituting these boundary conditions in equation L43; with PF equal 0.6, yields:

$$\text{L43A)} \quad \ln (KH T) \leq -3.3964 \quad \text{at } V_m = 1$$

$$\text{L43B) } \ln (KH T) \leq 1.9019 \quad \text{at } V_m = 200$$

Solving for KH in equation L43B yields:

$$\text{L44) } KH \leq 6.699 / T$$

This sets a limit on the effectiveness of the Lee and Johnson theory; for the calculation scheme used. An upper limit on the range of effectiveness of the calculation scheme used can be obtained by maximizing both terms of equation L43. The first term on the right side of equation L43 has a maximum value of 1.8 at PF equals one. The second term on the right side of equation L43 has a maximum value of 0.8910 at PF equal zero and V_m equals 200. Using both maximum values together yields an upper limit on the values of KH that are valid with the calculation scheme derived:

$$\text{L45) } KH \leq 14.746 / T$$

If equation L45 is followed by the experimental data, equation L35 can be used to calculate the radius of the solute atom.

Discussion

There are three noticable assumptions in the Lee & Johnson theory: 1) the average molecular volume of all solution molecules is equal to the molecular volume of the solvent molecules; 2) the attraction energies of the molecules in the gas phase are insignificant; 3) solute-solvent interactions in the liquid phase are insignificant.

For the solution average molecular volume to be equal to the solvent molecular volume requires that the solute concentration is dilute or that the solvent and solute are of the same relative size.

The neglect of the attractive energies of the gas molecule in equation L6 of the Lee and Campbell theory derivation is not serious. Including the factor would generate more pressure terms in equation L26 of the derivation. Pressure terms are cancelled out of equation L26 by a unit analysis.

The neglect of interaction energies of the solute and solvent

in the liquid solution is the source of largest error. The factor g in equation L4 of the Lee and Campbell theory represents solvent-solute interaction energies. If g was not assumed zero in equation L4, it would next show up on the right side of equation L28. Then g would appear in the equation L32, again on the right side of the equation. Assuming that g would be a constant, g would appear next in the expression for C in equation L33 above. Next g would appear in on the right side of equation L36. It would appear as $(-g)$. For organic solutes and metals, interaction would be exothermic. Energies would negative. Thus the factor $\ln(KH T)$ would be less limited by equation L36. This would expand the range of validity of the Lee and Johnson theory under the calculation scheme used.

Emi and Pehlke Theory Development

The following derivation is based on work found in Emi (79, 82). This model is similar to the Lee and Johnson theory of the previous section.

The chemical potential (μ) of a gas atom is given by:

$$\begin{aligned} \text{E1) } \mu_a^g &= (1/2) \mu_H^g + X_d / (2kT) \\ &= (1/2) d (-kT \ln (q_a^N / N!)) @ \text{ constant } T, V + \\ &\quad X_d / (2kT) \end{aligned}$$

Where μ_a and μ_H are the chemical potential of the gas atom and molecule. X_d is the dissociation energy of the diatomic gas. q_a is the total partition function for a system of N gas molecules. k is Boltzmann's constant and T is temperature.

Using the result $\ln N! = N \ln N - N$, equation E1 reduces to:

$$\text{E2) } \mu_a^g = - (\ln q_a - \ln N) kT / 2 + X_d / (2kT)$$

The partition function of a gas molecule can be expressed in by the following (Rushbrooke (94)):

$$E3) \quad q = (P.F.)_{trans} * (P.F.)_{rot} * (P.F.)_{vib} * (P.F.)_{elec}$$

Where q is the total partition function. $(P.F.)_{trans}$, $(P.F.)_{rot}$, and $(P.F.)_{vib}$ are the partition function of the translational, rotational, and vibrational motions of the molecule. $(P.F.)_{elec}$ is the partition function due to electronic permeations. They can be expressed:

$$E4A) \quad (P.F.)_{trans} = (2\pi mkT)^{3/2} V / (\sigma h^3)$$

$$E4B) \quad (P.F.)_{rot} = 8\pi^2 I kT / h^2$$

$$E4C) \quad (P.F.)_{vib} = 1 / (1 - \exp(-h\nu / (kT)))$$

$$E4D) \quad (P.F.)_{elec} = W_e \epsilon^2 / \delta$$

Where σ is a symmetry factor, two for homonuclear molecules and one for heteronuclear molecules. M , I , and ν are the mass, moment of inertia, and frequency of the molecule. W_e is the degeneracy of the molecule in its electronic ground state. ϵ is the spin degeneracy of the molecule. δ is a second symmetry factor of the molecule. T is temperature. V is

the volume of the system. h and k are Planck's and Boltzmann's constants.

The moment of inertia for a diatomic molecule is given by (Rushbrooke (94)):

$$E5) \quad I = m_a m_b / (m_a + m_b) * r_d^2$$

Where m_a and m_b are the mass of the atoms of the diatomic molecule. r_d is the radius separation of minimum potential energy. The factor r_d is obtainable directly from Lennard-Jones 6-12 data.

A diatomic molecule can be modeled as two weights (atoms) attached by springs to a fixed center point. The frequency of vibration in equation 4C is then the classical frequency of a harmonic oscillator:

$$E6) \quad \nu = \text{square root } (k / m) / 2\pi$$

Where m is the mass of the vibrating atom and k is the spring force constant. A possible technique for obtaining a value for k would be to use the Lennard-Jones 6-12 potential energy equation and plot the potential energy at different radial separations. A force constant could then be worked out. For more accuracy the speed of the atom could be used to take into account energy used to change the kinetic

energy of the molecule.

The chemical potential of a solute in a dilute solution is given by (Guggenheim (25)):

$$E7) \quad \mu_a^l = -\phi_{12} - kT \ln \left((2\pi mkT)^{3/2} / h^3 \right) + kT \ln (N/V)$$

Where ϕ_{12} is the potential energy of the solute. N is the number of solute molecules. m is the mass of the solute molecule. V is the system volume.

The approximation:

$$E8) \quad N / V = X_s / \bar{v}_1 = X_s N_A \rho_m$$

was discussed in the derivation of the Lee and Johnson theory. X_s is the mole fraction of the solute. $\bar{v}_1$ and ρ_m are the molecular volume and molar density of the solvent. N_A is Avogadro's number.

The potential energy of the solute can be modeled:

$$E9) \quad -\phi_{12} = g_1 + W(r)$$

Where g_1 is the energy of interaction between solute and solvent molecule. Emi (79, 82) assumes these to be zero. The factor $W(r)$ is the energy required to create a cavity in the solvent. $W(r)$ is modeled in the same manner as in the Lee and Johnson theory, using the work of Reiss. Note that equation E10 does not include any factor to account for the dispelling of interaction energies of the solute in the gas phase. This factor was accounted for in the Lee and Campbell theory development.

At equilibrium:

$$E10) \quad \mu_a^l = \mu_a^g$$

Combining equations E2, E3, E4A, E4B, E4C, E4D, E7, E8, and E9 with the following simplifications;

$$\bar{K} = (2\pi mkT)^{3/2} / h^3$$

$$\bar{I} = 8\pi^2 I k / h^2$$

$$\bar{V} = 1 / (1 - \exp(-h\nu / (kT)))$$

$$\bar{\epsilon} = w_e \epsilon / \gamma$$

yields the expression

$$\begin{aligned} \text{E11) } W(r) - kT (\ln \bar{K} + (3/2) \ln T) + kT \ln (X_s \text{ Navo } dm) = \\ - (kT/2) (\ln \bar{K} - \ln \theta + (5/2) \ln T + \ln \bar{I} + \\ \ln \bar{V} + \ln \bar{\epsilon} + \ln (V/N)) + X_d / (2kT) \end{aligned}$$

Equations E11 simplifies:

$$\begin{aligned} \text{E12) } \ln X_s = -W(r) / (kt) + (1/2) \ln (\bar{K} \theta / (\bar{I} \bar{V} \bar{\epsilon} \text{ Navo } dm)) + \\ \ln T / 4 - \ln (N/V) / 2 + X_d / (2kT) \end{aligned}$$

From the ideal gas law $N/V = P/kT$. Using this result:

$$\text{E13)} \quad \ln (X_s / P_s^{1/2}) = (1/2) \ln (\bar{K} \sigma / (\bar{I} \bar{J} \bar{E} \text{ Navo dm } T^{1/2} k)) - \\ (W(r) - X_d / 2) / (kT)$$

For a monatomic molecule X_d is zero and the rotational and vibrational partition functions; equations E4B and E4C, are one. Thus equation E13 is modified to:

$$\text{E14)} \quad \ln (X_s / P_s) = (1/2) \ln (\bar{K} \sigma / (\bar{E} \text{ Navo dm } T^2 k^2)) - \\ W(r) / (kT)$$

Surface Tension Theory Developement

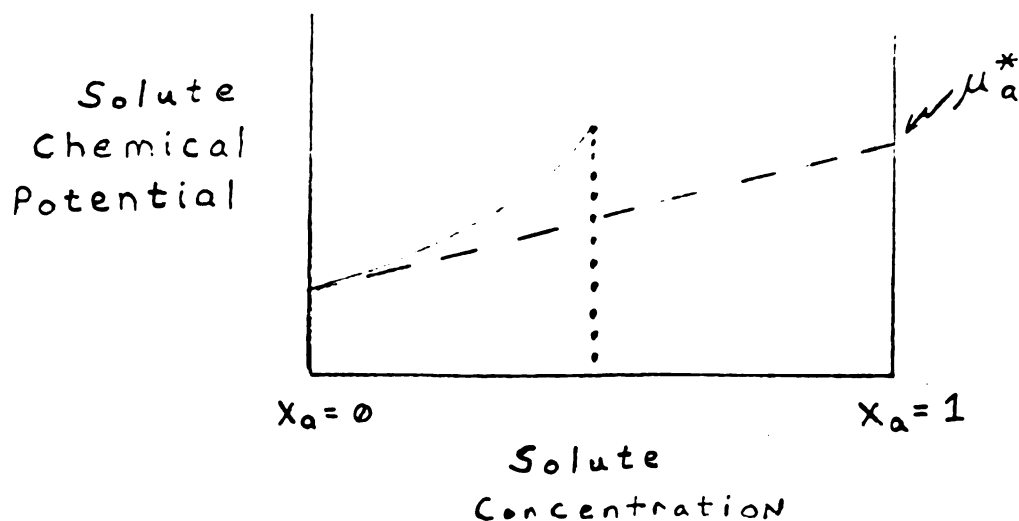
The chemical potential of a solute can be expressed:

$$B1) \quad \mu_a = \mu_a^* + RT \ln a$$

Where μ_a and μ_a^* are the absolute and reference chemical potentials of the solute. a is the activity of the solute. R and T are the ideal gas law constant and temperature.

μ_a^* is defined by choosing a state, a certain temperature, pressure, etc., to be the reference or standard state. Figure B1 shows a possible graph of solute chemical potential vs solubility (X_a). The dashed line on Figure B1 is the tangent to the curve at zero solute concentration. Where the dashed line intersects the $X_a = 1$ axis defines the reference state μ_a^* .

Figure B1



The standard state (μ_a^*) obtained from extrapolation in Figure B1 refers to a pure solution of solute, but with the solute molecules in the same configuration as when in an infinitely dilute solution. This is an hypothetical state.

At low solute concentrations the curve of solute chemical potential vs concentration follows the dashed line use to find μ_a^* . In this region the solute chemical potential is given by:

$$B2) \quad \mu_a = \mu_a^* + RT \ln X_a$$

Where X_a is the solute concentration. If equation B2 is followed up to the maximum concentration of the solute:

$$B3) \quad \mu_a^{max} = \mu_a^* + RT \ln X_{max}$$

Where μ_a^{max} is the chemical potential of the solute at its maximum solubility while X_{max} is that maximum solubility.

At maximum solubility the solute is in equilibrium with its vapor and with its precipitate. Thus:

$$B4) \quad \mu_a^{max} = \mu_a^\sigma$$

Where $\mu_a^\square$ is the chemical potential of the solute in its precipitate.

Chemical potential can be expressed in terms of molar enthalpy and entropy:

$$B5) \quad \mu^* = h^* - Ts^* \quad ; \quad \mu^\square = h^\square - Ts^\square$$

Where h is molar enthalpy and s is molar entropy. Combining equations B3, B4, and B5:

$$B6) \quad RT \ln X_{\max} = \mu_a^{\max} - \mu_a^* = \mu_a^\square - \mu_a^* \\ = h^\square - h^* - T(s^\square - s^*)$$

The term $(s^\square - s^*)$ in equation B6 is the change in entropic energy of the solute on going from the reference state to a precipitate. If entropic energies are modeled as due to random motion in a box, any change in entropic energy is equivalent to changing the size of the box. Box size would be dictated by the molecules surroundings. The surroundings of the solute in the reference state would be solvent molecules, since the reference state is extrapolated

from an infinitely dilute solution. For solutions of non metals dissolved in liquid metals the liquid metal solvent will carry positive charge due to electron delocalization; the non metal solute will carry a negative charge for the same reason. Thus the size of the box occupied by the solute in the reference state solution would be small. The size of the box occupied by the solute in a solid precipitate will also be small. If we assume the box sizes are of the same order, the term $(s^{\square} - s^*)$ becomes zero. Note that the random motion in a box model of entropy ignores the effect of degeneracy. The solute in liquid solution has freedom of movement and can occupy more positions. The solute in the precipitate is locked into a lattice. Thus s^* should be larger than $s^{\square}$, with a corresponding increase in $X_{\max}$.

Enthalpic energy can be modeled as an intrinsic portion to temperature and pressure only plus an external portion due to interactions with surroundings. These interactions can in turn be modeled as surface tension interactions between adjacent non-bonded molecules and bond energies of bonded atoms. Thus the enthalpy of the solute in the precipitate is:

$$B7) \quad h^{\square} = SA \text{ Navo} \left| \sigma_s - \sigma_a \right| + E^{\square} + h_{int}^{\square}$$

Where h_{int} is the intrinsic energy of the solute. $E^{\square}$ is the bond energy of any complex formed involving the solute. σ_a and σ_s are the surface tension of the solute and of the solute surroundings. SA is the surface area of solute exposed to the surroundings. Navo is Avogadro's

number.

The solute will precipitate as a pure crystal or as a solute-solvent complex. In the former the solute surroundings is other solute atoms. Thus the term $(\sigma_s - \sigma_a)$ is zero. If the precipitate is a solute-solvent complex the term $(\sigma_s - \sigma_a)$ can be again be assumed zero. Surface tension between bonded atom are defined as zero and surface tension between solute-solvent complexes is assumed zero. Thus for pure or hetero solute precipitates:

$$B8) \quad h^{\square} = E^{\square} + h_{int}^{\square}$$

The enthalpy of the solute in the reference state can be written:

$$B9) \quad h^* = SA \, \sigma_b - \sigma_a + E^* + h_{int}^*$$

Where σ_b and σ_a are the surface tension of the solvent and solute. E^* is the bond energy of any complex formed involving the solute. h_{int} is the intrinsic energy of the solute. SA is the surface area of solute exposed to solvent particles. Combining equations B9, B8, and B6 yields:

$$B10) \quad -RT \ln X_{\max} = SA \, N_{\text{avo}} \left[\sigma_b - \sigma_a \right] + E^* - E^\square$$

Note that $E^\square$ has dropped out of equation B10. This is because it is the internal energy of the solute atom, dependent only on temperature and pressure.

Calculation Scheme

Equation B10 of the derivation reads:

$$B11) \quad -RT \ln X_{\max} = SA \, N_{\text{avo}} \left[\sigma_b - \sigma_a \right] + E^* - E^\square$$

$X_{\max}$ is the maximum solubility of the solute. σ_b is the surface tension of the solvent, obtainable from the CRC Handbook of Chemistry and Physics (page F25). σ_a is the surface tension of the solute. T is temperature. R and N_{avo} are the ideal gas law constant and avogadro's number. SA is the surface area of the solute which is touched by solvent particles which the solute in question is not bonded to. $E^\square$ and E^* are the change in enthalpic energy of the solute on

going from an unassociated solute atom to a solvent-solute complex in the solid precipitate and in the liquid solution respectively.

Equation B13 shows two free floating parameters: the surface area term SA and the surface tension of the solute, (σ_a). The solute surface tension will be assumed zero. This will allow calculation of the surface area term SA

For organic-metal solution, the complex would be a organic-metal complex. $E^\square$ and E^* are thus the enthalpy of formation of the organic-metal complex. Enthalpy of formation data is defined as an energy that must be added to a system to create the complex. Thus:

$$\text{B12)} \quad E^\square = \Delta H_f \quad ; \quad E^* = \Delta H_f$$

Where ΔH_f is the enthalpy of formation of the organic-metal complex.

ΔH_f data can be obtained from the CRC Handbook of Chemistry and Physics (page D45 and D67). ΔH_f data for some systems was not found. For these systems $E^\square$ and E^* were assumed zero.

Calculation Scheme #1

It is logical to assume that the complex formed by the solute and solvent in the liquid solution is the same as the complex formed by

the solvent and solute in the solid precipitate. Thus the terms $E^\square$ and E^* are equal. The solute can be modeled as existing in a partially bounded state. This can be expressed mathematically:

$$- RT \ln X_{\max} = SA \text{ Navo} | \sigma_b | + \text{FRAC} * E^\square - E^*$$

Or:

$$\text{B13)} \quad - RT \ln X_{\max} = SA \text{ Navo} | \sigma_b | - (1 - \text{FRAC}) \text{ del Hf}$$

Where FRAC is the fractional existance of the solute in solution as the organic-metal complex.

Equation B13 can be solved for the surface area of the solute touched by solvent particles which the solute is not bonded to:

$$\text{B14)} \quad SA = (- RT \ln X_{\max} + (1 - \text{FRAC}) \text{ del Hf}) / (\text{Navo} | \sigma_b |)$$

If the solute is assumed spherical, the radius of the solute can be calculated from the surface area:

$$B15) \quad SA = 4 \pi r^2$$

$$B16) \quad r = (SA / 4 \pi)^{1/2}$$

Where r is the radius of the solute atom in the liquid solution.

Note that the above derivation does not take into account that the exposed surface area of the solute will be decreased by the solute's "fractional" existence in a complex.

Calculation Scheme #2

Calculation scheme 2 ignores the bound energy factors in equation B11. This is equivalent to calculation scheme one with FRAC equal one. The resulting equation is:

$$B17) \quad -RT \ln X_{\max} = SA \text{ Navo} \mid \sigma b \mid$$

Equation B17 can be solved for the surface area of the solute:

$$\text{B18)} \quad SA = - RT \ln X_{\text{max}} / (N_{\text{avo}} | \sigma b |)$$

Using equations B15 and B16 the results of equation B18 can be used to calculate the radius of the solute atom in solution.

Discussion

In development of equation B3 of the surface tension theory development section, the activity of the solute is assumed equal to the solubility of the solute over the entire solubility range of the solute. It is important to note that this is not equivalent to assuming an ideal solution. This assumption is equivalent to assuming that the activity coefficient is constant over the entire solubility range of the solute.

The activity coefficient is a measure of the deviation from the reference state. The reference state in turn is a set deviation from the ideal state. Thus assuming that the activity coefficient is constant assumes that the deviation of the solution from the ideal state is constant, that the environment of the solute is constant over the entire solubility range of the solute. At low solute concentration this assumption seems valid. As the solute concentration rises, and

the solute particles begin to affect each others environment, the assumption of a constant activity coefficient is suspect.

The surface tension of the solute is assumed zero to allow calculation of the surface area term SA (see equation B11 above). This could be a significant error if the solute surface tension varies with the solvent. The assumption was made to aid calculation.

The surface tension calculation scheme section shows how to calculate the surface area of the solute from experimental data (equations B14 and B18). Note that the areas defined by these equations are the surface area of the solute touched by solvent particles the solute is not bonded to. This area cannot be the entire surface area of the solute. Picture a rack of pool balls just before the break and a basket of apples. The objects rest against each other at points. The apples would mash against each other, thus the apples would have more area of contact than the pool balls. To model the percentage of solute surface area that could be touched, one must decide how soft the solute particles would be. This, combined with the lattice structure of solution and the relative positioning of the solvent and solute, would allow calculation the area of contact between solute and solvent.

Equation B16 above should read:

$$r = (SA * MORE / 4\pi)^{1/2}$$

Where MORE is the amount that the surface area supplied from the

surface tension theory should be increased to account for the fact that the solute cannot be touched on all of its surface by other particles.

Correlations Found

Regular Solution Theory

Figures 1 through 4 show the attempts made at finding a correlation involving W_{ab} , the free parameter of the regular solution theory. All of the graphs are weak, with the exception of the results for carbon with transition metals in Figure 1. For carbon in pure liquid transition metals Figure 1 predicts the correlation:

$$W_{ab} = 0.98858 * T + 361.98$$

where T is temperature.

Quasi-Chemical Solution Theory

Figures 5 through 8 show the attempts made at finding a correlation involving W_{ab} , the free parameter of the quasi-chemical solution theory. Figures 5 through 8 show that W_{ab} correlates well with temperature. The correlations predicted by Figures 5 through 8:

$$W_{ab} = 0.38889 * T + 94.444$$

$$W_{ab} = 0.34316 * T + 76.421$$

$$W_{ab} = 0.49412 * T + 60.000$$

$$W_{ab} = 0.33929 * T + 21.429$$

Where the equations are for carbon, oxygen, hydrogen, and nitrogen in pure liquid metals respectively.

A natural question is why would a interaction parameter such as W_{ab} (defined by equation H5 in the regular solution derivation section) would have such a strong dependance on temperature. An interaction energy parameter should be a function of the solute and the solvent. Figures 5 through 8 suggest that W_{ab} is a function of temperature alone.

Lee and Johnson Theory

The Lee and Johnson theory was found to be unusable. The use of experimental data in the calculations lead to the square root of a negative number. See the Lee and Johnson theory derivation for more complete explination.

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Surface Tension Theory

Figures 9 through 12 show the attempts made at finding a correlation involving the solute radius, the free parameter for the surface tension theory. Figures 9 through 12 were generated from surface tension calculation scheme two.

Figures 9 and 10 show that the surface tension calculation scheme two predicts a solute radius for carbon and oxygen with transition metals. It cannot be determined from Figures 11 and 12 if surface tension theory will predict a solute radius for nitrogen and hydrogen with transition metals. There is not enough data.

Surface tension calculation scheme one was found unusable. The enthalpy of formation (ΔH_f) of the solute-solvent complex is an input to the calculations (see equation B14 of the surface tension theory derivation). ΔH_f is a large negative number for almost all systems. The factor

$$- RT \ln(X_{\max}) + \text{FRAC} * \Delta H_f$$

is negative for almost all systems if FRAC is set to one. This negative feeds into the calculations where a negative surface area results from equation B14 .

Various values of FRAC were tried. Setting FRAC equal to 0.02 allowed all the experimental data to be mathematically viable. Unfortunately this led to results that were worse than when the enthalpy

factor was not taken into account (surface tension theory calculation scheme 2).

The enthalpy factor seems a logical inclusion in the derivation of the surface tension model. A manner in which to include it in the mathematics of the surface tension model was not found in this investigation.

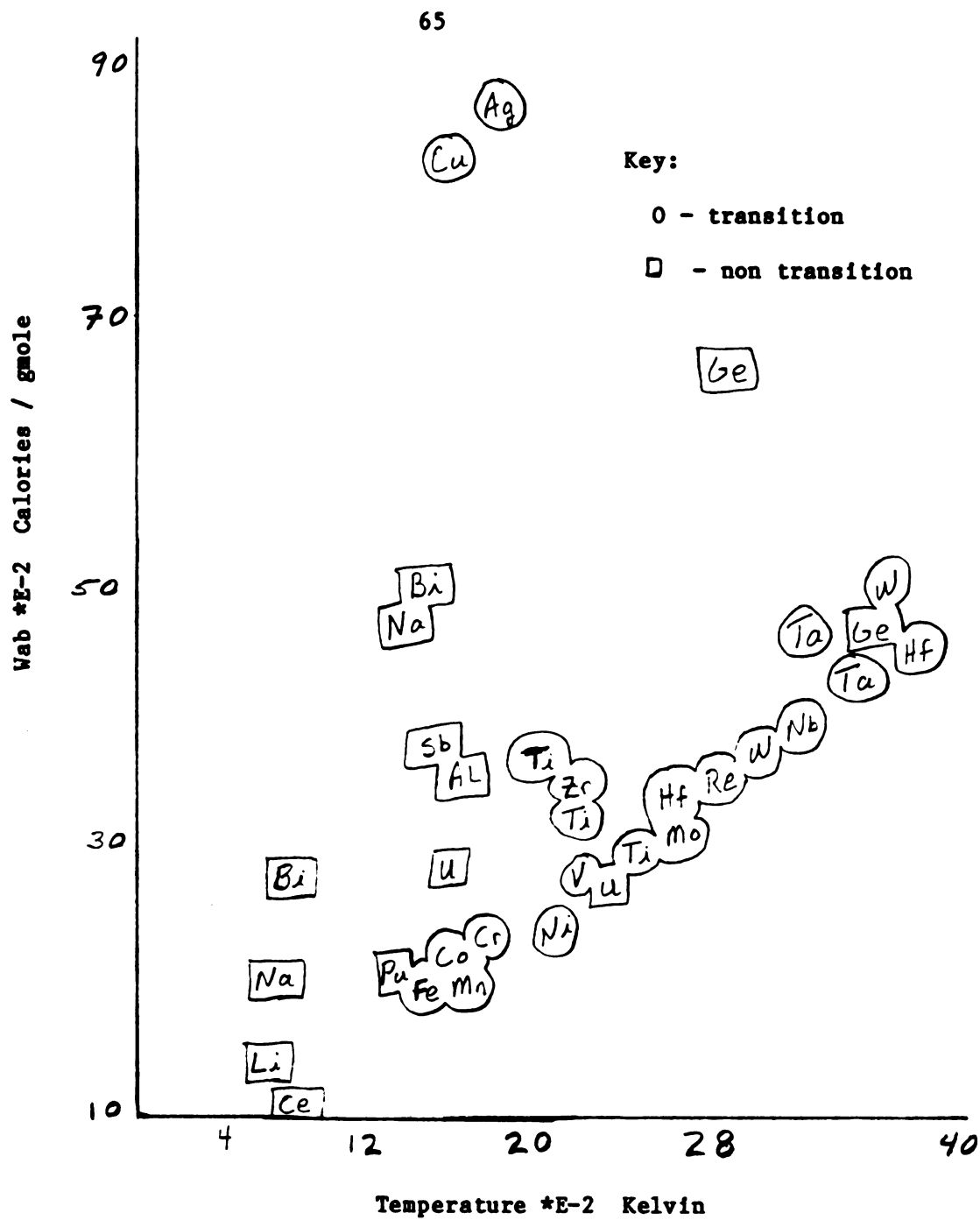


Figure 1

Wab Predicted by the Regular Solution

Theory for Metal-Carbon Systems

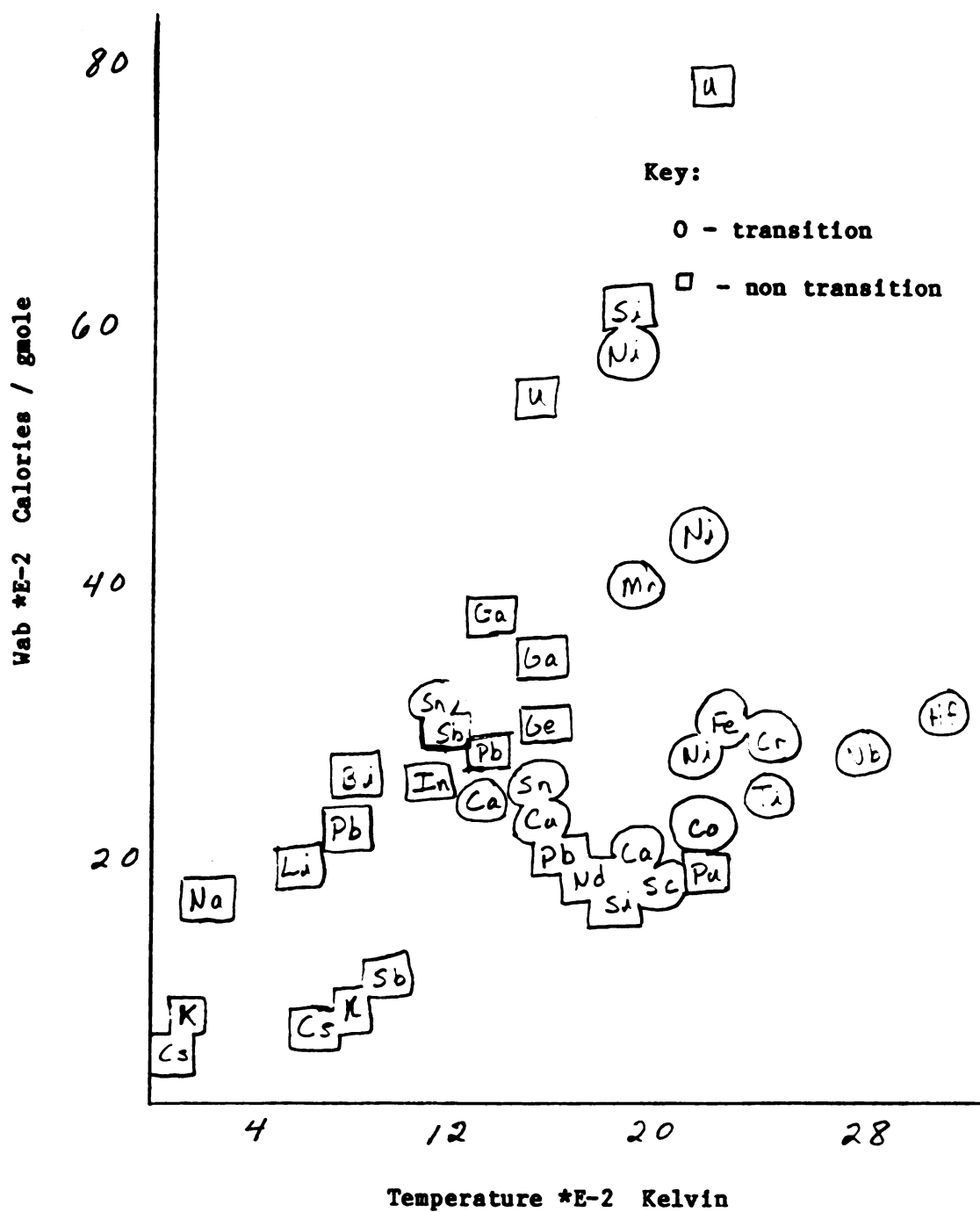


Figure 2

Wab Predicted by the Regular Solution

Theory for Metal-Oxygen Systems

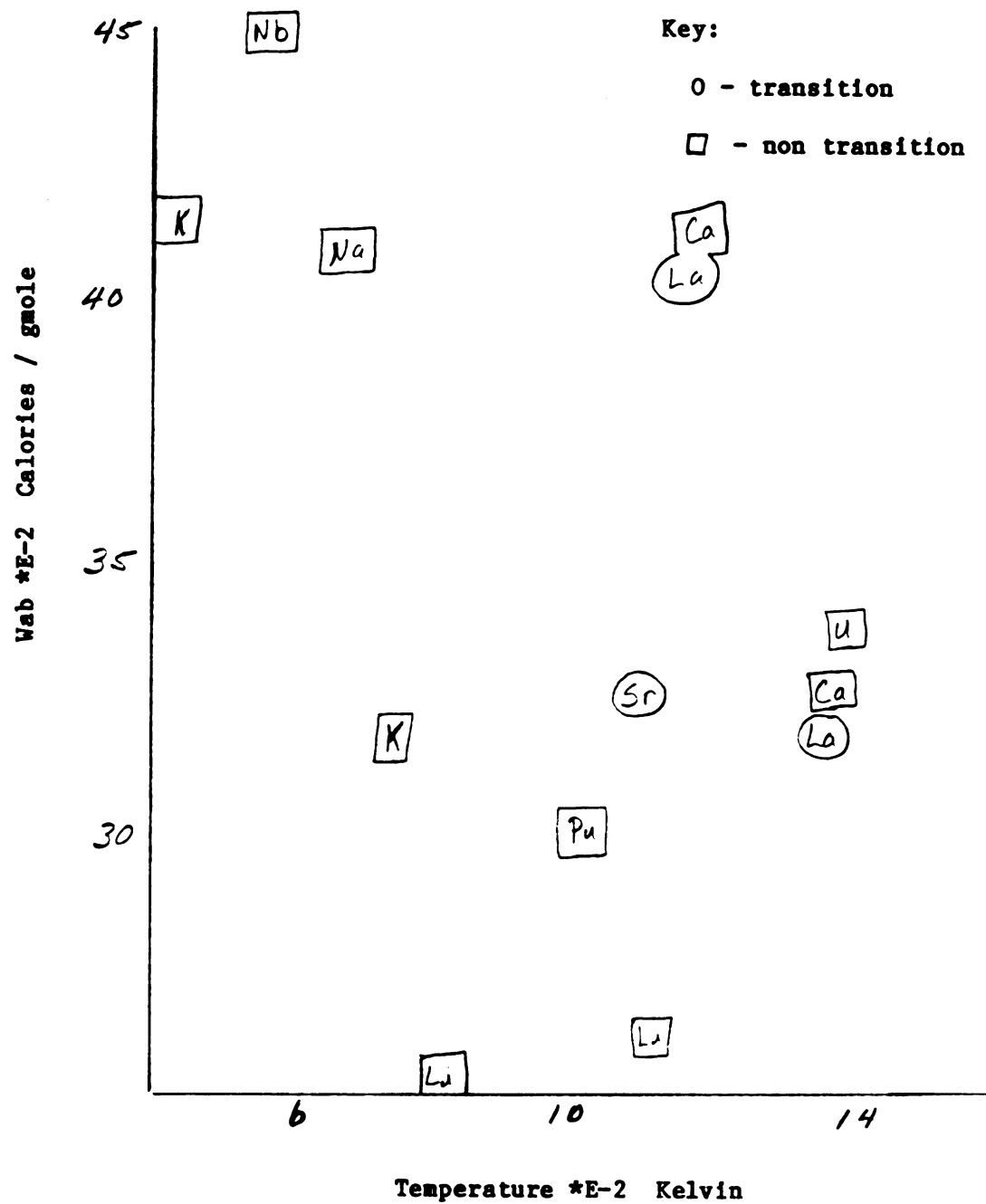


Figure 3

Wab Predicted by the Regular Solution
Theory for Metal-Hydrogen Systems

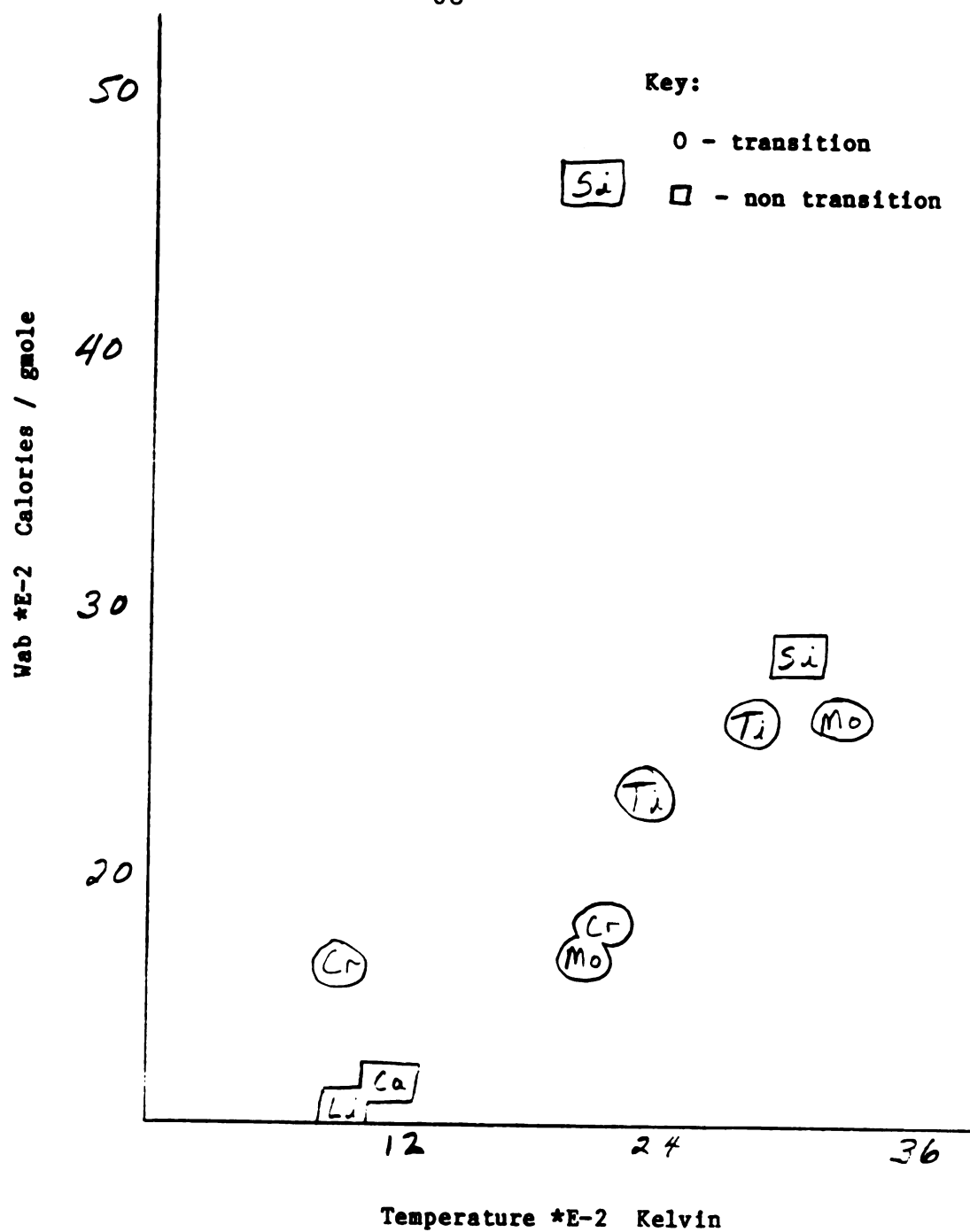


Figure 4

Wab Predicted by the Regular Solution
Theory for Metal-Nitrogen Systems

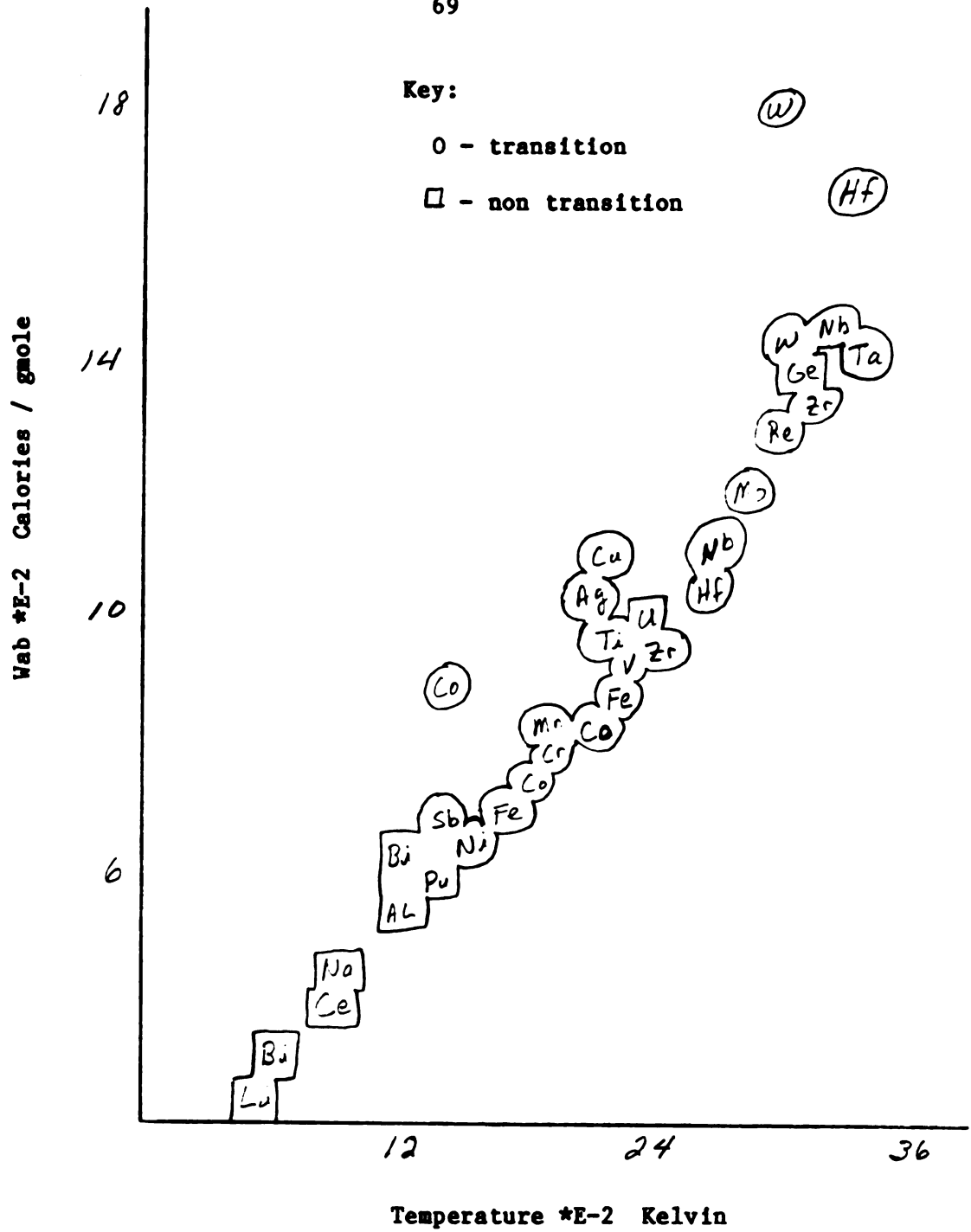


Figure 5

Wab Predicted by the Quasi-Chemical Solution

Theory for Metal-Carbon Systems

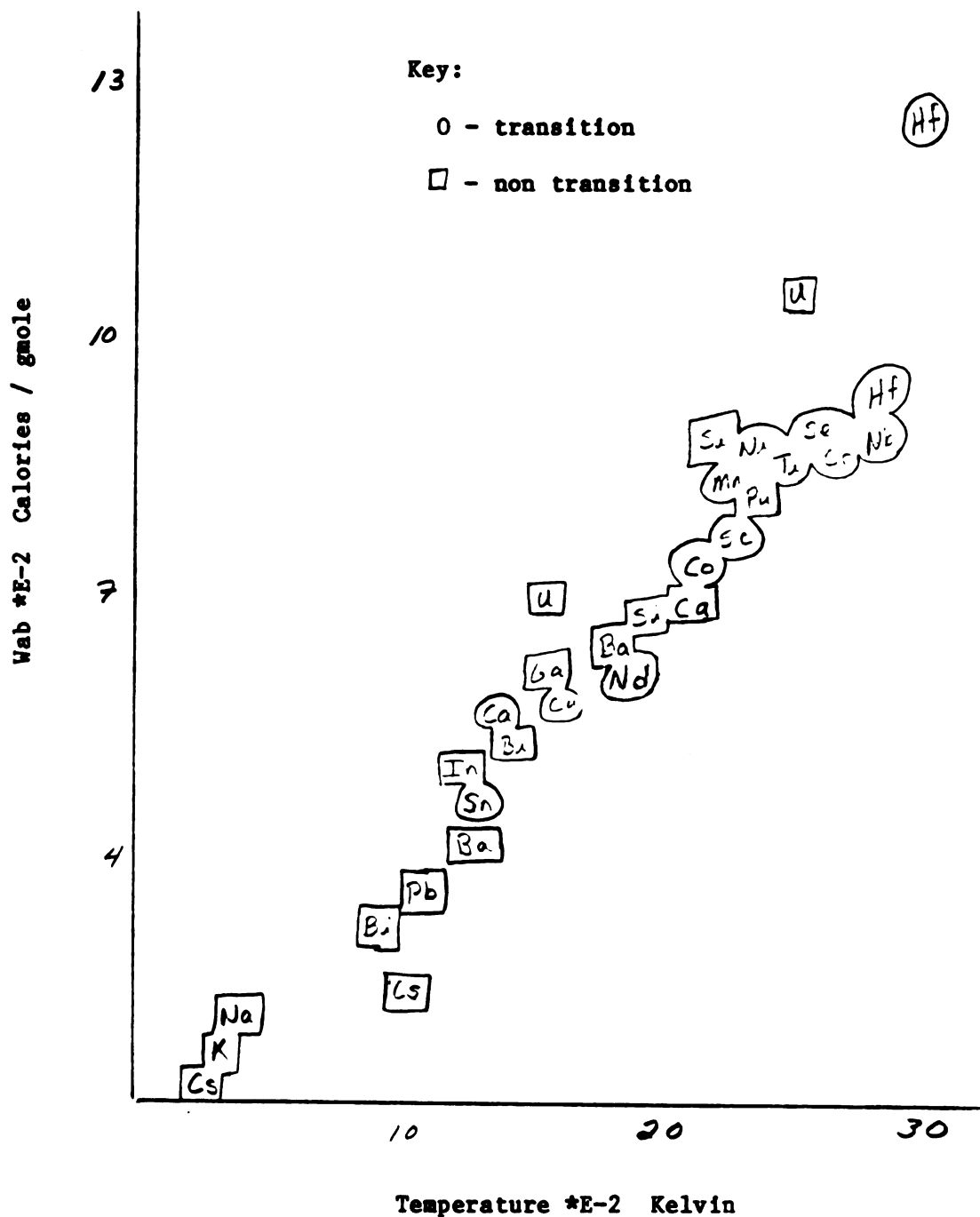


Figure 6

Wab Predicted by the Quasi-Chemical Solution

Theory for Metal-Oxygen Systems

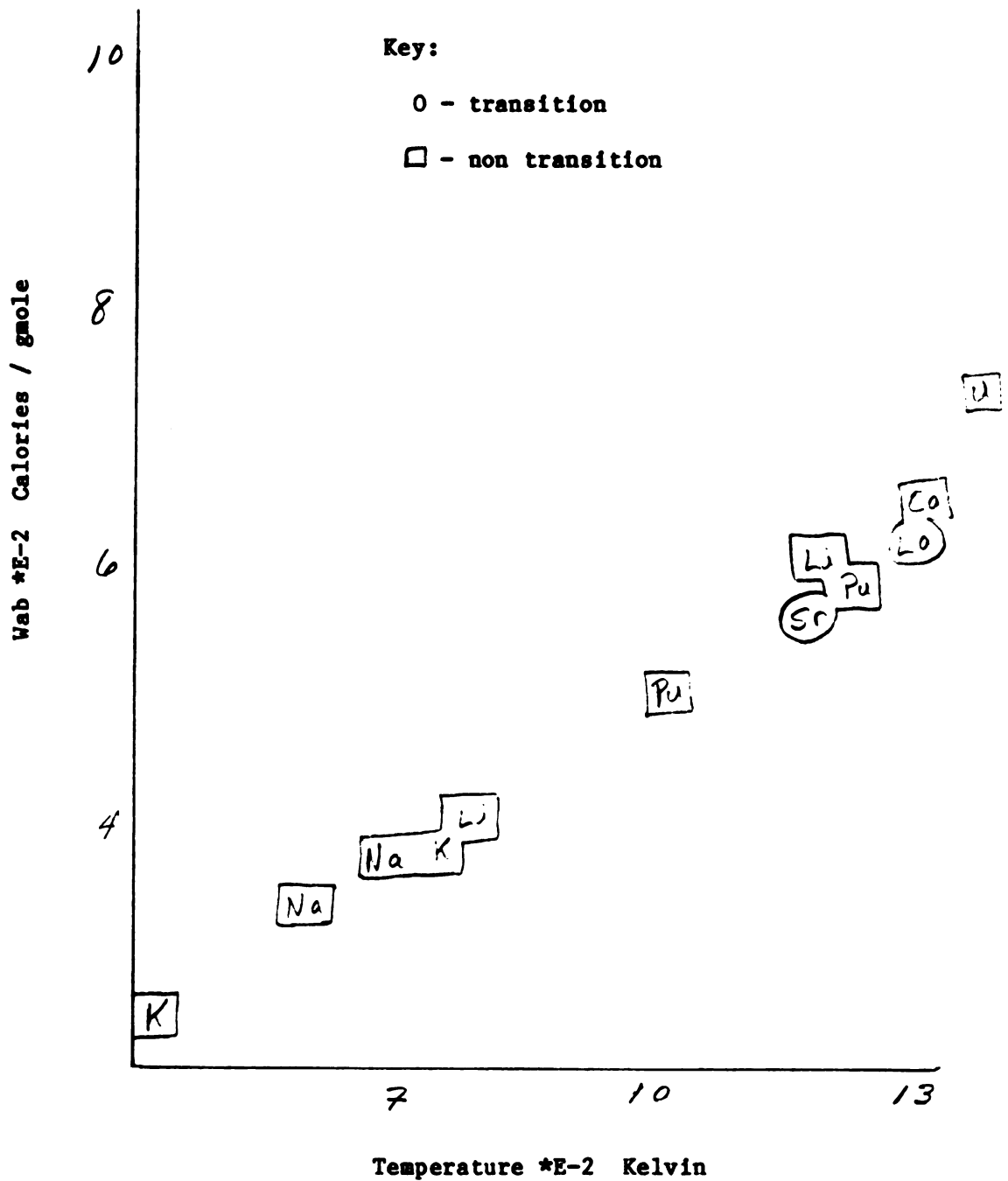


Figure 7

Wab Predicted by the Quasi-Chemical Solution

Theory for Metal-Hydrogen Systems

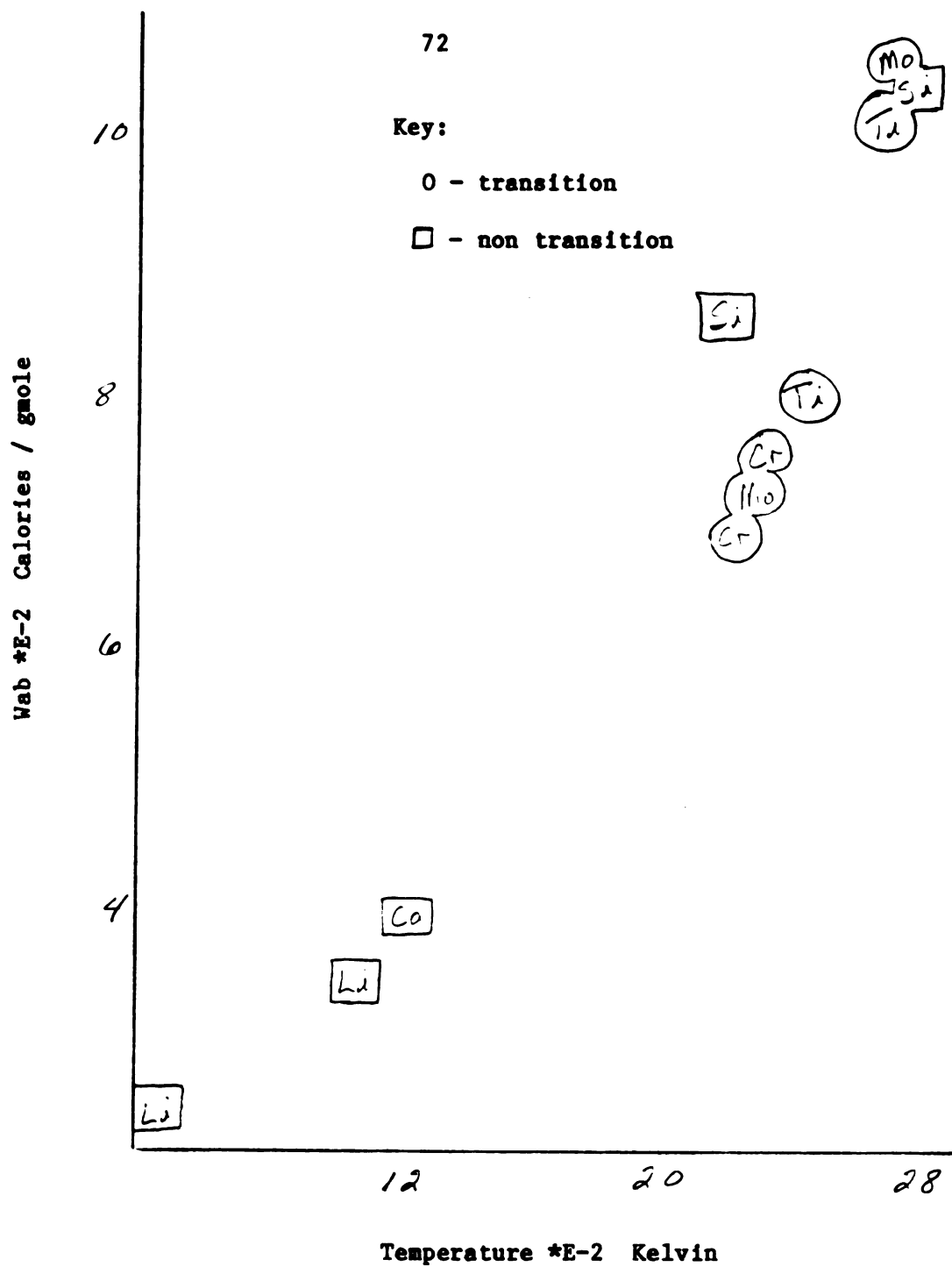


Figure 8

Wab Predicted by the Quasi-Chemical Solution
Theory for Metal-Nitrogen Systems

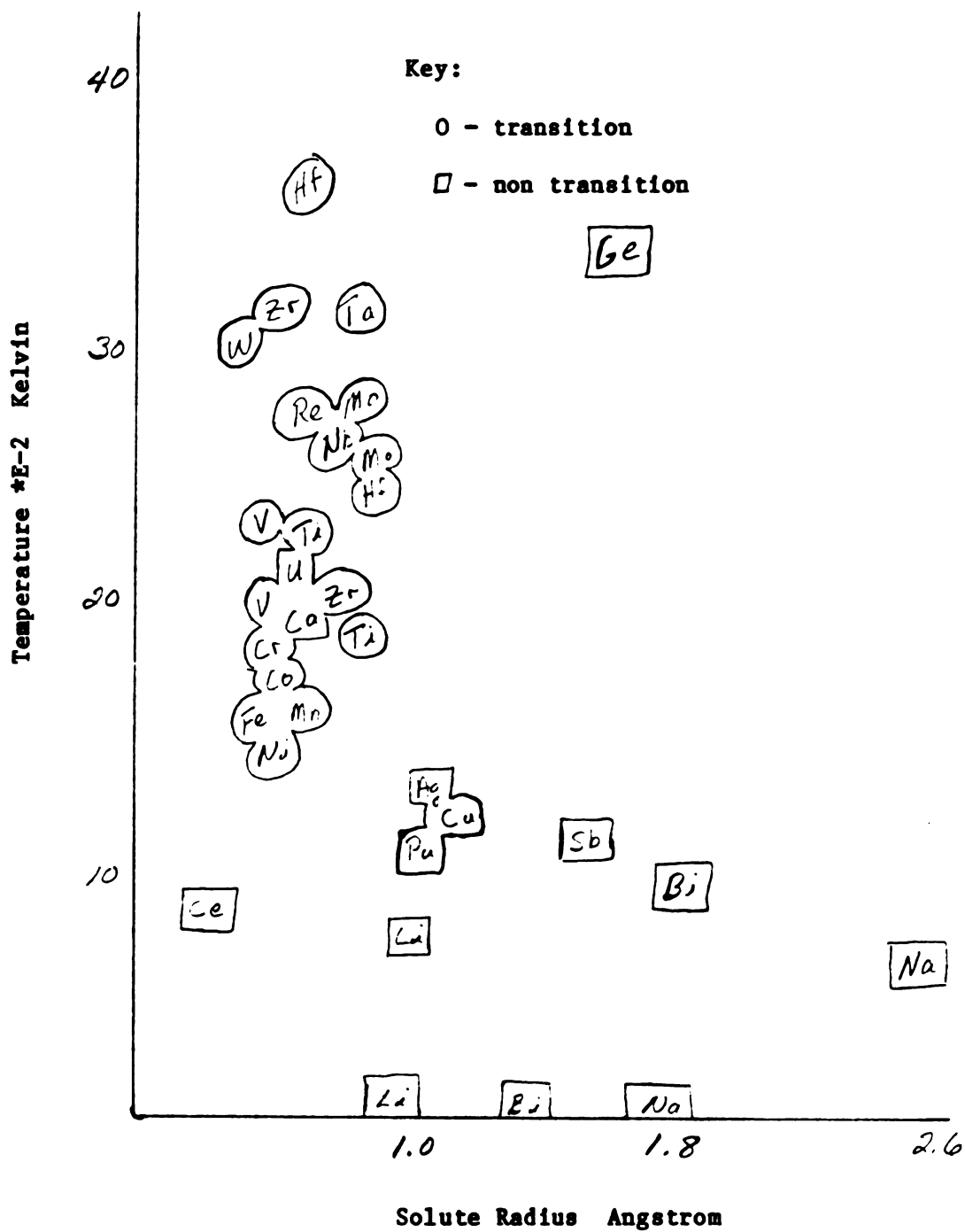


Figure 9

Solute Radius Predicted by the Surface Tension
Theory for Metal-Carbon Systems

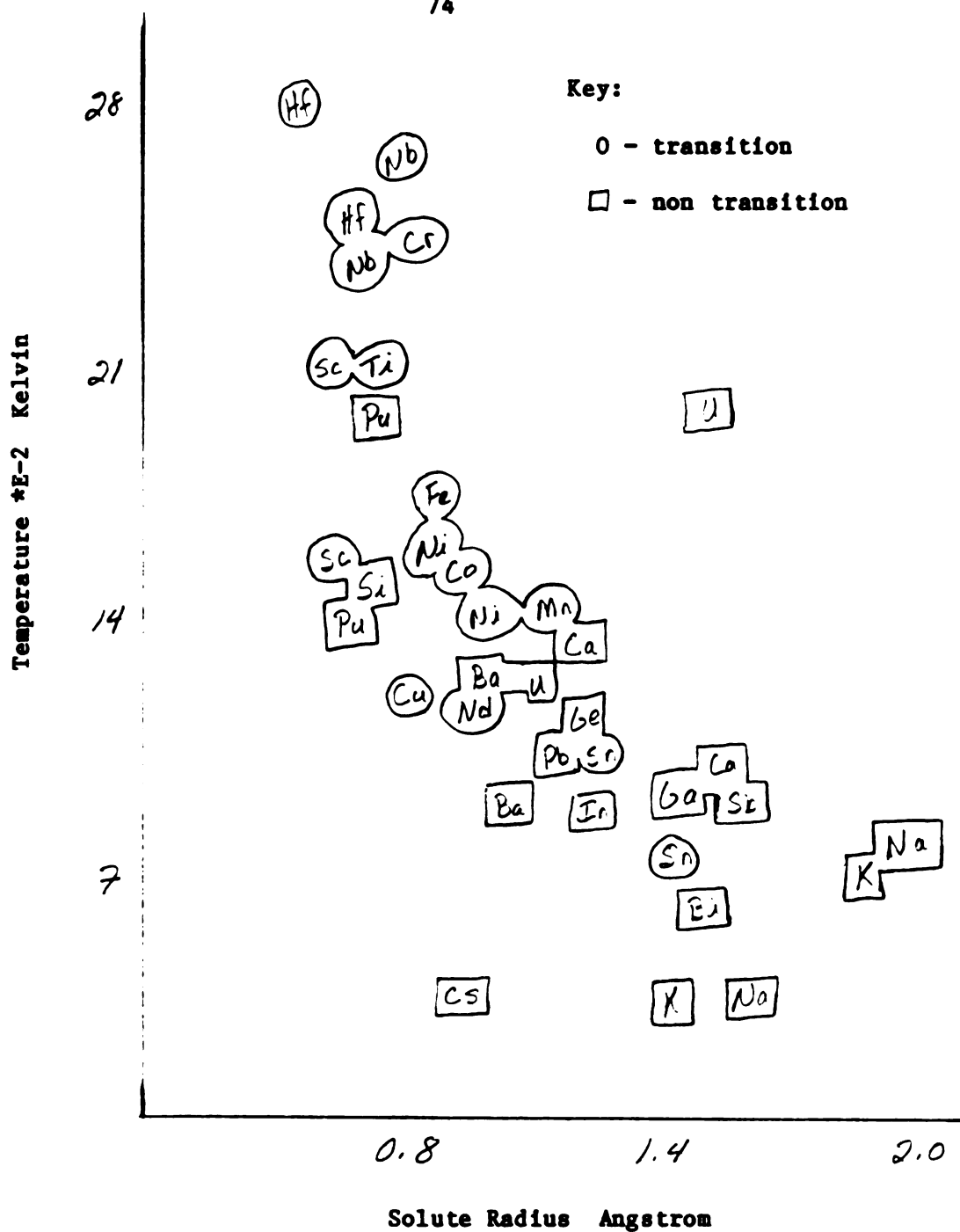


Figure 10

Solute Radius Predicted by the Surface Tension

Theory for Metal-Oxygen Systems

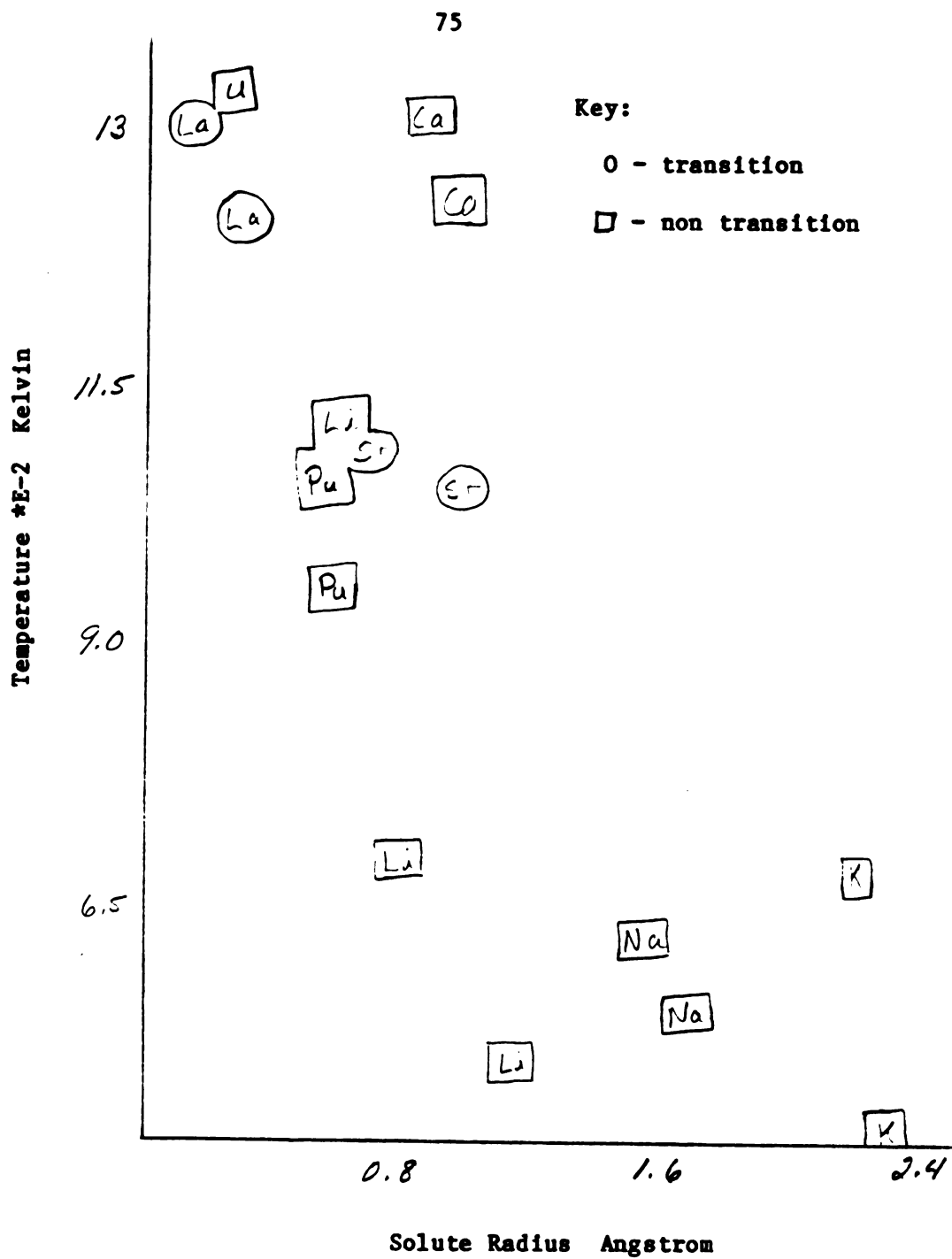


Figure 11

Solute Radius Predicted by the Surface Tension
 Theory for Metal-Hydrogen Systems

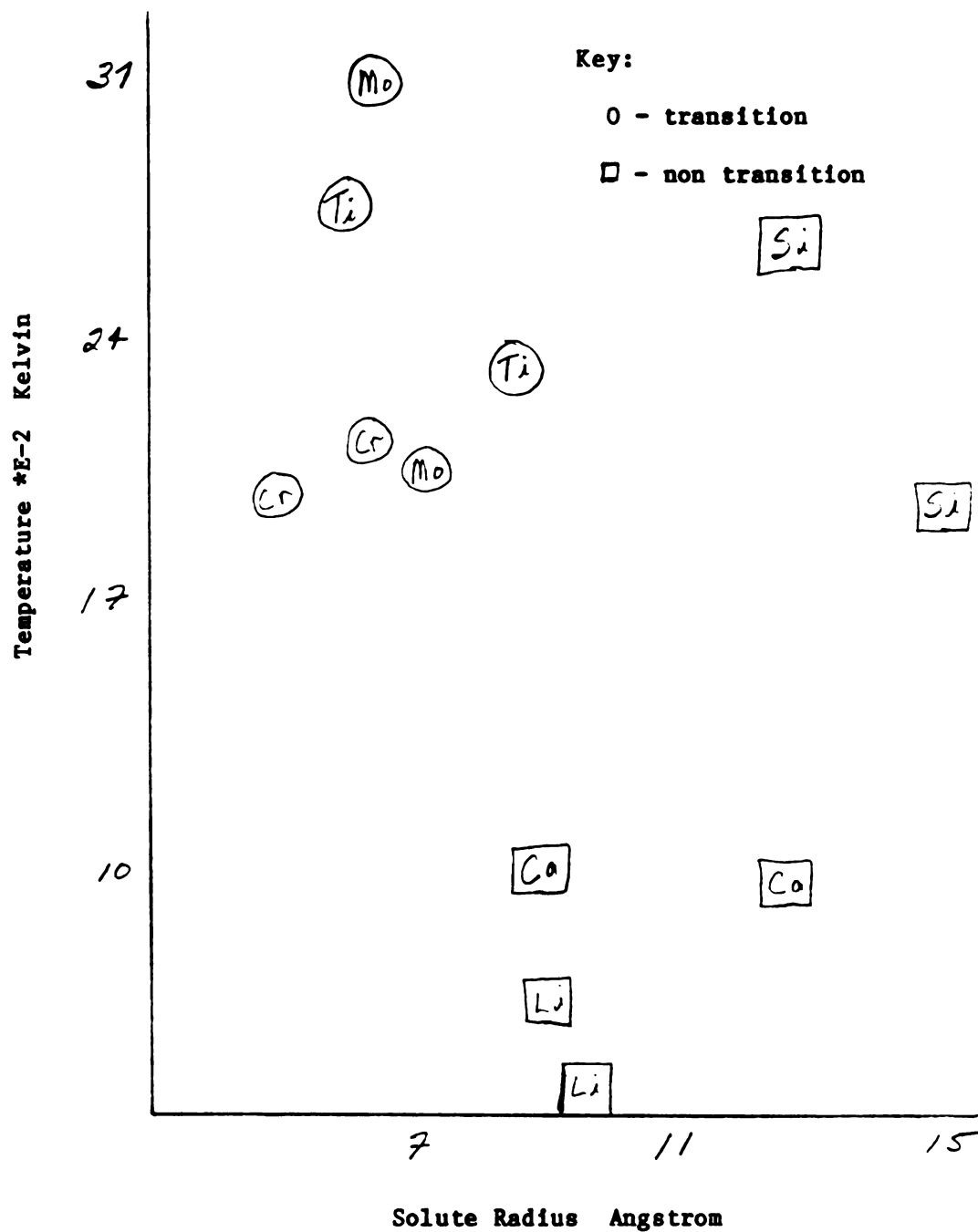


Figure 12

Solute Radius Predicted by the Surface Tension
Theory for Metal-Nitrogen Systems

Comparison of Theory Predictions with Experimental Data

Surface Tension Theory

The surface tension theory showed the best predictive abilities for carbon or oxygen with transition metals. The comparison of theory predictions with experimental data is shown in Figures 15 and 16. The systems in Figures 15 and 16 are examples of systems that showed good, fair, or poor fits in Figures 9 and 10. carbon with cobalt and oxygen with copper are example of good fit systems. The calculated maximum solubility for these systems are off by a factor two and three respectively. chromium with oxygen is an example of a fair fir system. The calculated value is off by a factor of four. carbon with titanium and oxygen with titanium are examples of poor fit systems. Their calculated values are off by five and four hundred respectively.

Quasi-Chemical Solution Theory

The quasi-chemical solution theory showed the best results for all other systems. The comparison of theory predictions with experimental data is shown in Figures 13 and 14. The systems aluminum with carbon, barium with oxygen, and copper with oxygen are examples of systems which show good fits in Figures 5 and 6. They calculated values of the activity coefficient are off by a factor of two for all three systems. bismuth with carbon and antimony with oxygen are

examples of systems with fair fits in Figures 5 and 6. Their calculated values are off by a factor of forty and twenty respectively. Copper with carbon and nickel with oxygen are examples of systems with poor fits in Figures 5 and 6. Their calculated values are off by a factor of seven hundred and two hundred.

It is evident, from Figures 5, 6, 13, and 14 that small deviations in W_{ab} produce large deviations in the predicted values of the activity coefficient. Example, the bismuth-carbon data entry at 1100 degrees Kelvin is only slightly off in Figure 5, but the predicted activity coefficient is off by a factor of eighty. The reason for this weakness can be seen by inspecting the key equation for the quasi-chemical theory, equation G25 of the quasi-chemical derivation:

$$(1) \quad \ln \gamma_a = (1/2) Z \lambda X_b^2 - Z \lambda^2 X_b^3 + (3/4) Z \lambda^2 X_b^4 \quad (1 + 20 \lambda / 3)$$

$$\lambda = \exp (2W_{ab} / kT) - 1$$

Where γ_a is the solute activity coefficient. Z is the solute coordination number. R is the ideal gas law constant. T is temperature.

For most systems the solubility of oxygen and carbon is small. The solvent concentration (X_b) is close to one. Thus the activity coefficient is mainly a function of W_{ab} . Equation (1) shortens to:

$$(2) \quad \ln a = K_1 * \exp (W_{ab} / T) + K_2 * (\exp (W_{ab} / T))^2 + \\ K_3 * (\exp (W_{ab} / T))^3 + K_0$$

Where K_1 , K_2 , K_3 , and K_4 are constants at low solute concentrations.

Equation (2) explains why small deviations in W_{ab} produce large deviations in the activity coefficient.

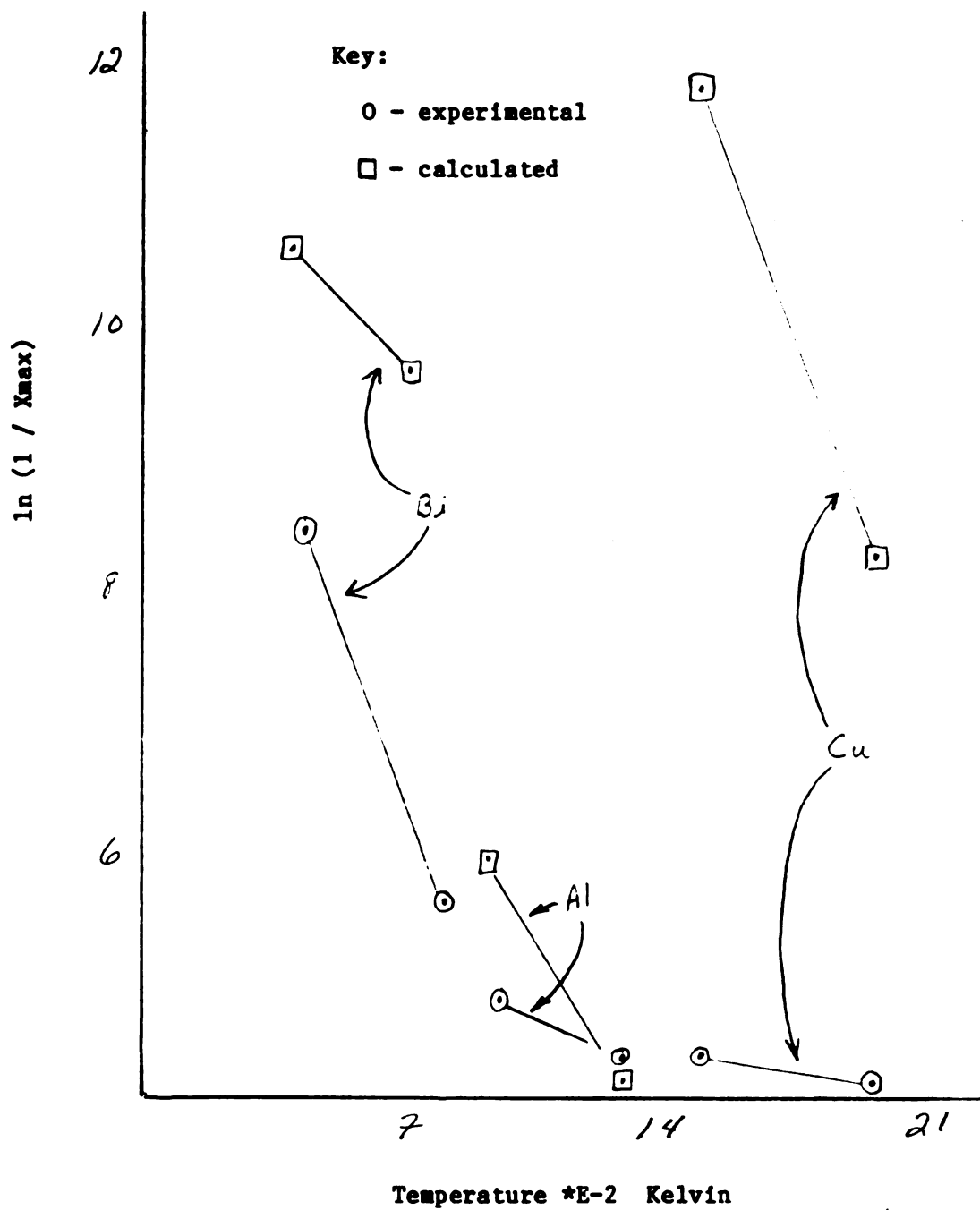


Figure 13
 Quasi-Chemical Solution Predictions for
 Metal-Carbon Systems

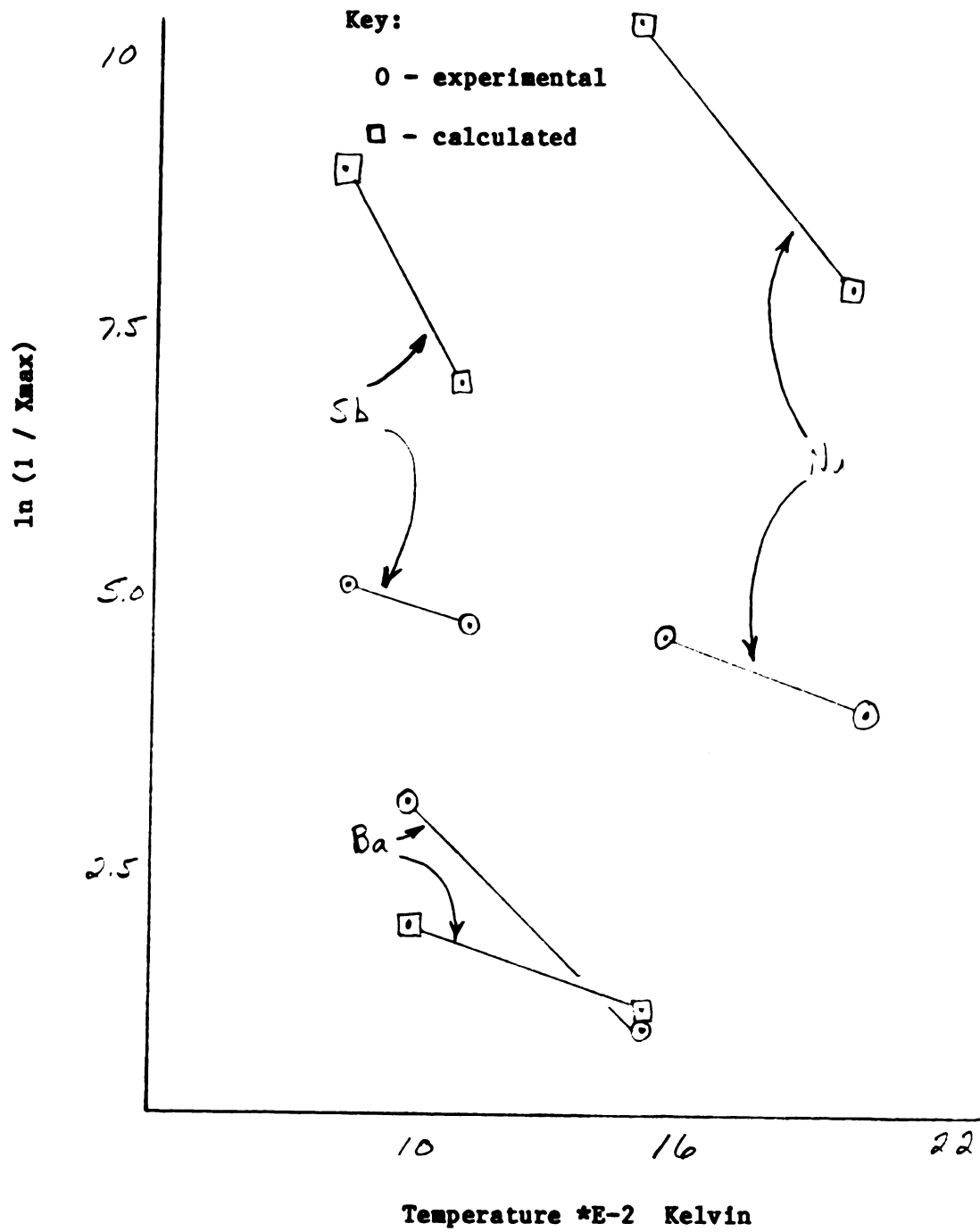


Figure 14
 Quasi-Chemical Solution Predictions for
 Metal-Oxygen Systems

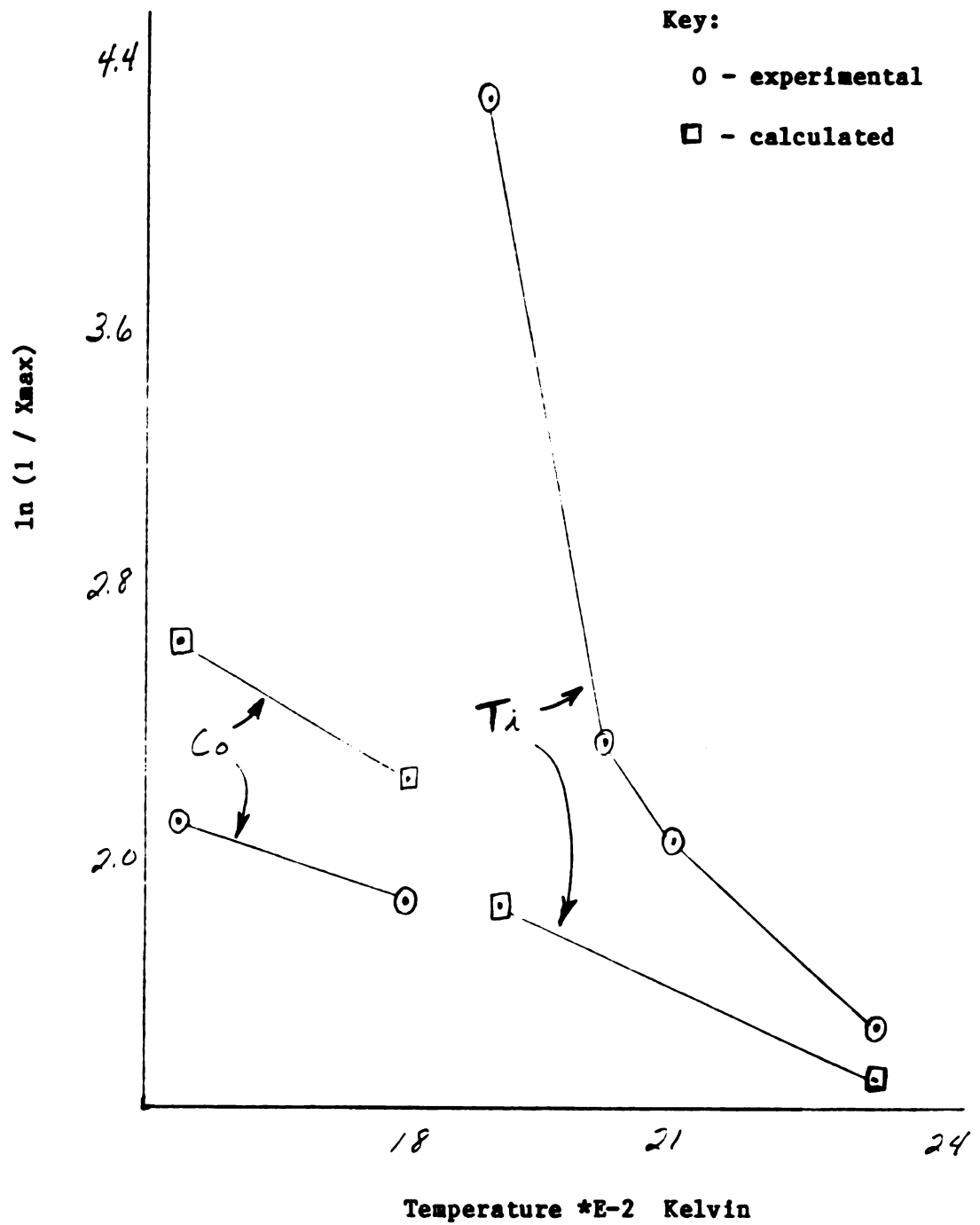


Figure 15

Surface Tension Theory Predictions for

Metal-Carbon Systems

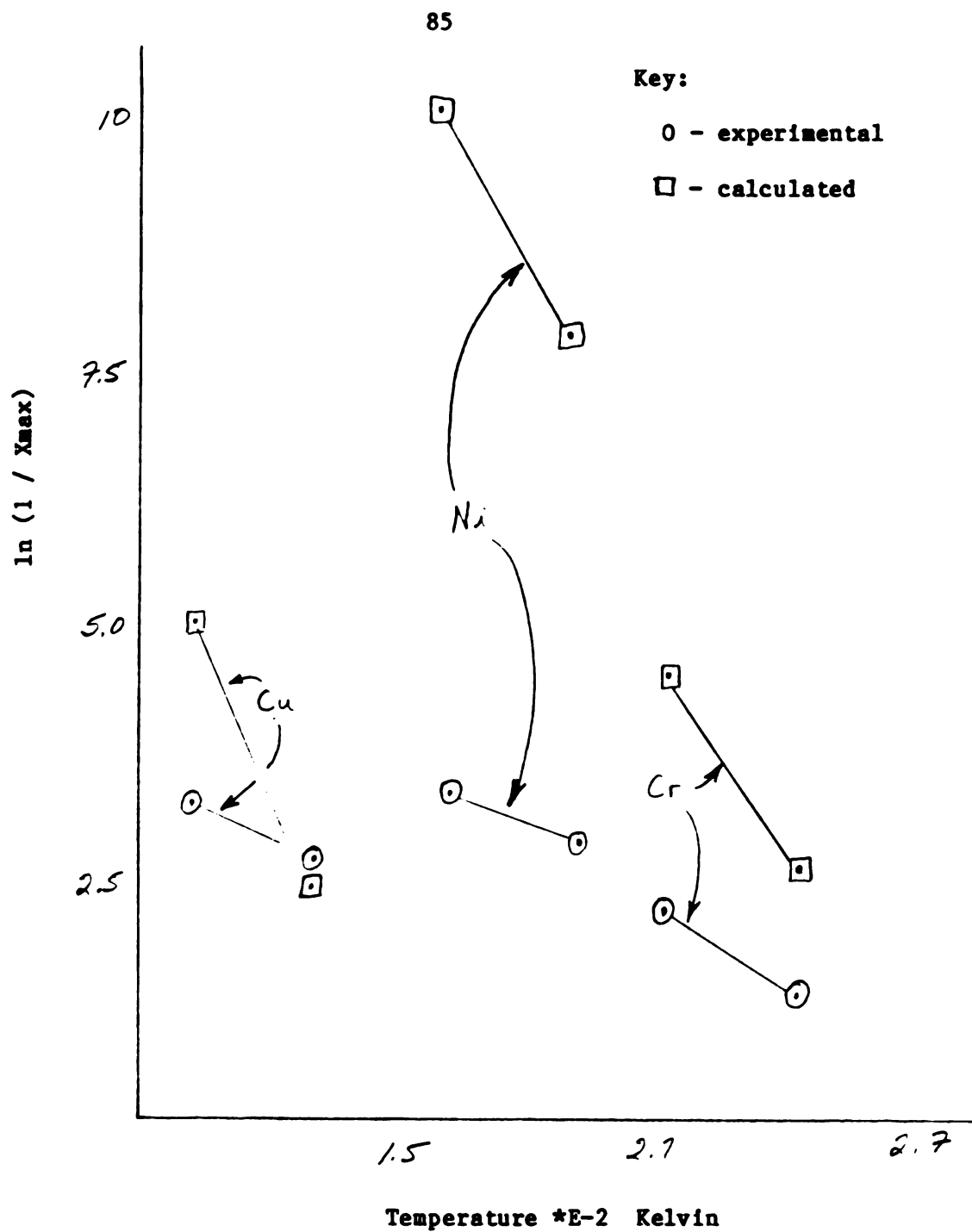


Figure 16

Surface Tension Theory Predictions for

Metal-Oxygen Systems

Conclusions

The surface tension theory showed to be the best for the isolated case of Carbon or Oxygen with transition metals. A logical question is whether the surface tension theory will prove to be the best for all solutes with transition metals. The amount of data for Nitrogen and Hydrogen was insufficient to draw any conclusions.

The surface tension theory is the theory of choice for further study. The results, unlike the quasi-chemical theories correlation of temperature and interaction energy, makes sense. The solute should have a radius in solution which is different than the radius the solute has normally. This solution radius would be a function of the solvent lattice, solvent-solute interaction energy, and the availability of free electrons for the solute to absorb or possible lose. It is logical that the solute radius in the transition metals showed such a single value; the chemistry of the transition metals is very similar. The results for the other periodic groups might be brought into shape further work with energy factors E^* and $E^\square$.

The quasi-chemical solution theory proved to be the best theory for all systems other than Carbon or Oxygen with transition metals. The correlations produced by the quasi-chemical theory are good, but the theory does shows a weakness in using correaltion predicted free parameter values to calculate the activity coefficient. The natural log of the activity coefficient is a function of the exponential of the free parameter.

Figures 5 through 8 show the correlation between

quasi-chemical free parameter, a solute-solvent interaction energy parameter W_{ab} , and temperature. It is difficult to understand why W_{ab} would correlate so well with temperature. Energy of interaction between the solvent and solute should be a function of solvent-solute bond energy, the lattice energy of the solvent, and the type of lattice the solvent forms.

The regular solution theory was surpassed in predictive ability for all systems by the surface tension theory or the quasi-chemical theory. The regular solution theory did predict a valid correlation for Carbon with transition metals.

The theory proposed by Lee and Johnson proved ineffective. But it must be stressed that the theory is ineffective with the calculation scheme used. See the Lee and Johnson theory derivation for a detailed analysis.

A theory by Emi and Pehlke was developed but not critiqued against experimental data. The theory requires data which was not easily found or modeled. The theory looks good. It would be worth the time to investigate it further.

Carbon proved to a solute quite susceptible to modeling. In each theories output it showed the best grouping. Possible this could be due to Carbon being more like a metal than the other solutes. Carbon systems would have simpler chemistry. If this analysis is true, the theories, or there derivatives, should hold more closly for

metal-metal systems.

VOLUME II

APPENDICES

Appendix A Computer Code and Print Out

This appendix contains the computer code used and the raw results generated by the the code. The computer used was an Apple 2e. The language is Applesoft Basic.

Computer code inputs and outputs:

Lee and Johnson code.....91

inputs - solvent radius (cm)
 solvent density (gmole/cm**3)
 temperature (degrees Kelvin)
 solute solubility ratio
 (atom fraction / atm ** (0.5))
output - solute radius (cm)

Regular solution and Quasi-chemical code.....94

inputs - solute coordination number
 solute maximum solubility
 (atol fraction)
 temperature (degrees Kelvin)
output - interaction energy (cal/gmole)

Surface tension code.....100

inputs - temperature (degrees Kelvin)
 solute maximum solubility
 (atopm fraction)

solvent surface tension**(dyne/cm)****output - solute radius (cm)****Print outs:****Regular and Quasi-chemical solution theories**

Carbon.....	105
Hydrogen.....	132
Nitrogen.....	141
Oxygen.....	148

Surface tension theory

Carbon.....	179
Hydrogen.....	202
Nitrogen.....	210
Oxygen.....	216

]LIST 10-500

```

10 REM          Lee and Johnson program
20 REM
30 REM  VARAIBLE LIST
40 REM  A - A.....INTERNAL CONSTANT
50 REM  B - B.....INTERNAL CONSTANT
60 REM  C - C.....INTERNAL CONSTANT
70 REM  CH - CHK.....USED FOR INTERNAL CHECK
80 REM  D - D.....INTERNAL CONSTANT
90 REM  D$ - D$.....CONTROL CHARACTER
100 REM  DE - DETR.....DETERMINATE OF QUADRATIC
110 REM  I$ - I$.....INPUT FILE
120 REM  KH - KH.....EXPERIMENTAL SOLUBILITY RATIO at frac / atm^2
130 REM  ME - MET.....LOOP INDEX
140 REM  M$ - M$.....NAME OF METAL
150 REM  NA - NAVO.....AVOGADROS NUMBER  molecules / mole
160 REM  ND - NDSET....NUMBER OF DATA SETS
170 REM  NM - NMET.....NUMBER OF METALS WHICH HAVE METAL FOR A SOLUTE
180 REM  NP - NPNT.....NUMBER OF DATA POINTS FOR A METAL-SOLUTE
190 REM  PF - PF.....PACKING FRACTION
200 REM  PI - PI.....THE CONSTANT PI
210 REM  PN - PNT.....LOOP INDEX
220 REM  O$ - O$.....OUTPUT FILE
230 REM  RG - RG.....IDEAL GAS CONSTANT  cm^3 - atm / gmole - degree K

240 REM  RH - RHO.....SOLVENT DENSITY  mole / cm^3
250 REM  RS - RSOLV....RADIUS OF THE SOLVENT
260 REM  R1 - R1.....POSSIBLE SOLUTION  cm
270 REM  R2 - R2.....POSSIBLE SOLUTION  cm
280 REM  SO - SOL.....LOOP INDEX
290 REM  TM - TMP.....TEMPERATURE  degree C
300 REM
310 REM          Set constants
320 REM
330 RG = 82.05
340 PF = .6
350 PI = 3.141593
360 NAVO = 6.023E23
370 REM
380 REM          Set input and output files
390 REM
400 O$ = "LAC3.OTP"
410 I$ = "K.DATA"
420 D$ = CHR$ (4)
430 PRINT D$"MON C,I,O"
440 PRINT D$"OPEN ";O$
450 PRINT D$"DELETE ";O$
460 PRINT D$"OPEN ";O$
470 PRINT D$"OPEN ";I$
480 REM
490 REM
500 PRINT D$;"WRITE ";O$

```

]

]LIST 510-1000

```

510 PRINT "          LAC THEORY OUTPUT"
520 PRINT " "
530 REM
540 REM          Start calculations
550 REM
560 FOR SOL = 1 TO 4
570 READ NMET
580 IF NMET = 0 THEN GOTO 1350
590 REM
600 REM
610 REM
620 FOR MET = 1 TO NMET
630 PRINT D$;"READ ";I$
640 INPUT M$,NDSET,RHO
650 REM
660 REM          Calc solvent radius
670 REM
680 RSOLV = (PF * 3 / (4 * PI * NAVO * RHO)) ^ .33333333
690 REM
700 PRINT D$;"WRITE ";O$
710 FOR I = 1 TO 6
720 PRINT " "
730 NEXT I
740 PRINT "          SOLUTE #";SOL;" METAL ";M$
750 PRINT " "
760 REM
770 REM
780 FOR SET = 1 TO NDSET
790 PRINT D$;"READ ";I$
800 INPUT A$,NPNT
810 PRINT D$;"WRITE ";O$
820 PRINT "INPUT FROM ";A$
830 REM
840 REM
850 REM
860 FOR PNT = 1 TO NPNT
870 PRINT D$;"READ ";I$
880 INPUT KH,TMP
890 PRINT D$;"WRITE ";O$
900 REM
910 REM          Check if data obeys equation L47 of
920 REM          Lee and Campbell calculation scheme
930 REM
940 CHK = 2.71828 ^ ((5 * PF + 4) / (2 * PF + 4) + LOG ((1 - PF) / RG /
    RHO))
950 IF KH < (CHK / TMP) GOTO 1010
960 PRINT "THIS DATA SHOULD NOT WORK"
970 REM
980 REM          Calc coefficients of equation L35 of
990 REM          Lee and Campbell calculation scheme
1000 REM

```

]

```
1010 D = PF / (1 - PF)
1020 A = (4.5 * D ^ 2 + 3 * D) / (RSOLV ^ 2)
1030 B = - (9 * D ^ 2 + 3 * D) / RSOLV
1040 C = LOG (KH * RG * TMP * RHO / (1 - PF)) + 4.5 * D ^ 2 - 1
1050 REM
1060 REM          Check if determinate is less than zero
1070 REM
1080 IF (B ^ 2 - 4 * A * C) < 0 THEN GOTO 1130
1090 REM
1100 R1(PNT) = ( - B + (B ^ 2 - 4 * A * C) ^ 0.5) / 2 / A - RSOLV
1110 R2(PNT) = ( - B - (B ^ 2 - 4 * A * C) ^ 0.5) / 2 / A - RSOLV
1120 GOTO 1140
1130 R1(PNT) = - 999
1140 REM
1150 PRINT "    TEMPERATURE: ";TMP
1160 PRINT "    SOLVENT DENSITY: ";RHO
1170 PRINT "    SOLUBILITY RATIO: ";KH
1180 PRINT " "
1190 NEXT PNT
1200 PRINT " "
1210 PRINT "OUTPUTS"
1220 FOR I = 1 TO NPNT
1230 IF R1(I) = - 999 THEN GOTO 1260
1240 PRINT "    POSSIBLE SOLUTIONS: ";R1(I);" ";R2(I)
1250 GOTO 1270
1260 PRINT "    NO SOLUTIONS...UNABLE TO SOLVE QUADRATIC"
1270 NEXT I
1280 PRINT " "
1290 PRINT " "
1300 REM
1310 REM
1320 REM
1330 NEXT SET
1340 NEXT MET
1350 NEXT SOL
1360 PRINT D$;"CLOSE ";O$
1370 PRINT D$;"CLOSE ";I$
1380 PRINT D$;"NOMON C,I,O"
1390 DATA 17, 0, 11, 4
1400 END

]PR#1
]PR#0
```


]LIST 10-500

```

10 REM          Regular solution and Qausi-chemical solution
20 REM          calulation programs
30 REM
40 REM  VARIABLE LIST
50 REM  AC - ACSOL...ACTIVITY COEFF OF THE SOLUTE
60 REM  BE - BE.....OUTPUT FROM REGULAR SOLUTION THEORY
70 REM  CH - CHK....NEXT VALUE CALC
80 REM  CA - CA.....MULTIPLIER OF THE CUBED TERM IN THE CUBIC TO BE SOLV
  ED
90 REM  CB - CB.....MULTIPLIER OF SQUARED TERM IN CUBIC
100 REM  CC - CC.....MULTIPLIER OF LINEAR TERM IN CUBIC
110 REM  CD - CD.....CONSTANT IN CUBIC
120 REM  D$ - D$.....CONTROL D
130 REM  DE - DETR...DETERMINATE OF QUADRATIC TO BE SOLVED
140 REM  LA - LAM....FIRST ROOT FOUND
150 REM  IT - ITER...INCREASE IN LAM PER ITERATION
160 REM  I  - I.....LOOP INDEX
170 REM  I$ - I$.....NAME OF INPUT FILE
180 REM  ME - MET....METAL LOOP INDEX
190 REM  M$ - M$.....NAME OF METAL
200 REM  NM - NMET...NUMBER OF METALS FORA SOLUTER HAS DATA
210 REM  NP - NPNT...NUMBER OF DATA POINTS FOR A SPECIFIC METAL-SOLUTE S
  YSTEM
220 REM  ND - NDSET..NUMBER OF DATA SETS
230 REM  O$ - O$.....NAME OF OUTPUT FILE
240 REM  PA - PTH....FLAG
250 REM  PT - PTH....LOCAL FLAG
260 REM  PN - PNT....INDEX IN DATA POINTS LOOP
270 REM  QB - QB.....COEFFICIENT
280 REM  QC - QC.....CONSTANT IN QUADRATIC EQUATION
290 REM  R1 - R1.....ROOT OF CUBIC
300 REM  R2 - R2.....ROOT OF CUBIC
310 REM  RG - RG....IDEAL GAS LAW CONSTANT
320 REM  SE - SET....LOOP INDEX
330 REM  SO - SOL....SOLUTE NUMBER
340 REM  SL - SLTE...CONCENTRATION FO THE SOLUTE  at frac
350 REM  SP - SP.....SPREAD ON OUTPUT
360 REM  ST - STR....VALUE OF STARTING CALCULATED STARTING POINT
370 REM  TM - TMP....TEMP  degree C
380 REM  XS - XSLV...CONCENTRATION OF THE SOLUTE  at frac
390 REM  ZE - ZERO...REMAINDER AFTER LONG DEVISION
400 REM  ZS - ZSOL...COORDINATION NUMBER OF THE SOLUTES
410 REM  E1, E2, E3..POSSIBLE SOLUTIONS  cal/gmole
420 REM
430 REM          Set input and output files
440 REM
450 O$ = "RQ.OTP"
460 I$ = "AC.DATA"
470 D$ = CHR$(4)
480 PRINT D$;"MON C,I,0"
490 PRINT D$;"OPEN ";O$
500 PRINT D$;"DELETE ";O$

```

```
510 PRINT D$;"OPEN ";O$
520 PRINT D$;"OPEN ";I$
530 REM
540 REM          Set constants
550 REM
560 RG = 1.987
570 REM
580 REM          Print output header
590 REM
600 PRINT D$;"WRITE ";O$
610 PRINT "          REGULAR SOLUTION AND QUASI-CHEMICAL SOLUTION RESULTS
"
620 PRINT " "
630 PRINT "UNIT KEY:"
640 PRINT "TEMPERATURE - DEGREE K"
650 PRINT "Wab          - CA;/GMOLE"
660 PRINT " "
670 PRINT " "
680 PRINT " "
690 FOR SOL = 1 TO 4
700 READ ZSOL(SOL),NMET
710 IF NMET = 0 THEN GOTO 2290
720 PRINT D$;"WRITE ";O$
730 PRINT " "
740 PRINT " "
750 FOR MET = 1 TO NMET
760 PRINT D$;"READ ";I$
770 INPUT M$,NDSET
780 PRINT D$;"WRITE ";O$
790 PRINT " "
800 PRINT " "
810 PRINT " "
820 PRINT " "
830 PRINT " "
840 PRINT " "
850 PRINT "          SOLUTE #";SOL;" METAL ";M$
860 REM
870 REM
880 FOR SET = 1 TO NDSET
890 PRINT D$;"READ ";I$
900 INPUT A$,NPNT
910 PRINT D$;"WRITE ";O$
920 PRINT "INPUT FROM ";A$
930 REM
940 REM
950 REM
960 FOR PNT = 1 TO NPNT
970 PRINT D$;"READ ";I$
980 INPUT ACSOL,SLTE,TMP
990 XSLV = 1 - SLTE
1000 REM
```

```
1010 REM          Begin quais-chemical calculation
1020 REM
1030 REM          Calculate coeffs in cubic defined by equation
1040 REM          G28 of quasi-chemical calculation scheme
1050 REM
1060 CA = 5 * ZSOL(SOL) * XSLV ^ 4
1070 CB = 3 / 4 * ZSOL(SOL) * XSL ^ 4 - ZSOL(SOL) * XSL ^ 3
1080 CC = 1 / 2 * ZSOL(SOL) * XSLV ^ 2
1090 CD = - LOG (ACSOL)
1100 REM
1110 REM          Normalize coeffs
1120 REM
1130 CB = CB / CA
1140 CC = CC / CA
1150 CD = CD / CA
1160 CA = CA / CA
1170 REM
1180 REM          Solve for first root by iterative loop technique
1190 REM
1200 LAM = - 1
1210 ITER = 1
1220 STR = CA * LAM ^ 3 + CB * LAM ^ 2 + CC * LAM + CD
1230 IF ABS (STR) < .001 GOTO 1550
1240 PTH = 0
1250 IF STR < 0.0 THEN PTH = 1
1260 REM
1270 REM
1280 REM
1290 LAM = LAM + ITER
1300 CHK = CA * LAM ^ 3 + CB * LAM ^ 2 + CC * LAM + CD
1310 IF ABS (CHK) < .001 GOTO 1550
1320 IF PTH = 1 GOTO 1400
1330 REM
1340 REM WHEN PTH EQUALS ONE, THE STARTING POINT WAS LESS THEN ZERO
1350 REM
1360 REM
1370 IF CHK > 0 THEN GOTO 1290
1380 GOTO 1440
1390 REM
1400 IF CHK < 0 THEN GOTO 1290
1410 REM
1420 REM          Overshot reset LAM
1430 REM
1440 LAM = LAM - 2 * ITER
1450 IF LAM < - 1 THEN LAM = - 1
1460 ITER = ITER / 10
1470 GOTO 1220
1480 REM
1490 REM
1500 REM
```

]

```
1010 REM          Begin quais-chemical calculation
1020 REM
1030 REM          Calculate coeffs in cubic defined by equation
1040 REM          G28 of quasi-chemical calculation scheme
1050 REM
1060 CA = 5 * ZSOL(SOL) * XSLV ^ 4
1070 CB = 3 / 4 * ZSOL(SOL) * XSL ^ 4 - ZSOL(SOL) * XSL ^ 3
1080 CC = 1 / 2 * ZSOL(SOL) * XSLV ^ 2
1090 CD = - LOG (ACSOL)
1100 REM
1110 REM          Normalize coeffs
1120 REM
1130 CB = CB / CA
1140 CC = CC / CA
1150 CD = CD / CA
1160 CA = CA / CA
1170 REM
1180 REM          Solve for first root by iterative loop technique
1190 REM
1200 LAM = - 1
1210 ITER = 1
1220 STR = CA * LAM ^ 3 + CB * LAM ^ 2 + CC * LAM + CD
1230 IF ABS (STR) < .001 GOTO 1550
1240 PTH = 0
1250 IF STR < 0.0 THEN PTH = 1
1260 REM
1270 REM
1280 REM
1290 LAM = LAM + ITER
1300 CHK = CA * LAM ^ 3 + CB * LAM ^ 2 + CC * LAM + CD
1310 IF ABS (CHK) < .001 GOTO 1550
1320 IF PTH = 1 GOTO 1400
1330 REM
1340 REM  WHEN PTH EQUALS ONE, THE STARTING POINT WAS LESS THEN ZERO
1350 REM
1360 REM
1370 IF CHK > 0 THEN GOTO 1290
1380 GOTO 1440
1390 REM
1400 IF CHK < 0 THEN GOTO 1290
1410 REM
1420 REM          Overshot reset LAM
1430 REM
1440 LAM = LAM - 2 * ITER
1450 IF LAM < - 1 THEN LAM = - 1
1460 ITER = ITER / 10
1470 GOTO 1220
1480 REM
1490 REM
1500 REM
```

```
1510 REM      ***FIRST ROOT OF CUBIC FOUND ***
1520 REM
1530 REM      Calc coeff of square
1540 REM
1550 QB = CB + LAM
1560 QC = CC + LAM * QB
1570 ZERO = CD + QC * LAM
1580 DETR = QB ^ 2 - 4 * QC
1590 REM
1600 REM      Solve square
1610 REM
1620 IF DETR < 0 GOTO 1710
1630 IF DETR = 0 GOTO 1780
1640 R1 = ( - QB + DETR ^ (0.5)) / 2
1650 R2 = ( - QB - DETR ^ .5) / 2
1660 PRINT "ROOT ARE ";R1;R2;LAM
1670 GOTO 1870
1680 REM
1690 REM
1700 REM
1710 PRINT "ONE ROOT ONLY, EQUALS ";LAM
1720 R1 = - 2
1730 R2 = - 2
1740 GOTO 1870
1750 REM
1760 REM
1770 REM
1780 R1 = - QB / 2
1790 PRINT "ROOTS ARE: ";R1;LAM
1800 R2 = - 2
1810 GOTO 1870
1820 REM
1830 REM
1840 REM
1850 REM      Calculate Wab values
1860 REM
1870 E1(PNT) = 0
1880 E2(PNT) = 0
1890 E3(PNT) = 0
1900 IF R1 < - 1 GOTO 1920
1910 E1(PNT) = LOG (R1 + 1) * RG * TMP / 2
1920 IF R2 < - 1 GOTO 1940
1930 E2(PNT) = LOG (R2 + 1) * RG * TMP / 2
1940 E3(PNT) = LOG (LAM + 1) * RG * TMP / 2
1950 PRINT D$;"WRITE ";O$
1960 REM
1970 REM      REGULAR SOLN CALC:
1980 REM
1990 BE(PNT) = LOG (ACSOL) * RG * TMP / XSLV ^ 2 / ZSOL(SOL)
2000 REM
```

```
2010 REM
2020 PRINT "    TEMPERATURE:          ";TMP
2030 PRINT "    SOLUTE ACTIVITY COEFF:    ";ACSOL
2040 PRINT "    SOLUTE CONCENTRATION        ";SLTE
2050 PRINT "    SOLUTE COORDINATION NUMBER: ";ZSOL(SOL)
2060 PRINT " "
2070 NEXT PNT
2080 REM
2090 REM
2100 PRINT "OUTPUT"
2110 FOR I = 1 TO NPNT
2120 PRINT "    QUASI-CHEMICAL PREDICTIONS OF Wab: ";E1(I);" ";E2(I);"
      ";E3(I)
2130 NEXT I
2140 SP = (E3(NPNT) - E3(1)) / E3(1) * 100
2150 IF SP < 0 THEN SP = - SP
2160 PRINT "    SPREAD ON OUTPUT: ";SP
2170 PRINT " "
2180 PRINT " "
2190 FOR I = 1 TO NPNT
2200 PRINT "    REGULAR SOLUTION PREDITIONS OF Wab: ";BE(I)
2210 NEXT I
2220 SP = (BE(NPNT) - BE(1)) / BE(1) * 100
2230 IF SP < 0 THEN SP = - SP
2240 PRINT "    SPREAD ON OUTPUT: ";SP
2250 PRINT " "
2260 PRINT " "
2270 NEXT SET
2280 NEXT MET
2290 NEXT SOL
2300 PRINT D$;"CLOSE ";I$
2310 PRINT D$;"CLOSE ";O$
2320 PRINT D$;"NOMON C,I,O"
2330 END
2340 DATA 2, 0
2350 DATA 4, 0
2360 DATA 6, 0
2370 DATA 6, 9
```

]PR#0

]LIST 10 - 500

```

10 REM          BUX THEORY CALC
20 REM
30 REM
40 REM
50 REM VARIABLE LIST
60 REM A - A.....CONS FOR DELTA H CALC
70 REM B - B.....CONS FOR DELTA H CACL
80 REM C - C.....CONS FOR DELTA H CALC
90 REM CE - CEC.....CONV FACTOR  erg/cal
100 REM CH - CHOICE..=0 FOR CALC FROM EXP DATA; =1 FOR PREDICTIONS
130 REM EC - ECOM....DELTA H  cal/gmole
140 REM DH - DH.....CONS FOR DELTA H CALC
150 REM I - I.....CONS FOR DELTA H CALC
160 REM IN - IN.....LOOP INDEX
170 REM LA - LAST....NUMBER OF POINTS DATA TABLES
180 REM ME - MET.....LOOP INDEX
190 REM MN - MNUM....METAL NUMBER
200 REM NA - NAVO.....AVOGODROS NUMBER  molecule/mole
205 REM NC - NC.....NUMBER OF ATOMS IN SOLUTE-SOLVENT COMPLEX
210 REM ND - NDSET...NUMBER OF DATA SETS
220 REM NM - NMET....NUMBER OF METALS SOLUTE HAS DATA FOR
230 REM NP - NPNT....NUMBER OF DATA POINTS FOR A METAL-SOLUTE
240 REM RA - RAD(4)...SOLUTE RADIUS  cm
250 REM RC - RC.....CALC SOLUTE RADIUS WITHOUT ECOM
260 REM RE - RE.....CALC SOLUTE RADIUS USING ECOM
270 REM RG - RG.....IDEAL GAS CONSTANT  cal/gmole /degree C
280 REM PE - PE.....PERCENT ERROR ON XMAX PREDICTION
290 REM PI - PI.....THE CONSTANT PI
300 REM PN - PNT.....LOOP INDEX
310 REM SE - SET....LOOP INDEX
340 REM T1 - T1.....INDEPENDENT VARIABLE DATA TABLE
350 REM T2 - T2.....DEPENDENT VARIABLE DATA TABLE
360 REM TH - THMET....METAL SURFACE TENSION  dyne/cm
380 REM TM - TMP.....TEMPERATURE  degree C
400 REM XC - XC.....CALC MAX SOLUBILTY
410 REM XM - XMAX.....SOLUTE MAXIMUM SOLUBITY  at frac
420 REM A$ - A$.....NAME AUTHOR FOR DATA SET
430 REM D$ - D$.....CONTROL D
440 REM I$ - I$.....NAME OF INPUT FILE
450 REM M$ - M$.....NAME OF METAL
460 REM O$ - O$.....NAME OF OUTPUT FILE
470 REM S$ - S$.....NAME OF SOLUTE
480 REM T$ - T$.....NAME OF TABLE INPUT FILE
490 REM
500 REM

```

]

```
510 D$ = CHR$ (4)
520 O$ = "BUXC.OTP"
525 I$ = "XC.DATA"
530 READ CHOICE
550 PRINT D$;"MON C,I,O"
560 PRINT D$;"OPEN ";O$
570 PRINT D$;"DELETE ";O$
580 PRINT D$;"OPEN ";O$
590 PRINT D$;"OPEN ";I$
600 REM
610 REM
615 GOTO 750
620 REM FOR PREDICTIVE PURPOSES ONLY
630 IF CHOICE = 0 THEN GOTO 740
640 T$ = "TABLE.DAT"
650 PRINT D$;"OPEN ";T$
660 PRINT D$;"READ ";T$
670 INPUT LAST
680 REM
690 FOR IN = 1 TO LAST
700 INPUT T1(IN),T2(IN)
705 T2(IN) = T2(IN) * 10 ^ ( - 8)
710 NEXT IN
720 REM
730 REM
740 REM
750 PRINT D$;"READ ";I$
760 INPUT S$,NMET
770 REM
780 REM
790 REM
800 REM SET CONSTANTA
850 RG = 1.987
860 NAVO = 6.023E23
870 PI = 3.141593
880 CEC = 4.184E7
890 REM
900 REM
910 REM
920 REM START CALCULATIONS
940 REM
950 REM
960 REM
970 IF NMET = 0 THEN GOTO 2060
980 REM
990 REM
1000 PRINT D$;"WRITE ";O$
```

]


```
1010 PRINT "          BUX THEORY OUTPUT"
1020 PRINT " "
1030 PRINT "UNITS KEY:"
1040 PRINT "  RADIUS          - CM"
1050 PRINT "  SOLUBILITY       - AT FRAC"
1070 PRINT "  TEMPERATURE      - DEGREE C"
1080 PRINT "  SURFACE TENSION - DYNE/CM"
1090 REM
1100 REM
1110 REM
1120 FOR MET = 1 TO NMET
1130 PRINT D$;"READ ";I$
1140 INPUT M$,NDSET
1150 INPUT DH,A,B,C,I,NC
1160 REM
1170 REM
1200 REM
1210 REM
1220 REM
1230 PRINT D$;"WRITE ";O$
1240 FOR IN = 1 TO 6
1250 PRINT " "
1260 NEXT IN
1270 PRINT "          OUTPUT FOR ";S$;" AND METAL ";M$
1280 PRINT " "
1290 FOR SET = 1 TO NDSET
1300 PRINT D$;"READ ";I$
1310 INPUT A$,NPNT
1320 PRINT D$;"WRITE ";O$
1330 PRINT "INPUT FROM ";A$
1340 REM
1350 REM
1360 REM
1370 FOR PNT = 1 TO NPNT
1380 PRINT D$;"READ ";I$
1390 INPUT XMAX,TMP,THMET
1400 REM
1410 REM
1420 REM
1430 IF CHOICE = 0 THEN GOTO 1840
1450 REM
1460 REM
1465 GOTO 1765
1470 REM THIS WILL SEARCH A TABLE
1480 REM
1490 REM
1500 REM T1 ARE THE INDEPDENT OR SEARCHED TABLE VALUES
```

```

1510 REM      IT IS ASSUMED THEY STARTS SMALL AND GETS LARGER
1520 REM
1530 REM      RAD IS THE DEPENDENT OR OUTPUT TABLE VALUES
1540 REM
1550 REM      INPUTS
1560 REM      NUMBER OF TABLE VALUES
1570 REM      THE TABLE VALUES
1580 REM      THE VALUE TO BE SEARCHED FOR
1590 REM
1600 REM
1610 REM
1620 IF TMP > T1(1) THEN GOTO 1650
1630 RAD(SOL) = T2(1)
1640 GOTO 1760
1650 IF TMP < T1(LAST) THEN GOTO 1680
1660 RAD(SOL) = T2(LAST)
1670 GOTO 1760
1680 IN = 1
1690 IN = IN + 1
1700 IF TMP > T1(IN) THEN GOTO 1690
1710 REM
1720 REM
1730 RC(PNT) = T2(IN) + (TMP - T1(IN)) / (T1(IN - 1) - T1(IN)) * (T2(IN -
1) - T2(IN))
1740 REM
1750 REM
1760 REM
1765 RC(PNT) = 0.5E - 8
1770 XC(PNT) = 2.7128 ^ ( - 4 * PI * RC(PNT) ^ 2 * NAVO * THMET / (RG * T
MP * CEC))
1780 PE(PNT) = (XMAX - XC(PNT)) / XMAX * 100
1790 ECOM = 0
1800 GOTO 1868
1810 REM
1820 REM
1830 REM
1840 ECOM = DH + A / 2.303 * LOG (TMP) + B * 1E - 3 * TMP ^ 2 + C * 1E5 /
TMP + I * TMP
1845 IF ECOM = 0 GOTO 1868
1850 ECOM = ECOM / NC
1860 RE(PNT) = (CEC * ( - RG * TMP * LOG (XMAX) + ECOM) / THMET / NAVO /
4 / PI) ^ 0.5
1865 GOTO 1870
1868 RE(PNT) = 0
1870 RC(PNT) = (CEC * ( - RG * TMP * LOG (XMAX)) / THMET / NAVO / 4 / PI
) ^ 0.5
1930 REM
1940 REM
1950 REM
1960 PRINT D$;"WRITE ";O$
1970 PRINT "      TEMPERATURE:          ";TMP
2000 PRINT "      SOLUTE MAXIMUM SOL:    ";XMAX

```

```
2010 PRINT " METAL SURFACE TENSION: ";THMET
2020 PRINT " "
2030 NEXT PNT
2040 REM
2050 REM
2060 REM
2070 PRINT " "
2080 PRINT "OUTPUT"
2090 IF CHOICE = 0 THEN GOTO 2180
2100 REM
2110 REM
2120 FOR IN = 1 TO NPNT
2130 PRINT " CALC MAX SOLUBILITY: ";XC(IN)
2140 NEXT IN
2150 PRINT " "
2160 REM
2170 REM
2180 FOR IN = 1 TO NPNT
2190 PRINT " SOLUTE RADIUS N/ECOM: ";RC(IN)
2200 NEXT IN
2210 REM
2215 GOTO 2310
2220 PRINT " "
2230 FOR IN = 1 TO NPNT
2240 PRINT " SOLUTE RADIUS W/ECOM: ";RE(IN)
2250 NEXT IN
2260 REM
2310 PRINT " "
2320 PRINT " "
2330 NEXT SET
2340 NEXT MET
2350 PRINT D$;"CLOSE ";O$
2360 PRINT D$;"CLOSE ";I$
2370 PRINT D$"NOMON C,I,O"
2380 DATA 1
2390 END
```

]PR#0

REGULAR SOLUTION AND QUASI-CHEMICAL SOLUTION RESULTS
WITH MAXIMUM SOLUBILITY DATA AS INPUT

UNIT KEY:

SOLUBILITY - AT FRAC

TEMPERATURE - DEGREE K

Wab - CA;/GMOLE

SOLUTE CARBON METAL ALUMINUM - NONE??

INPUT FROM HANSEN

TEMPERATURE: 1070
SOLUTE ACTIVITY COEFF: 454.545455
SOLUTE CONCENTRATION 2.2E-03
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1270
SOLUTE ACTIVITY COEFF: 322.580645
SOLUTE CONCENTRATION 3.1E-03
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1370
SOLUTE ACTIVITY COEFF: 285.714286
SOLUTE CONCENTRATION 3.5E-03
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1470
SOLUTE ACTIVITY COEFF: 140.84507
SOLUTE CONCENTRATION 7.1E-03
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 527.179973
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 616.463392
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 659.984406
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 682.758767
SPREAD ON OUTPUT: 29.5115143

REGULAR SOLUTION PREDICTIONS OF Wab: 3266.90309
REGULAR SOLUTION PREDICTIONS OF Wab: 3666.84154
REGULAR SOLUTION PREDICTIONS OF Wab: 3875.57241
REGULAR SOLUTION PREDICTIONS OF Wab: 3664.74769
SPREAD ON OUTPUT: 12.178035

SOLUTE CARBON METAL ANTIMONY - NONE

INPUT FROM HANSEN

TEMPERATURE: 1330
SOLUTE ACTIVITY COEFF: 297.619048
SOLUTE CONCENTRATION 3.36E-03
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1540
SOLUTE ACTIVITY COEFF: 144.7178
SOLUTE CONCENTRATION 6.91E-03
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1600
SOLUTE ACTIVITY COEFF: 104.602511
SOLUTE CONCENTRATION 9.56E-03
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 642.341071
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 716.229428
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 731.141755
SPREAD ON OUTPUT: 13.8245378

REGULAR SOLUTION PREDICTIONS OF Wab: 3788.51239
REGULAR SOLUTION PREDICTIONS OF Wab: 3858.83093
REGULAR SOLUTION PREDICTIONS OF Wab: 3767.64622
SPREAD ON OUTPUT: .550774632

SOLUTE CARBON METAL BISMUTH - NONE

INPUT FROM GRIFFITH

TEMPERATURE: 570
SOLUTE ACTIVITY COEFF: 36363.6364
SOLUTE CONCENTRATION 2.75E-05
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 670
SOLUTE ACTIVITY COEFF: 29239.7661
SOLUTE CONCENTRATION 3.42E-05
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 770
SOLUTE ACTIVITY COEFF: 24937.6559
SOLUTE CONCENTRATION 4.01E-05
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 870

SOLUTE ACTIVITY COEFF: 22026.4317
 SOLUTE CONCENTRATION 4.54E-05
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 970
 SOLUTE ACTIVITY COEFF: 19960.0798
 SOLUTE CONCENTRATION 5.01E-05
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1070
 SOLUTE ACTIVITY COEFF: 19157.0881
 SOLUTE CONCENTRATION 5.22E-05
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 327.169194
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 382.322288
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 437.228577
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 492.546102
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 547.523979
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 603.367288
 SPREAD ON OUTPUT: 84.4205684

REGULAR SOLUTION PREDITIONS OF Wab: 2973.58734
 REGULAR SOLUTION PREDITIONS OF Wab: 3422.7427
 REGULAR SOLUTION PREDITIONS OF Wab: 3872.76662
 REGULAR SOLUTION PREDITIONS OF Wab: 4322.11677
 REGULAR SOLUTION PREDITIONS OF Wab: 4771.48608
 REGULAR SOLUTION PREDITIONS OF Wab: 5241.58658
 SPREAD ON OUTPUT: 76.2714857

SOLUTE CARBON METAL CERIUM - NONE - S.T. GUESS
 INPUT FROM GTE

TEMPERATURE: 870
 SOLUTE ACTIVITY COEFF: 3.92156863
 SOLUTE CONCENTRATION .255
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1070
 SOLUTE ACTIVITY COEFF: 3.33333333
 SOLUTE CONCENTRATION .3
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 373.770054
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 474.763393

SPREAD ON OUTPUT: 27.0201796

REGULAR SOLUTION PREDITIONS OF Wab: 1064.02441

REGULAR SOLUTION PREDITIONS OF Wab: 1305.99721

SPREAD ON OUTPUT: 22.741283

SOLUTE CARBON METAL CHROMIUM - NONE - UNSURE S.T. DATA
INPUT FROM HANSEN

TEMPERATURE: 1750
SOLUTE ACTIVITY COEFF: 7.35294118
SOLUTE CONCENTRATION .136
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1830
SOLUTE ACTIVITY COEFF: 6.66666667
SOLUTE CONCENTRATION .15
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1950
SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2080
SOLUTE ACTIVITY COEFF: 3.33333333
SOLUTE CONCENTRATION .3
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 716.504143
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 749.258618
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 812.452136
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 922.904541
SPREAD ON OUTPUT: 28.8065882

REGULAR SOLUTION PREDITIONS OF Wab: 2323.34227

REGULAR SOLUTION PREDITIONS OF Wab: 2386.96424

REGULAR SOLUTION PREDITIONS OF Wab: 2435.94086

REGULAR SOLUTION PREDITIONS OF Wab: 2538.76094

SPREAD ON OUTPUT: 9.27193009

INPUT FROM GTE

TEMPERATURE: 1800
SOLUTE ACTIVITY COEFF: 6.89655173

SOLUTE CONCENTRATION .145
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1910
SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1990
SOLUTE ACTIVITY COEFF: 4
SOLUTE CONCENTRATION .25
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 736.975689
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 795.786451
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 853.661905
SPREAD ON OUTPUT: 15.833116

REGULAR SOLUTION PREDICTIONS OF Wab: 2361.92046
REGULAR SOLUTION PREDICTIONS OF Wab: 2385.97284
REGULAR SOLUTION PREDICTIONS OF Wab: 2436.26139
SPREAD ON OUTPUT: 3.14747793

SOLUTE CARBON METAL COBALT - Co3C - DENSITY IS GUESS
INPUT FROM HANSEN - CHECKS WITH ONE SOURCE

TEMPERATURE: 1620
SOLUTE ACTIVITY COEFF: 8.33333333
SOLUTE CONCENTRATION .12
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1720
SOLUTE ACTIVITY COEFF: 7.57575758
SOLUTE CONCENTRATION .132
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1820
SOLUTE ACTIVITY COEFF: 6.99300699
SOLUTE CONCENTRATION .143
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 660.077317
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 701.956376
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 745.164308
SPREAD ON OUTPUT: 12.8904583

REGULAR SOLUTION PREDITIONS OF Wab: 2203.31906
REGULAR SOLUTION PREDITIONS OF Wab: 2296.37017
REGULAR SOLUTION PREDITIONS OF Wab: 2394.12749
SPREAD ON OUTPUT: 8.66004567

SOLUTE CARBON METAL COPPER - NONE
INPUT FROM HANSEN

TEMPERATURE: 1370
SOLUTE ACTIVITY COEFF: 188679.245
SOLUTE CONCENTRATION 5.3E-06
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1570
SOLUTE ACTIVITY COEFF: 125944.584
SOLUTE CONCENTRATION 7.94E-06
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1770
SOLUTE ACTIVITY COEFF: 37735.849
SOLUTE CONCENTRATION 2.65E-05
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1970
SOLUTE ACTIVITY COEFF: 6289.30818
SOLUTE CONCENTRATION 1.59E-04
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 818.061503
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 928.911505
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1016.93298
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1073.91148
SPREAD ON OUTPUT: 31.2751519

REGULAR SOLUTION PREDITIONS OF Wab: 8267.24509
REGULAR SOLUTION PREDITIONS OF Wab: 9158.94761
REGULAR SOLUTION PREDITIONS OF Wab: 9266.32292
REGULAR SOLUTION PREDITIONS OF Wab: 8562.12965
SPREAD ON OUTPUT: 3.56690235

SOLUTE CARBON METAL GERMANIUM - NONE - S.T. UNSURE DUE TO HIGH

TEMPS

INPUT FROM SCARCE

TEMPERATURE: 3000
 SOLUTE ACTIVITY COEFF: 75.1879699
 SOLUTE CONCENTRATION .0133
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3100
 SOLUTE ACTIVITY COEFF: 39.2156863
 SOLUTE CONCENTRATION .0255
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3200
 SOLUTE ACTIVITY COEFF: 21.2765958
 SOLUTE CONCENTRATION .047
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3300
 SOLUTE ACTIVITY COEFF: 12.0048019
 SOLUTE CONCENTRATION .0833
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1346.32869
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1339.80839
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1339.51922
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1351.1221
 SPREAD ON OUTPUT: .356035701

REGULAR SOLUTION PREDITIONS OF Wab: 6612.5922
 REGULAR SOLUTION PREDITIONS OF Wab: 5949.66739
 REGULAR SOLUTION PREDITIONS OF Wab: 5351.60207
 REGULAR SOLUTION PREDITIONS OF Wab: 4848.16452
 SPREAD ON OUTPUT: 26.6828443

SOLUTE CARBON METAL HAFNIUM - NONE - S.T. UNSURE

INPUT FROM HANSEN

TEMPERATURE: 2480
 SOLUTE ACTIVITY COEFF: 10.5263158
 SOLUTE CONCENTRATION .095
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2820
SOLUTE ACTIVITY COEFF: 6.66666667
SOLUTE CONCENTRATION .15
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3160
SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3400
SOLUTE ACTIVITY COEFF: 4
SOLUTE CONCENTRATION .25
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3685
SOLUTE ACTIVITY COEFF: 3.33333333
SOLUTE CONCENTRATION .3
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1012.12315
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1154.59525
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1316.5891
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1458.51783
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1635.04963
SPREAD ON OUTPUT: 61.5465109

REGULAR SOLUTION PREDICTIONS OF Wab: 3540.59637
REGULAR SOLUTION PREDICTIONS OF Wab: 3678.27276
REGULAR SOLUTION PREDICTIONS OF Wab: 3947.4734
REGULAR SOLUTION PREDICTIONS OF Wab: 4162.45664
REGULAR SOLUTION PREDICTIONS OF Wab: 4497.75676
SPREAD ON OUTPUT: 27.0338748

INPUT FROM GTE

TEMPERATURE: 2630
SOLUTE ACTIVITY COEFF: 20
SOLUTE CONCENTRATION .05
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3110
SOLUTE ACTIVITY COEFF: 14.2857143
SOLUTE CONCENTRATION .07
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3680
SOLUTE ACTIVITY COEFF: 6.66666667
SOLUTE CONCENTRATION .15
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 4080

SOLUTE ACTIVITY COEFF: 3.33333333
SOLUTE CONCENTRATION .3
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1097.4861
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1279.46277
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1506.70585
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1810.31275
SPREAD ON OUTPUT: 64.9508592

REGULAR SOLUTION PREDICTIONS OF Wab: 4336.60046
REGULAR SOLUTION PREDICTIONS OF Wab: 4749.99524
REGULAR SOLUTION PREDICTIONS OF Wab: 4800.01552
REGULAR SOLUTION PREDICTIONS OF Wab: 4979.87723
SPREAD ON OUTPUT: 14.8336645

SOLUTE CARBON METAL IRON - Fe3C
INPUT FROM TURKOGAN

TEMPERATURE: 1570
SOLUTE ACTIVITY COEFF: 5.39083558
SOLUTE CONCENTRATION .1855
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1670
SOLUTE ACTIVITY COEFF: 5.13347022
SOLUTE CONCENTRATION .1948
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1770
SOLUTE ACTIVITY COEFF: 4.91400491
SOLUTE CONCENTRATION .2035
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1870
SOLUTE ACTIVITY COEFF: 4.72589792
SOLUTE CONCENTRATION .2116
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 650.020701
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 694.701159
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 738.612318
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 784.000204
SPREAD ON OUTPUT: 20.6115748

REGULAR SOLUTION PREDITIONS OF Wab: 1980.51451
 REGULAR SOLUTION PREDITIONS OF Wab: 2093.01437
 REGULAR SOLUTION PREDITIONS OF Wab: 2206.51558
 REGULAR SOLUTION PREDITIONS OF Wab: 2320.99288
 SPREAD ON OUTPUT: 17.19141

INPUT FROM .GRIGOROVICH - Fe-GRAPHITE EQUIL

TEMPERATURE: 1420
 SOLUTE ACTIVITY COEFF: 5.84795322
 SOLUTE CONCENTRATION .171
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1710
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2300
 SOLUTE ACTIVITY COEFF: 4
 SOLUTE CONCENTRATION .25
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2600
 SOLUTE ACTIVITY COEFF: 3.33333333
 SOLUTE CONCENTRATION .3
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 585.12413
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 712.458027
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 986.644413
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1153.63068
 SPREAD ON OUTPUT: 97.15999

REGULAR SOLUTION PREDITIONS OF Wab: 1812.71869
 REGULAR SOLUTION PREDITIONS OF Wab: 2136.13275
 REGULAR SOLUTION PREDITIONS OF Wab: 2815.77949
 REGULAR SOLUTION PREDITIONS OF Wab: 3173.45117
 SPREAD ON OUTPUT: 75.065838

INPUT FROM GIRGOROVICH - Fe₃C-Fe EQUIL

TEMPERATURE: 1420
 SOLUTE ACTIVITY COEFF: 5.84795322
 SOLUTE CONCENTRATION .171
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1500
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1670
 SOLUTE ACTIVITY COEFF: 4
 SOLUTE CONCENTRATION .25
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 585.12413
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 624.963181
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 716.389639
 SPREAD ON OUTPUT: 22.4337884

REGULAR SOLUTION PREDITIONS OF Wab: 1812.71869
 REGULAR SOLUTION PREDITIONS OF Wab: 1873.80066
 REGULAR SOLUTION PREDITIONS OF Wab: 2044.50076
 SPREAD ON OUTPUT: 12.7864334

SOLUTE CARBON METAL LITHIUM - NONE

INPUT FROM ADAMS

TEMPERATURE: 570
 SOLUTE ACTIVITY COEFF: 95.2380953
 SOLUTE CONCENTRATION .0105
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 670
 SOLUTE ACTIVITY COEFF: 58.8235294
 SOLUTE CONCENTRATION .017
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 770
 SOLUTE ACTIVITY COEFF: 42.5531915
 SOLUTE CONCENTRATION .0235
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 870
 SOLUTE ACTIVITY COEFF: 33.3333333
 SOLUTE CONCENTRATION .03
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 259.037404
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 296.429452
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 334.275103
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 373.208973
 SPREAD ON OUTPUT: 44.0753217

REGULAR SOLUTION PREDITIONS OF Wab: 1317.65305
REGULAR SOLUTION PREDITIONS OF Wab: 1403.40957
REGULAR SOLUTION PREDITIONS OF Wab: 1504.5367
REGULAR SOLUTION PREDITIONS OF Wab: 1610.62588
SPREAD ON OUTPUT: 22.2344438

INPUT FROM HANSEN

TEMPERATURE: 680
SOLUTE ACTIVITY COEFF: 62.5
SOLUTE CONCENTRATION .016
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 830
SOLUTE ACTIVITY COEFF: 50
SOLUTE CONCENTRATION .02
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 970
SOLUTE ACTIVITY COEFF: 31.25
SOLUTE CONCENTRATION .032
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1070
SOLUTE ACTIVITY COEFF: 19.2307692
SOLUTE CONCENTRATION .052
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1170
SOLUTE ACTIVITY COEFF: 10.989011
SOLUTE CONCENTRATION .091
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 301.718792
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 363.512479
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 414.227397
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 445.80707
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 479.034198
SPREAD ON OUTPUT: 58.768433

REGULAR SOLUTION PREDITIONS OF Wab: 1442.61219
REGULAR SOLUTION PREDITIONS OF Wab: 1679.4428
REGULAR SOLUTION PREDITIONS OF Wab: 1769.99568
REGULAR SOLUTION PREDITIONS OF Wab: 1748.57619
REGULAR SOLUTION PREDITIONS OF Wab: 1685.95167
SPREAD ON OUTPUT: 16.867976

INPUT FROM HANSEN

TEMPERATURE: 1010
SOLUTE ACTIVITY COEFF: 20

SOLUTE CONCENTRATION .05
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1055
SOLUTE ACTIVITY COEFF: 10
SOLUTE CONCENTRATION .1
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1070
SOLUTE ACTIVITY COEFF: 6.66666667
SOLUTE CONCENTRATION .15
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1090
SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 421.468046
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 430.560452
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 438.091104
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 454.139912
SPREAD ON OUTPUT: 7.75192002

REGULAR SOLUTION PREDICTIONS OF Wab: 1665.38649
REGULAR SOLUTION PREDICTIONS OF Wab: 1489.77611
REGULAR SOLUTION PREDICTIONS OF Wab: 1395.65669
REGULAR SOLUTION PREDICTIONS OF Wab: 1361.62848
SPREAD ON OUTPUT: 18.2394904

SOLUTE CARBON METAL MANGANESE - Mn₃C - S.T. UNSURE INPUT FROM HANSEN

TEMPERATURE: 1620
SOLUTE ACTIVITY COEFF: 3.79362671
SOLUTE CONCENTRATION .2636
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1720
SOLUTE ACTIVITY COEFF: 3.67647059
SOLUTE CONCENTRATION .272
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1820
SOLUTE ACTIVITY COEFF: 3.57653791
SOLUTE CONCENTRATION .2796

SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1870
 SOLUTE ACTIVITY COEFF: 3.48675035
 SOLUTE CONCENTRATION .2868
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 700.157933
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 748.898793
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 794.771037
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 821.387507
 SPREAD ON OUTPUT: 17.314604

REGULAR SOLUTION PREDITIONS OF Wab: 1978.61151
 REGULAR SOLUTION PREDITIONS OF Wab: 2098.93477
 REGULAR SOLUTION PREDITIONS OF Wab: 2220.06661
 REGULAR SOLUTION PREDITIONS OF Wab: 2280.91384
 SPREAD ON OUTPUT: 15.2785085

INPUT FROM HANSEN

TEMPERATURE: 1500
 SOLUTE ACTIVITY COEFF: 17.5438597
 SOLUTE CONCENTRATION .057
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1565
 SOLUTE ACTIVITY COEFF: 6.66666667
 SOLUTE CONCENTRATION .15
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1590
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1610
 SOLUTE ACTIVITY COEFF: 4
 SOLUTE CONCENTRATION .25
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 622.02093
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 640.759419
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 662.460973
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 690.651089
 SPREAD ON OUTPUT: 11.0334164

REGULAR SOLUTION PREDITIONS OF Wab: 2400.41043
 REGULAR SOLUTION PREDITIONS OF Wab: 2041.31095
 REGULAR SOLUTION PREDITIONS OF Wab: 1986.2287

REGULAR SOLUTION PREDITIONS OF Wab: 1971.04565
SPREAD ON OUTPUT: 17.8871405

INPUT FROM HANSEN

TEMPERATURE: 1580
SOLUTE ACTIVITY COEFF: 3.77358491
SOLUTE CONCENTRATION .265
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1620
SOLUTE ACTIVITY COEFF: 3.67647059
SOLUTE CONCENTRATION .272
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1720
SOLUTE ACTIVITY COEFF: 3.57142857
SOLUTE CONCENTRATION .28
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1870
SOLUTE ACTIVITY COEFF: 3.42465754
SOLUTE CONCENTRATION .292
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 683.88576
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 705.358165
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 752.202987
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 826.157331
SPREAD ON OUTPUT: 20.8034118

REGULAR SOLUTION PREDITIONS OF Wab: 1929.41959
REGULAR SOLUTION PREDITIONS OF Wab: 1976.90368
REGULAR SOLUTION PREDITIONS OF Wab: 2098.06057
REGULAR SOLUTION PREDITIONS OF Wab: 2281.24296
SPREAD ON OUTPUT: 18.2346738

SOLUTE CARBON METAL MOLYBDENUM - Mo₂C - S.T. UNSURE

INPUT FROM RUDY

TEMPERATURE: 2470
SOLUTE ACTIVITY COEFF: 5.88235294
SOLUTE CONCENTRATION .17
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2600

SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2700
SOLUTE ACTIVITY COEFF: 4
SOLUTE CONCENTRATION .25
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1017.78634
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1083.26951
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1158.23475
SPREAD ON OUTPUT: 13.7993999

REGULAR SOLUTION PREDICTIONS OF Wab: 3155.96214
REGULAR SOLUTION PREDICTIONS OF Wab: 3247.92115
REGULAR SOLUTION PREDICTIONS OF Wab: 3305.48027
SPREAD ON OUTPUT: 4.73764049

SOLUTE CARBON METAL NICKEL - N13C
INPUT FROM HANSEN

TEMPERATURE: 1620
SOLUTE ACTIVITY COEFF: 10.3092784
SOLUTE CONCENTRATION .097
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1720
SOLUTE ACTIVITY COEFF: 9.61538462
SOLUTE CONCENTRATION .104
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1820
SOLUTE ACTIVITY COEFF: 9.00900901
SOLUTE CONCENTRATION .111
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1920
SOLUTE ACTIVITY COEFF: 8.47457627
SOLUTE CONCENTRATION .118
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2020
SOLUTE ACTIVITY COEFF: 8.06451613
SOLUTE CONCENTRATION .124
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 661.144959
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 700.82283
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 741.568343
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 782.313857
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 823.05937
 SPREAD ON OUTPUT: 24.4900016

REGULAR SOLUTION PREDICTIONS OF Wab: 2302.50391
 REGULAR SOLUTION PREDICTIONS OF Wab: 2408.82239
 REGULAR SOLUTION PREDICTIONS OF Wab: 2514.65205
 REGULAR SOLUTION PREDICTIONS OF Wab: 2620.11778
 REGULAR SOLUTION PREDICTIONS OF Wab: 2729.6191
 SPREAD ON OUTPUT: 18.5500312

SOLUTE CARBON METAL NIOBIUM - NONE - S.T. UNSURE
 INPUT FROM KIMURA

TEMPERATURE: 2610
 SOLUTE ACTIVITY COEFF: 7.40740741
 SOLUTE CONCENTRATION .135
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2880
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3110
 SOLUTE ACTIVITY COEFF: 4
 SOLUTE CONCENTRATION .25
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3280
 SOLUTE ACTIVITY COEFF: 3.33333333
 SOLUTE CONCENTRATION .3
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1068.61475
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1199.92931
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1334.11484
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1455.34947
 SPREAD ON OUTPUT: 36.1902844

REGULAR SOLUTION PREDITIONS OF Wab: 3469.88006
REGULAR SOLUTION PREDITIONS OF Wab: 3597.69727
REGULAR SOLUTION PREDITIONS OF Wab: 3807.42358
REGULAR SOLUTION PREDITIONS OF Wab: 4003.43071
SPREAD ON OUTPUT: 15.3766308

SOLUTE CARBON METAL PLUTONIUM - NONE
INPUT FROM HANSEN

TEMPERATURE: 1275
SOLUTE ACTIVITY COEFF: 20
SOLUTE CONCENTRATION .05
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1420
SOLUTE ACTIVITY COEFF: 10
SOLUTE CONCENTRATION .1
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1550
SOLUTE ACTIVITY COEFF: 6.66666667
SOLUTE CONCENTRATION .15
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1650
SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 532.051246
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 579.522124
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 634.617954
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 687.4595
SPREAD ON OUTPUT: 29.2092641

REGULAR SOLUTION PREDITIONS OF Wab: 2102.34433
REGULAR SOLUTION PREDITIONS OF Wab: 2005.19628
REGULAR SOLUTION PREDITIONS OF Wab: 2021.74567
REGULAR SOLUTION PREDITIONS OF Wab: 2061.18073
SPREAD ON OUTPUT: 1.95798573

SOLUTE CARBON METAL RHENIUM - NONE - S.T. UNSURE
INPUT FROM HUGES

TEMPERATURE: 2770
SOLUTE ACTIVITY COEFF: 5.91715977
SOLUTE CONCENTRATION .169
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2870
SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2970
SOLUTE ACTIVITY COEFF: 4.34782609
SOLUTE CONCENTRATION .23
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3040
SOLUTE ACTIVITY COEFF: 4
SOLUTE CONCENTRATION .25
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1139.58581
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1195.76289
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1256.76331
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1304.08653
SPREAD ON OUTPUT: 14.4351318

REGULAR SOLUTION PREDICTIONS OF Wab: 3542.52005
REGULAR SOLUTION PREDICTIONS OF Wab: 3585.20527
REGULAR SOLUTION PREDICTIONS OF Wab: 3657.08006
REGULAR SOLUTION PREDICTIONS OF Wab: 3721.72594
SPREAD ON OUTPUT: 5.05871217

SOLUTE CARBON METAL SILVER - NONE
INPUT FROM HANSEN

TEMPERATURE: 1930
SOLUTE ACTIVITY COEFF: 9259.25926
SOLUTE CONCENTRATION 1.08E-04
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2005
SOLUTE ACTIVITY COEFF: 4444.44445

SOLUTE CONCENTRATION 2.25E-04
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1065.35289
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1081.45015
SPREAD ON OUTPUT: 1.51097874

REGULAR SOLUTION PREDICTIONS OF Wab: 8758.31363
REGULAR SOLUTION PREDICTIONS OF Wab: 8369.44185
SPREAD ON OUTPUT: 4.44003019

SOLUTE CARBON METAL SODIUM - NONE
INPUT FROM SALZANO

TEMPERATURE: 850
SOLUTE ACTIVITY COEFF: 61312.0785
SOLUTE CONCENTRATION 1.631E-05
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 970
SOLUTE ACTIVITY COEFF: 27063.5995
SOLUTE CONCENTRATION 3.695E-05
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 494.022116
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 552.425519
SPREAD ON OUTPUT: 11.8220221

REGULAR SOLUTION PREDICTIONS OF Wab: 4654.78494
REGULAR SOLUTION PREDICTIONS OF Wab: 4918.07248
SPREAD ON OUTPUT: 5.65627723

INPUT FROM HANSEN

TEMPERATURE: 420
SOLUTE ACTIVITY COEFF: 16129.0323
SOLUTE CONCENTRATION 6.2E-05
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 570
SOLUTE ACTIVITY COEFF: 11111.1111
SOLUTE CONCENTRATION 9E-05
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 770
 SOLUTE ACTIVITY COEFF: 8196.72132
 SOLUTE CONCENTRATION 1.22E-04
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 970
 SOLUTE ACTIVITY COEFF: 6944.44445
 SOLUTE CONCENTRATION 1.44E-04
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 235.65134
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 316.260058
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 423.279563
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 530.447486
 SPREAD ON OUTPUT: 125.098438

REGULAR SOLUTION PREDICTIONS OF Wab: 2021.58503
 REGULAR SOLUTION PREDICTIONS OF Wab: 2638.19227
 REGULAR SOLUTION PREDICTIONS OF Wab: 3447.7134
 REGULAR SOLUTION PREDICTIONS OF Wab: 4263.50491
 SPREAD ON OUTPUT: 110.899113

SOLUTE CARBON METAL TANTALUM - NONE
 INPUT FROM HANSEN - UNSURE PHASE DIAG

TEMPERATURE: 3070
 SOLUTE ACTIVITY COEFF: 12.5
 SOLUTE CONCENTRATION .08
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3150
 SOLUTE ACTIVITY COEFF: 10
 SOLUTE CONCENTRATION .1
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3305
 SOLUTE ACTIVITY COEFF: 6.66666667
 SOLUTE CONCENTRATION .15
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3455
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1256.95298
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1285.55964
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1353.16925
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1439.49853
SPREAD ON OUTPUT: 14.522862

REGULAR SOLUTION PREDITIONS OF Wab: 4550.79515
REGULAR SOLUTION PREDITIONS OF Wab: 4448.14667
REGULAR SOLUTION PREDITIONS OF Wab: 4310.88351
REGULAR SOLUTION PREDITIONS OF Wab: 4315.98753
SPREAD ON OUTPUT: 5.1597054

INPUT FROM GTE

TEMPERATURE: 3120
SOLUTE ACTIVITY COEFF: 8.33333333
SOLUTE CONCENTRATION .12
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3255
SOLUTE ACTIVITY COEFF: 6.66666667
SOLUTE CONCENTRATION .15
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3450
SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1271.26002
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1332.6977
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1437.41532
SPREAD ON OUTPUT: 13.0701271

REGULAR SOLUTION PREDITIONS OF Wab: 4243.42929
REGULAR SOLUTION PREDITIONS OF Wab: 4245.6659
REGULAR SOLUTION PREDITIONS OF Wab: 4309.74152
SPREAD ON OUTPUT: 1.56270376

SOLUTE CARBON METAL TITANIUM - TiC

INPUT FROM GTE

TEMPERATURE: 1920
SOLUTE ACTIVITY COEFF: 66.6666667
SOLUTE CONCENTRATION .015

SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1950
 SOLUTE ACTIVITY COEFF: 20
 SOLUTE CONCENTRATION .05
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2020
 SOLUTE ACTIVITY COEFF: 10
 SOLUTE CONCENTRATION .1
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2115
 SOLUTE ACTIVITY COEFF: 6.66666667
 SOLUTE CONCENTRATION .15
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2320
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 855.56964
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 813.725435
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 824.390628
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 865.946435
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 966.609721
 SPREAD ON OUTPUT: 12.9784971

REGULAR SOLUTION PREDICTIONS OF Wab: 4128.43486
 REGULAR SOLUTION PREDICTIONS OF Wab: 3215.35015
 REGULAR SOLUTION PREDICTIONS OF Wab: 2852.46231
 REGULAR SOLUTION PREDICTIONS OF Wab: 2758.70457
 REGULAR SOLUTION PREDICTIONS OF Wab: 2898.14502
 SPREAD ON OUTPUT: 29.8003935

INPUT FROM HANSEN

TEMPERATURE: 2110
 SOLUTE ACTIVITY COEFF: 20
 SOLUTE CONCENTRATION .05
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2210
 SOLUTE ACTIVITY COEFF: 10
 SOLUTE CONCENTRATION .1
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2350
 SOLUTE ACTIVITY COEFF: 6.66666667
 SOLUTE CONCENTRATION .15
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2490
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 880.492651
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 901.93232
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 962.162706
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1037.43888
 SPREAD ON OUTPUT: 17.82482

REGULAR SOLUTION PREDICTIONS OF Wab: 3479.17375
 REGULAR SOLUTION PREDICTIONS OF Wab: 3120.76322
 REGULAR SOLUTION PREDICTIONS OF Wab: 3065.2273
 REGULAR SOLUTION PREDICTIONS OF Wab: 3110.5091
 SPREAD ON OUTPUT: 10.5963278

SOLUTE CARBON METAL URANIUM - UC2 - S.T. UNSURE
 INPUT FROM HANSEN

TEMPERATURE: 1670
 SOLUTE ACTIVITY COEFF: 20
 SOLUTE CONCENTRATION .05
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 1870
 SOLUTE ACTIVITY COEFF: 10
 SOLUTE CONCENTRATION .1
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2030
 SOLUTE ACTIVITY COEFF: 6.66666667
 SOLUTE CONCENTRATION .15
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2170
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 696.882809
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 763.173502
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 831.144806
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 904.113403

SPREAD ON OUTPUT: 29.7367923

REGULAR SOLUTION PREDITIONS OF Wab: 2753.65885
REGULAR SOLUTION PREDITIONS OF Wab: 2640.6458
REGULAR SOLUTION PREDITIONS OF Wab: 2647.83465
REGULAR SOLUTION PREDITIONS OF Wab: 2710.76496
SPREAD ON OUTPUT: 1.55770536

SOLUTE CARBON METAL VANADIUM - NONE - S.T. UNSURE
INPUT FROM STORMS - CHECKED BY ONE SOURCE

TEMPERATURE: 1920
SOLUTE ACTIVITY COEFF: 6.89655173
SOLUTE CONCENTRATION .145
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2000
SOLUTE ACTIVITY COEFF: 5.98802395
SOLUTE CONCENTRATION .167
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2120
SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2250
SOLUTE ACTIVITY COEFF: 4.34782609
SOLUTE CONCENTRATION .23
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 786.107402
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 822.805642
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 883.281296
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 952.093416
SPREAD ON OUTPUT: 21.1149283

REGULAR SOLUTION PREDITIONS OF Wab: 2519.38183
REGULAR SOLUTION PREDITIONS OF Wab: 2562.55398
REGULAR SOLUTION PREDITIONS OF Wab: 2648.30494
REGULAR SOLUTION PREDITIONS OF Wab: 2770.5152
SPREAD ON OUTPUT: 9.96805513

SOLUTE CARBON METAL WOLFRAM - WC - S.T. UNSURE
 INPUT FROM HANSEN

TEMPERATURE: 3070
 SOLUTE ACTIVITY COEFF: 2.5
 SOLUTE CONCENTRATION .4
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3350
 SOLUTE ACTIVITY COEFF: 2
 SOLUTE CONCENTRATION .5
 SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1492.06165
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1831.95781
 SPREAD ON OUTPUT: 22.7803026

REGULAR SOLUTION PREDICTIONS OF Wab: 3881.56662
 REGULAR SOLUTION PREDICTIONS OF Wab: 4613.89955
 SPREAD ON OUTPUT: 18.8669423

SOLUTE CARBON METAL ZIRCONIUM - ZrC - S.T. GUESSED FROM T1
 DATA

INPUT FROM HANSEN

TEMPERATURE: 2100
 SOLUTE ACTIVITY COEFF: 20
 SOLUTE CONCENTRATION .05
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2270
 SOLUTE ACTIVITY COEFF: 14.9253731
 SOLUTE CONCENTRATION .067
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 2670
 SOLUTE ACTIVITY COEFF: 6.99300699
 SOLUTE CONCENTRATION .143
 SOLUTE COORDINATION NUMBER: 4

TEMPERATURE: 3070
 SOLUTE ACTIVITY COEFF: 3.62318841

SOLUTE CONCENTRATION .276
SOLUTE COORDINATION NUMBER: 4

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 876.3197
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 935.374489
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1093.18061
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1338.6644
SPREAD ON OUTPUT: 52.7598202

REGULAR SOLUTION PREDICTIONS OF Wab: 3462.68478
REGULAR SOLUTION PREDICTIONS OF Wab: 3501.51958
REGULAR SOLUTION PREDICTIONS OF Wab: 3512.26396
REGULAR SOLUTION PREDICTIONS OF Wab: 3745.39171
SPREAD ON OUTPUT: 8.16438536

SOLUTE HYDROGEN METAL CALCIUM - CaH₂

INPUT FROM HANSEN

TEMPERATURE: 1235
 SOLUTE ACTIVITY COEFF: 20
 SOLUTE CONCENTRATION .05
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1250
 SOLUTE ACTIVITY COEFF: 10
 SOLUTE CONCENTRATION .1
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1270
 SOLUTE ACTIVITY COEFF: 6.66666667
 SOLUTE CONCENTRATION .15
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1320
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 639.463609
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 636.862842
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 651.577739
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 690.465388
 SPREAD ON OUTPUT: 7.97571263

REGULAR SOLUTION PREDICTIONS OF Wab: 4072.77686
 REGULAR SOLUTION PREDICTIONS OF Wab: 3530.27514
 REGULAR SOLUTION PREDICTIONS OF Wab: 3313.05419
 REGULAR SOLUTION PREDICTIONS OF Wab: 3297.88916
 SPREAD ON OUTPUT: 19.0260287

SOLUTE HYDROGEN METAL LANTANUM - NONE

INPUT FROM PETERSON - S.T. IFY

TEMPERATURE: 1200
 SOLUTE ACTIVITY COEFF: 20
 SOLUTE CONCENTRATION .05
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1210
 SOLUTE ACTIVITY COEFF: 10
 SOLUTE CONCENTRATION .1

SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1220
 SOLUTE ACTIVITY COEFF: 6.66666667
 SOLUTE CONCENTRATION .15
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1240
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1300
 SOLUTE ACTIVITY COEFF: 3.33333333
 SOLUTE CONCENTRATION .3
 SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 621.341158
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 616.483231
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 625.925072
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 648.619001
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 724.246986
 SPREAD ON OUTPUT: 16.5618882

REGULAR SOLUTION PREDICTIONS OF Wab: 3957.35403
 REGULAR SOLUTION PREDICTIONS OF Wab: 3417.30633
 REGULAR SOLUTION PREDICTIONS OF Wab: 3182.61899
 REGULAR SOLUTION PREDICTIONS OF Wab: 3098.01709
 REGULAR SOLUTION PREDICTIONS OF Wab: 3173.45117
 SPREAD ON OUTPUT: 19.8087625

SOLUTE HYDROGEN METAL LITHIUM - LiH INPUT FROM HANSEN

TEMPERATURE: 760
 SOLUTE ACTIVITY COEFF: 20
 SOLUTE CONCENTRATION .05
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 920
 SOLUTE ACTIVITY COEFF: 10
 SOLUTE CONCENTRATION .1
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 960
 SOLUTE ACTIVITY COEFF: 6.66666667

SOLUTE CONCENTRATION .15
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1090
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 393.516067
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 468.731052
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 492.531204
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 570.157025
 SPREAD ON OUTPUT: 44.8878644

REGULAR SOLUTION PREDITIONS OF Wab: 2506.32422
 REGULAR SOLUTION PREDITIONS OF Wab: 2598.2825
 REGULAR SOLUTION PREDITIONS OF Wab: 2504.35592
 REGULAR SOLUTION PREDITIONS OF Wab: 2723.25696
 SPREAD ON OUTPUT: 8.65541415

INPUT FROM HUBBERTY

TEMPERATURE: 470
 SOLUTE ACTIVITY COEFF: 2439.02439
 SOLUTE CONCENTRATION 4.1E-04
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 550
 SOLUTE ACTIVITY COEFF: 471.698113
 SOLUTE CONCENTRATION 2.12E-03
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 650
 SOLUTE ACTIVITY COEFF: 106.609808
 SOLUTE CONCENTRATION 9.38E-03
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 750
 SOLUTE ACTIVITY COEFF: 35.8422939
 SOLUTE CONCENTRATION .0279
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 870
 SOLUTE ACTIVITY COEFF: 13.4952767
 SOLUTE CONCENTRATION .0741
 SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 299.956159
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 330.213353
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 364.698503
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 398.446238

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 444.80786
SPREAD ON OUTPUT: 48.2909575

REGULAR SOLUTION PREDITIONS OF Wab: 3644.85724
REGULAR SOLUTION PREDITIONS OF Wab: 3378.28639
REGULAR SOLUTION PREDITIONS OF Wab: 3072.60861
REGULAR SOLUTION PREDITIONS OF Wab: 2822.17896
REGULAR SOLUTION PREDITIONS OF Wab: 2623.75301
SPREAD ON OUTPUT: 28.0149306

INPUT FROM ADAMS

TEMPERATURE: 900
SOLUTE ACTIVITY COEFF: 8.54700855
SOLUTE CONCENTRATION .117
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 950
SOLUTE ACTIVITY COEFF: 5.31914894
SOLUTE CONCENTRATION .188
SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 458.541246
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 494.13429
SPREAD ON OUTPUT: 7.76223377

REGULAR SOLUTION PREDITIONS OF Wab: 2460.55999
REGULAR SOLUTION PREDITIONS OF Wab: 2392.41927
SPREAD ON OUTPUT: 2.76931781

SOLUTE HYDROGEN METAL PLUTONIUM - PuH₂ - DENSITY DATA BASED ON
URANIUM

INPUT FROM HANSEN

TEMPERATURE: 970
SOLUTE ACTIVITY COEFF: 20
SOLUTE CONCENTRATION .05
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1070
SOLUTE ACTIVITY COEFF: 13.3333333
SOLUTE CONCENTRATION .075
SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 502.25077
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 547.06254
SPREAD ON OUTPUT: 8.92219053

REGULAR SOLUTION PREDITIONS OF Wab: 3198.86118
REGULAR SOLUTION PREDITIONS OF Wab: 3218.19788
SPREAD ON OUTPUT: .604487015

SOLUTE HYDROGEN METAL POTASSIUM - NONE
INPUT FROM HUBBERTY

TEMPERATURE: 400
SOLUTE ACTIVITY COEFF: 151285.93
SOLUTE CONCENTRATION 6.61E-06
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 500
SOLUTE ACTIVITY COEFF: 4807.69231
SOLUTE CONCENTRATION 2.08E-04
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 600
SOLUTE ACTIVITY COEFF: 483.091788
SOLUTE CONCENTRATION 2.07E-03
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 700
SOLUTE ACTIVITY COEFF: 93.457944
SOLUTE CONCENTRATION .0107
SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 284.357376
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 326.108028
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 360.558397
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 390.375979
SPREAD ON OUTPUT: 37.2835778

REGULAR SOLUTION PREDITIONS OF Wab: 4739.82341
REGULAR SOLUTION PREDITIONS OF Wab: 4213.18533
REGULAR SOLUTION PREDITIONS OF Wab: 3699.32053
REGULAR SOLUTION PREDITIONS OF Wab: 3224.24203
SPREAD ON OUTPUT: 31.9754819

INPUT FROM ARNILDOV - RUSSIAN

TEMPERATURE: 570
SOLUTE ACTIVITY COEFF: 558.659218
SOLUTE CONCENTRATION 1.79E-03
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 670
SOLUTE ACTIVITY COEFF: 95.2380953
SOLUTE CONCENTRATION .0105
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 770
SOLUTE ACTIVITY COEFF: 25.9067358
SOLUTE CONCENTRATION .0386
SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 344.691321
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 373.64558
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 403.223201
SPREAD ON OUTPUT: 16.9809554

REGULAR SOLUTION PREDICTIONS OF Wab: 3594.97999
REGULAR SOLUTION PREDICTIONS OF Wab: 3097.64051
REGULAR SOLUTION PREDICTIONS OF Wab: 2693.612
SPREAD ON OUTPUT: 25.0729627

SOLUTE HYDROGEN METAL SODIUM - NaH
INPUT FROM McCLURE

TEMPERATURE: 530
SOLUTE ACTIVITY COEFF: 5265.92944
SOLUTE CONCENTRATION 1.899E-04
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 630
SOLUTE ACTIVITY COEFF: 763.941941
SOLUTE CONCENTRATION 1.309E-03
SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 346.493201
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 385.724056
SPREAD ON OUTPUT: 11.3222582

REGULAR SOLUTION PREDICTIONS OF Wab: 4513.77078
REGULAR SOLUTION PREDICTIONS OF Wab: 4165.96456

SPREAD ON OUTPUT: 7.70544697

INPUT FROM ADDISON

TEMPERATURE: 520
SOLUTE ACTIVITY COEFF: 12112.4031
SOLUTE CONCENTRATION 8.256E-05
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 593
SOLUTE ACTIVITY COEFF: 7843.13725
SOLUTE CONCENTRATION 1.275E-04
SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 348.183469
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 392.238925
SPREAD ON OUTPUT: 12.6529432

REGULAR SOLUTION PREDICTIONS OF Wab: 4858.05575
REGULAR SOLUTION PREDICTIONS OF Wab: 5284.44738
SPREAD ON OUTPUT: 8.77700163

INPUT FROM HUBBERTY

TEMPERATURE: 400
SOLUTE ACTIVITY COEFF: 537634.408
SOLUTE CONCENTRATION 1.86E-06
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 500
SOLUTE ACTIVITY COEFF: 16583.7479
SOLUTE CONCENTRATION 6.03E-05
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 600
SOLUTE ACTIVITY COEFF: 1636.66121
SOLUTE CONCENTRATION 6.11E-04
SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 700
SOLUTE ACTIVITY COEFF: 312.5
SOLUTE CONCENTRATION 3.2E-03
SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 291.615761
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 337.569059
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 377.884374
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 413.013275
SPREAD ON OUTPUT: 41.6292704

REGULAR SOLUTION PREDITIONS OF Wab: 5243.6863
 REGULAR SOLUTION PREDITIONS OF Wab: 4827.09377
 REGULAR SOLUTION PREDITIONS OF Wab: 4416.7822
 REGULAR SOLUTION PREDITIONS OF Wab: 4020.77698
 SPREAD ON OUTPUT: 23.3215577

SOLUTE HYDROGEN METAL STRONTIUM - SrH₂
 INPUT FROM HANSEN - SCEWY PHASE DIAG

TEMPERATURE: 1050
 SOLUTE ACTIVITY COEFF: 20
 SOLUTE CONCENTRATION .05
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1065
 SOLUTE ACTIVITY COEFF: 10
 SOLUTE CONCENTRATION .1
 SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1080
 SOLUTE ACTIVITY COEFF: 6.66666667
 SOLUTE CONCENTRATION .15
 SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 543.673513
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 542.607141
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 554.097605
 SPREAD ON OUTPUT: 1.91734389

REGULAR SOLUTION PREDITIONS OF Wab: 3462.68478
 REGULAR SOLUTION PREDITIONS OF Wab: 3007.79442
 REGULAR SOLUTION PREDITIONS OF Wab: 2817.40042
 SPREAD ON OUTPUT: 18.635377

SOLUTE HYDROGEN METAL URANIUM - UH₃ - UNSURE S.T. DATA
 INPUT FROM HANSEN

TEMPERATURE: 1400
 SOLUTE ACTIVITY COEFF: 3.44827586
 SOLUTE CONCENTRATION .29

SOLUTE COORDINATION NUMBER: 2

TEMPERATURE: 1470
SOLUTE ACTIVITY COEFF: 3.003003
SOLUTE CONCENTRATION .333
SOLUTE COORDINATION NUMBER: 2

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 773.592606
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 840.470233
SPREAD ON OUTPUT: 8.6450706

REGULAR SOLUTION PREDICTIONS OF Wab: 3415.51169
REGULAR SOLUTION PREDICTIONS OF Wab: 3609.71838
SPREAD ON OUTPUT: 5.68602025

SOLUTE NITROGEN METAL CALCIUM - Ca₃N₂

INPUT FROM HANSEN

TEMPERATURE: 1050
 SOLUTE ACTIVITY COEFF: 52.631579
 SOLUTE CONCENTRATION .019
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1110
 SOLUTE ACTIVITY COEFF: 20
 SOLUTE CONCENTRATION .05
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1150
 SOLUTE ACTIVITY COEFF: 10
 SOLUTE CONCENTRATION .1
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 403.314427
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 402.122956
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 404.650152
 SPREAD ON OUTPUT: .331187177

REGULAR SOLUTION PREDICTIONS OF Wab: 1432.0449
 REGULAR SOLUTION PREDICTIONS OF Wab: 1220.18416
 REGULAR SOLUTION PREDICTIONS OF Wab: 1082.61771
 SPREAD ON OUTPUT: 24.4005749

SOLUTE NITROGEN METAL CHROMIUM - DELTA H DATA FOR CrN₂ -
 DENSITY DATA FOR CrN - UNSURE S.T.

INPUT FROM HUMBERT

TEMPERATURE: 1960
 SOLUTE ACTIVITY COEFF: 5.81395349
 SOLUTE CONCENTRATION .172
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2000
 SOLUTE ACTIVITY COEFF: 6.41025641
 SOLUTE CONCENTRATION .156
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2040
 SOLUTE ACTIVITY COEFF: 7.04225353
 SOLUTE CONCENTRATION .142
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2080
SOLUTE ACTIVITY COEFF: 7.75193798
SOLUTE CONCENTRATION .129
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2130
SOLUTE ACTIVITY COEFF: 8.84955753
SOLUTE CONCENTRATION .113
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 696.48514
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 705.133292
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 717.814183
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 730.438302
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 747.996915
SPREAD ON OUTPUT: 7.39596183

REGULAR SOLUTION PREDICTIONS OF Wab: 1666.55263
REGULAR SOLUTION PREDICTIONS OF Wab: 1727.4834
REGULAR SOLUTION PREDICTIONS OF Wab: 1791.29062
REGULAR SOLUTION PREDICTIONS OF Wab: 1859.47986
REGULAR SOLUTION PREDICTIONS OF Wab: 1954.82855
SPREAD ON OUTPUT: 17.2977388

INPUT FROM HANSEN - 1ST SAMPLE EXPOSED TO AIR - 2ND TO HYDROGEN

TEMPERATURE: 1900
SOLUTE ACTIVITY COEFF: 13.5501355
SOLUTE CONCENTRATION .0738
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1920
SOLUTE ACTIVITY COEFF: 8.10372771
SOLUTE CONCENTRATION .1234
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 675.164166
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 674.25074
SPREAD ON OUTPUT: .135289455

REGULAR SOLUTION PREDICTIONS OF Wab: 1911.75025
REGULAR SOLUTION PREDICTIONS OF Wab: 1731.3062
SPREAD ON OUTPUT: 9.43868335

SOLUTE NITROGEN METAL LITHIUM - Li3N - DENISITY DATA GUESS
INPUT FROM ADAMS

TEMPERATURE: 500
SOLUTE ACTIVITY COEFF: 800
SOLUTE CONCENTRATION 1.25E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 600
SOLUTE ACTIVITY COEFF: 168.067227
SOLUTE CONCENTRATION 5.95E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 700
SOLUTE ACTIVITY COEFF: 54.9450549
SOLUTE CONCENTRATION .0182
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 223.121702
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 247.235548
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 269.348577
SPREAD ON OUTPUT: 20.7182333

REGULAR SOLUTION PREDITIONS OF Wab: 1109.63264
REGULAR SOLUTION PREDITIONS OF Wab: 1030.43686
REGULAR SOLUTION PREDITIONS OF Wab: 963.486689
SPREAD ON OUTPUT: 13.1706607

INPUT FROM ADAMS

TEMPERATURE: 570
SOLUTE ACTIVITY COEFF: 1333.33333
SOLUTE CONCENTRATION 7.5E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 670
SOLUTE ACTIVITY COEFF: 149.253731
SOLUTE CONCENTRATION 6.7E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 770
SOLUTE ACTIVITY COEFF: 26.6666667
SOLUTE CONCENTRATION .0375
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 870
SOLUTE ACTIVITY COEFF: 15.3846154
SOLUTE CONCENTRATION .065
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 260.46925
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 274.318729
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 284.244263
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 310.96553
 SPREAD ON OUTPUT: 19.3866568

REGULAR SOLUTION PREDITIONS OF Wab: 1360.2864
 REGULAR SOLUTION PREDITIONS OF Wab: 1125.69525
 REGULAR SOLUTION PREDITIONS OF Wab: 903.777566
 REGULAR SOLUTION PREDITIONS OF Wab: 900.825673
 SPREAD ON OUTPUT: 33.7767638

INPUT FROM HANSEN

TEMPERATURE: 520
 SOLUTE ACTIVITY COEFF: 5000
 SOLUTE CONCENTRATION 2E-04
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 620
 SOLUTE ACTIVITY COEFF: 169.491525
 SOLUTE CONCENTRATION 5.9E-03
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 720
 SOLUTE ACTIVITY COEFF: 153.846154
 SOLUTE CONCENTRATION 6.5E-03
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 249.868406
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 255.476733
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 295.26384
 SPREAD ON OUTPUT: 18.1677367

REGULAR SOLUTION PREDITIONS OF Wab: 1467.30431
 REGULAR SOLUTION PREDITIONS OF Wab: 1066.43097
 REGULAR SOLUTION PREDITIONS OF Wab: 1216.53623
 SPREAD ON OUTPUT: 17.0903935

SOLUTE NITROGEN METAL MOLYBDENUM - Mo2N - DENSITY GUESS - S.T.

UNSURE

INPUT FROM HERMAN

TEMPERATURE: 2090
 SOLUTE ACTIVITY COEFF: 5

SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2180
SOLUTE ACTIVITY COEFF: 4
SOLUTE CONCENTRATION .25
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 3250
SOLUTE ACTIVITY COEFF: 3.33333333
SOLUTE CONCENTRATION .3
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 747.032135
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 800.25783
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1235.16611
SPREAD ON OUTPUT: 65.3431021

REGULAR SOLUTION PREDICTIONS OF Wab: 1740.55261
REGULAR SOLUTION PREDICTIONS OF Wab: 1779.24617
REGULAR SOLUTION PREDICTIONS OF Wab: 2644.54264
SPREAD ON OUTPUT: 51.9369551

SOLUTE NITROGEN METAL SILICON - Si3N4 - DENSITY GUESS
INPUT FROM SCARCE

TEMPERATURE: 2000
SOLUTE ACTIVITY COEFF: 1333.33333
SOLUTE CONCENTRATION 7.5E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2200
SOLUTE ACTIVITY COEFF: 370.37037
SOLUTE CONCENTRATION 2.7E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2500
SOLUTE ACTIVITY COEFF: 75.1879699
SOLUTE CONCENTRATION .0133
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2700
SOLUTE ACTIVITY COEFF: 31.9488818
SOLUTE CONCENTRATION .0313
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2900
 SOLUTE ACTIVITY COEFF: 15.3139357
 SOLUTE CONCENTRATION .0653
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 913.927194
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 946.583557
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 982.111443
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1004.09034
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1036.55177
 SPREAD ON OUTPUT: 13.417324

REGULAR SOLUTION PREDICTIONS OF Wab: 4772.93472
 REGULAR SOLUTION PREDICTIONS OF Wab: 4332.47388
 REGULAR SOLUTION PREDICTIONS OF Wab: 3673.66233
 REGULAR SOLUTION PREDICTIONS OF Wab: 3300.85816
 REGULAR SOLUTION PREDICTIONS OF Wab: 2999.61824
 SPREAD ON OUTPUT: 37.1535876

SOLUTE NITROGEN METAL TITANIUM - TiN

INPUT FROM HANSEN

TEMPERATURE: 2330
 SOLUTE ACTIVITY COEFF: 20
 SOLUTE CONCENTRATION .05
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2484
 SOLUTE ACTIVITY COEFF: 10
 SOLUTE CONCENTRATION .1
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2565
 SOLUTE ACTIVITY COEFF: 6.66666667
 SOLUTE CONCENTRATION .15
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2830
 SOLUTE ACTIVITY COEFF: 5
 SOLUTE CONCENTRATION .2
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 844.095935
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 874.044328
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 902.545774

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1011.53155
SPREAD ON OUTPUT: 19.8360884

REGULAR SOLUTION PREDITIONS OF Wab: 2561.28747
REGULAR SOLUTION PREDITIONS OF Wab: 2338.45425
REGULAR SOLUTION PREDITIONS OF Wab: 2230.442
REGULAR SOLUTION PREDITIONS OF Wab: 2356.82483
SPREAD ON OUTPUT: 7.98280713

SOLUTE OXYGEN METAL ANTIMONY - Sb2O3

INPUT FROM JACOB

TEMPERATURE: 1000
SOLUTE ACTIVITY COEFF: 5586.59218
SOLUTE CONCENTRATION 1.79E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1100
SOLUTE ACTIVITY COEFF: 1760.56338
SOLUTE CONCENTRATION 5.68E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1175
SOLUTE ACTIVITY COEFF: 847.457628
SOLUTE CONCENTRATION 1.18E-03
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 482.352015
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 508.16551
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 526.568763
SPREAD ON OUTPUT: 9.16690436

REGULAR SOLUTION PREDICTIONS OF Wab: 2858.37052
REGULAR SOLUTION PREDICTIONS OF Wab: 2725.52642
REGULAR SOLUTION PREDICTIONS OF Wab: 2629.74892
SPREAD ON OUTPUT: 7.99831919

SOLUTE OXYGEN METAL BARIUM - BaO2

INPUT FROM HANSEN

TEMPERATURE: 1000
SOLUTE ACTIVITY COEFF: 5.98802395
SOLUTE CONCENTRATION .167
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1170
SOLUTE ACTIVITY COEFF: 4.73933649
SOLUTE CONCENTRATION .211
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1370
SOLUTE ACTIVITY COEFF: 3.6101083
SOLUTE CONCENTRATION .277
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1520
 SOLUTE ACTIVITY COEFF: 3.14465409
 SOLUTE CONCENTRATION .318
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 355.349561
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 420.625966
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 511.353797
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 585.896048
 SPREAD ON OUTPUT: 64.8787875

REGULAR SOLUTION PREDICTIONS OF Wab: 854.184659
 REGULAR SOLUTION PREDICTIONS OF Wab: 968.410202
 REGULAR SOLUTION PREDICTIONS OF Wab: 1114.20963
 REGULAR SOLUTION PREDICTIONS OF Wab: 1239.92051
 SPREAD ON OUTPUT: 45.1583684

SOLUTE OXYGEN METAL BISMUTH - B10
 INPUT FROM GRIFFITH

TEMPERATURE: 670
 SOLUTE ACTIVITY COEFF: 30120.4819
 SOLUTE CONCENTRATION 3.32E-05
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 770
 SOLUTE ACTIVITY COEFF: 6622.51655
 SOLUTE CONCENTRATION 1.51E-04
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 870
 SOLUTE ACTIVITY COEFF: 2114.16491
 SOLUTE CONCENTRATION 4.73E-04
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 970
 SOLUTE ACTIVITY COEFF: 813.00813
 SOLUTE CONCENTRATION 1.23E-03
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1020
 SOLUTE ACTIVITY COEFF: 546.448088
 SOLUTE CONCENTRATION 1.83E-03
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 340.959774
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 373.761269
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 405.16418
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 433.470899
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 447.378074
 SPREAD ON OUTPUT: 31.2113944

REGULAR SOLUTION PREDICTIONS OF Wab: 2288.40885
 REGULAR SOLUTION PREDICTIONS OF Wab: 2244.21187
 REGULAR SOLUTION PREDICTIONS OF Wab: 2208.01635
 REGULAR SOLUTION PREDICTIONS OF Wab: 2157.79515
 REGULAR SOLUTION PREDICTIONS OF Wab: 2137.05322
 SPREAD ON OUTPUT: 6.61401169

SOLUTE OXYGEN METAL CALCIUM - DELTA H FOR CaO - DENSITY FOR
 CaO2

INPUT FROM HANSEN

TEMPERATURE: 1110
 SOLUTE ACTIVITY COEFF: 666.666667
 SOLUTE CONCENTRATION 1.5E-03
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1620
 SOLUTE ACTIVITY COEFF: 10
 SOLUTE CONCENTRATION .1
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 491.805775
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 570.02891
 SPREAD ON OUTPUT: 15.9052902

REGULAR SOLUTION PREDICTIONS OF Wab: 2397.39615
 REGULAR SOLUTION PREDICTIONS OF Wab: 1525.07886
 SPREAD ON OUTPUT: 36.3860303

SOLUTE OXYGEN METAL CESIUM - Cs20
 INPUT FROM ADAMS

TEMPERATURE: 320
SOLUTE ACTIVITY COEFF: 5.07614213
SOLUTE CONCENTRATION .197
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 420
SOLUTE ACTIVITY COEFF: 4.40528634
SOLUTE CONCENTRATION .227
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 520
SOLUTE ACTIVITY COEFF: 3.90625
SOLUTE CONCENTRATION .256
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 620
SOLUTE ACTIVITY COEFF: 3.73134329
SOLUTE CONCENTRATION .268
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 720
SOLUTE ACTIVITY COEFF: 3.28947369
SOLUTE CONCENTRATION .304
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 114.378126
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 152.154632
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 191.957165
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 230.145108
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 274.124573
SPREAD ON OUTPUT: 139.665207

REGULAR SOLUTION PREDICTIONS OF Wab: 266.992463
REGULAR SOLUTION PREDICTIONS OF Wab: 345.160458
REGULAR SOLUTION PREDICTIONS OF Wab: 423.901945
REGULAR SOLUTION PREDICTIONS OF Wab: 504.574741
REGULAR SOLUTION PREDICTIONS OF Wab: 586.101788
SPREAD ON OUTPUT: 119.519975

SOLUTE OXYGEN METAL CHROMIUM - Cr2O3
INPUT FROM HANSEN - CHECKS ONE SOURCE

TEMPERATURE: 2100
SOLUTE ACTIVITY COEFF: 50
SOLUTE CONCENTRATION .02
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2173
SOLUTE ACTIVITY COEFF: 33.3333333
SOLUTE CONCENTRATION .03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2373
SOLUTE ACTIVITY COEFF: 25
SOLUTE CONCENTRATION .04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2473
SOLUTE ACTIVITY COEFF: 20
SOLUTE CONCENTRATION .05
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 803.792211
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 811.074307
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 869.476497
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 895.900965
SPREAD ON OUTPUT: 11.4592743

REGULAR SOLUTION PREDICTIONS OF Wab: 2832.79508
REGULAR SOLUTION PREDICTIONS OF Wab: 2681.90808
REGULAR SOLUTION PREDICTIONS OF Wab: 2744.77097
REGULAR SOLUTION PREDICTIONS OF Wab: 2718.48237
SPREAD ON OUTPUT: 4.03533299

SOLUTE OXYGEN METAL COBALT - CoO
INPUT FROM HANSEN

TEMPERATURE: 1720
SOLUTE ACTIVITY COEFF: 118.063754
SOLUTE CONCENTRATION 8.47E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1760
SOLUTE ACTIVITY COEFF: 50
SOLUTE CONCENTRATION .02
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1820
SOLUTE ACTIVITY COEFF: 25
SOLUTE CONCENTRATION .04
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 694.005721
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 673.654425
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 666.85513
 SPREAD ON OUTPUT: 3.91215667

REGULAR SOLUTION PREDICTIONS OF Wab: 2764.35123
 REGULAR SOLUTION PREDICTIONS OF Wab: 2374.15207
 REGULAR SOLUTION PREDICTIONS OF Wab: 2105.13408
 SPREAD ON OUTPUT: 23.8470837

INPUT FROM HANSEN - FROM RUSSIAN

TEMPERATURE: 1820
 SOLUTE ACTIVITY COEFF: 142.857143
 SOLUTE CONCENTRATION 7E-03
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1920
 SOLUTE ACTIVITY COEFF: 100
 SOLUTE CONCENTRATION .01
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 745.164308
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 767.063784
 SPREAD ON OUTPUT: 2.93887876

REGULAR SOLUTION PREDICTIONS OF Wab: 3032.93227
 REGULAR SOLUTION PREDICTIONS OF Wab: 2987.60474
 SPREAD ON OUTPUT: 1.49451178

SOLUTE OXYGEN METAL COPPER - Cu2O

INPUT FROM PARLEE

TEMPERATURE: 1223
 SOLUTE ACTIVITY COEFF: 143.061517
 SOLUTE CONCENTRATION 6.99E-03
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 500.734038
 SPREAD ON OUTPUT: 0

REGULAR SOLUTION PREDICTIONS OF Wab: 2038.60997

SPREAD ON OUTPUT: 0

SOLUTE OXYGEN METAL COPPER - Cu₂O - DIFF DELTA H USED HERE
INPUT FROM HANSEN

TEMPERATURE: 1373
SOLUTE ACTIVITY COEFF: 43.4782609
SOLUTE CONCENTRATION .023
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1473
SOLUTE ACTIVITY COEFF: 14.9253731
SOLUTE CONCENTRATION .067
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF W_{ab}: 0 0 520.879381
QUASI-CHEMICAL PREDICTIONS OF W_{ab}: 0 0 525.475223
SPREAD ON OUTPUT: .88232345

REGULAR SOLUTION PREDICTIONS OF W_{ab}: 1796.92424
REGULAR SOLUTION PREDICTIONS OF W_{ab}: 1514.75428
SPREAD ON OUTPUT: 15.7029412

SOLUTE OXYGEN METAL GALLIUM - Ga₂O₃
INPUT FROM ALCOCK

TEMPERATURE: 1050
SOLUTE ACTIVITY COEFF: 58139.5349
SOLUTE CONCENTRATION 1.72E-05
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1150
SOLUTE ACTIVITY COEFF: 14245.0143
SOLUTE CONCENTRATION 7.02E-05
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1250
SOLUTE ACTIVITY COEFF: 4366.81223
SOLUTE CONCENTRATION 2.29E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1350
SOLUTE ACTIVITY COEFF: 1594.89633
SOLUTE CONCENTRATION 6.27E-04
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 543.673513
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 572.148287
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 597.578848
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 621.971657
SPREAD ON OUTPUT: 14.4016844

REGULAR SOLUTION PREDICTIONS OF Wab: 3814.88352
REGULAR SOLUTION PREDICTIONS OF Wab: 3642.94294
REGULAR SOLUTION PREDICTIONS OF Wab: 3471.3009
REGULAR SOLUTION PREDICTIONS OF Wab: 3301.12151
SPREAD ON OUTPUT: 13.4673052

INPUT FROM STEVENSON

TEMPERATURE: 1023
SOLUTE ACTIVITY COEFF: 15174.5068
SOLUTE CONCENTRATION 6.59E-05
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1123
SOLUTE ACTIVITY COEFF: 5555.55556
SOLUTE CONCENTRATION 1.8E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1223
SOLUTE ACTIVITY COEFF: 2403.84615
SOLUTE CONCENTRATION 4.16E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1323
SOLUTE ACTIVITY COEFF: 1661.12957
SOLUTE CONCENTRATION 6.02E-04
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 510.194408
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 541.681313
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 571.837314
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 609.532224
SPREAD ON OUTPUT: 19.470581

REGULAR SOLUTION PREDICTIONS OF Wab: 3262.02474
REGULAR SOLUTION PREDICTIONS OF Wab: 3207.8839
REGULAR SOLUTION PREDICTIONS OF Wab: 3155.61021
REGULAR SOLUTION PREDICTIONS OF Wab: 3252.78598

SPREAD ON OUTPUT: .283221816

SOLUTE OXYGEN METAL GERMANIUM GeO₂

INPUT FROM JACOB

TEMPERATURE: 1230
SOLUTE ACTIVITY COEFF: 1047.12042
SOLUTE CONCENTRATION 9.55E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1330
SOLUTE ACTIVITY COEFF: 421.940928
SOLUTE CONCENTRATION 2.37E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1400
SOLUTE ACTIVITY COEFF: 240.384615
SOLUTE CONCENTRATION 4.16E-03
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 555.877844
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 575.675988
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 588.774961
SPREAD ON OUTPUT: 5.91804792

REGULAR SOLUTION PREDICTIONS OF Wab: 2837.94369
REGULAR SOLUTION PREDICTIONS OF Wab: 2675.13612
REGULAR SOLUTION PREDICTIONS OF Wab: 2563.02935
SPREAD ON OUTPUT: 9.68709634

SOLUTE OXYGEN METAL HAFNIUM - HfO₂ - S.T. UNSURE

INPUT FROM KARNILOV - RUSSIAN

TEMPERATURE: 2570
SOLUTE ACTIVITY COEFF: 3.33333333
SOLUTE CONCENTRATION .3
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2670
SOLUTE ACTIVITY COEFF: 2.85714286

SOLUTE CONCENTRATION .35
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2770
 SOLUTE ACTIVITY COEFF: 2.5
 SOLUTE CONCENTRATION .4
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2860
 SOLUTE ACTIVITY COEFF: 2.22222222
 SOLUTE CONCENTRATION .45
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2950
 SOLUTE ACTIVITY COEFF: 2
 SOLUTE CONCENTRATION .5
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 976.731352
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1057.81148
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1152.28875
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1258.06523
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1382.98854
 SPREAD ON OUTPUT: 41.5935442

REGULAR SOLUTION PREDICTIONS OF Wab: 2091.22295
 REGULAR SOLUTION PREDICTIONS OF Wab: 2197.08513
 REGULAR SOLUTION PREDICTIONS OF Wab: 2334.84029
 REGULAR SOLUTION PREDICTIONS OF Wab: 2500.15179
 REGULAR SOLUTION PREDICTIONS OF Wab: 2708.65745
 SPREAD ON OUTPUT: 29.525044

SOLUTE OXYGEN METAL INDIUM - In₂O₃

INPUT FROM JACOB

TEMPERATURE: 920
 SOLUTE ACTIVITY COEFF: 2551.02041
 SOLUTE CONCENTRATION 3.92E-04
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1000
 SOLUTE ACTIVITY COEFF: 990.09901
 SOLUTE CONCENTRATION 1.01E-03
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1100

SOLUTE ACTIVITY COEFF: 369.00369
SOLUTE CONCENTRATION 2.71E-03
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 431.3049
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 450.671619
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 473.291778
SPREAD ON OUTPUT: 9.7348484

REGULAR SOLUTION PREDICTIONS OF Wab: 2391.80821
REGULAR SOLUTION PREDICTIONS OF Wab: 2288.9444
REGULAR SOLUTION PREDICTIONS OF Wab: 2164.92635
SPREAD ON OUTPUT: 9.48578843

SOLUTE OXYGEN METAL IRON Fe(.947)O...WUSTITE
INPUT FROM WRIDT - CHECKS ONE SOURCE

TEMPERATURE: 1820
SOLUTE ACTIVITY COEFF: 159.235669
SOLUTE CONCENTRATION 6.28E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1920
SOLUTE ACTIVITY COEFF: 102.354145
SOLUTE CONCENTRATION 9.77E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1970
SOLUTE ACTIVITY COEFF: 84.0336134
SOLUTE CONCENTRATION .0119
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 747.55765
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 768.33929
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 780.482628
SPREAD ON OUTPUT: 4.40433972

REGULAR SOLUTION PREDICTIONS OF Wab: 3094.78801
REGULAR SOLUTION PREDICTIONS OF Wab: 3001.30556
REGULAR SOLUTION PREDICTIONS OF Wab: 2960.97029
SPREAD ON OUTPUT: 4.32397041

SOLUTE OXYGEN METAL LEAD - PbO

INPUT FROM RAPP

TEMPERATURE: 1050
SOLUTE ACTIVITY COEFF: 2906.97674
SOLUTE CONCENTRATION 3.44E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1150
SOLUTE ACTIVITY COEFF: 1000
SOLUTE CONCENTRATION 1E-03
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 494.849972
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 518.998005
SPREAD ON OUTPUT: 4.87986939

REGULAR SOLUTION PREDICTIONS OF Wab: 2774.97014
REGULAR SOLUTION PREDICTIONS OF Wab: 2636.03046
SPREAD ON OUTPUT: 5.00688927

INPUT FROM HANSEN

TEMPERATURE: 670
SOLUTE ACTIVITY COEFF: 7692.30769
SOLUTE CONCENTRATION 1.3E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 770
SOLUTE ACTIVITY COEFF: 3846.15385
SOLUTE CONCENTRATION 2.6E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 870
SOLUTE ACTIVITY COEFF: 1724.13793
SOLUTE CONCENTRATION 5.8E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 970
SOLUTE ACTIVITY COEFF: 854.700855
SOLUTE CONCENTRATION 1.17E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1070
SOLUTE ACTIVITY COEFF: 429.184549
SOLUTE CONCENTRATION 2.33E-03
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 326.852328
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 366.688845
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 401.369621
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 434.699319
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 463.825213
 SPREAD ON OUTPUT: 41.9066573

REGULAR SOLUTION PREDICTIONS OF Wab: 1985.90815
 REGULAR SOLUTION PREDICTIONS OF Wab: 2106.06263
 REGULAR SOLUTION PREDICTIONS OF Wab: 2149.66487
 REGULAR SOLUTION PREDICTIONS OF Wab: 2173.6385
 REGULAR SOLUTION PREDICTIONS OF Wab: 2158.06442
 SPREAD ON OUTPUT: 8.66889381

INPUT FROM HANSEN

TEMPERATURE: 870
 SOLUTE ACTIVITY COEFF: 5000
 SOLUTE CONCENTRATION 2E-04
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 970
 SOLUTE ACTIVITY COEFF: 1666.66667
 SOLUTE CONCENTRATION 6E-04
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1030
 SOLUTE ACTIVITY COEFF: 1000
 SOLUTE CONCENTRATION 1E-03
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 418.049064
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 446.898154
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 464.841691
 SPREAD ON OUTPUT: 11.1930945

REGULAR SOLUTION PREDICTIONS OF Wab: 2454.91298
 REGULAR SOLUTION PREDICTIONS OF Wab: 2385.94538
 REGULAR SOLUTION PREDICTIONS OF Wab: 2360.96641
 SPREAD ON OUTPUT: 3.82687994

INPUT FROM ALCOCK

TEMPERATURE: 780
 SOLUTE ACTIVITY COEFF: 13513.5135
 SOLUTE CONCENTRATION 7.4E-05
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 870
 SOLUTE ACTIVITY COEFF: 3144.65409

SOLUTE CONCENTRATION 3.18E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 970
SOLUTE ACTIVITY COEFF: 735.294117
SOLUTE CONCENTRATION 1.36E-03
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 387.595997
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 411.630632
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 431.625329
SPREAD ON OUTPUT: 11.3595941

REGULAR SOLUTION PREDICTIONS OF Wab: 2457.26514
REGULAR SOLUTION PREDICTIONS OF Wab: 2321.79882
REGULAR SOLUTION PREDICTIONS OF Wab: 2125.99469
SPREAD ON OUTPUT: 13.481266

INPUT FROM CHARLE - GERMAN

TEMPERATURE: 1000
SOLUTE ACTIVITY COEFF: 578.034683
SOLUTE CONCENTRATION 1.73E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1100
SOLUTE ACTIVITY COEFF: 199.600798
SOLUTE CONCENTRATION 5.01E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1143
SOLUTE ACTIVITY COEFF: 133.868809
SOLUTE CONCENTRATION 7.47E-03
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 439.882947
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 457.58759
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 464.967438
SPREAD ON OUTPUT: 5.70253779

REGULAR SOLUTION PREDICTIONS OF Wab: 2113.4048
REGULAR SOLUTION PREDICTIONS OF Wab: 1948.83933
REGULAR SOLUTION PREDICTIONS OF Wab: 1881.58254
SPREAD ON OUTPUT: 10.9691367

SOLUTE OXYGEN METAL LEAD - PbO - NEW DELTA H
 INPUT FROM RAPP

TEMPERATURE: 1250
 SOLUTE ACTIVITY COEFF: 408.163265
 SOLUTE CONCENTRATION 2.45E-03
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1350
 SOLUTE ACTIVITY COEFF: 182.815356
 SOLUTE CONCENTRATION 5.47E-03
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 540.245319
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 558.934998
 SPREAD ON OUTPUT: 3.45948003

REGULAR SOLUTION PREDITIONS OF Wab: 2500.81876
 REGULAR SOLUTION PREDITIONS OF Wab: 2354.26492
 SPREAD ON OUTPUT: 5.86023431

INPUT FROM HANSEN

TEMPERATURE: 1170
 SOLUTE ACTIVITY COEFF: 202.42915
 SOLUTE CONCENTRATION 4.94E-03
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 487.471282
 SPREAD ON OUTPUT: 0

REGULAR SOLUTION PREDITIONS OF Wab: 2078.07087
 SPREAD ON OUTPUT: 0

INPUT FROM CHARLE - GERMAN

TEMPERATURE: 1240
 SOLUTE ACTIVITY COEFF: 53.4759358
 SOLUTE CONCENTRATION .0187
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1340
 SOLUTE ACTIVITY COEFF: 28.9017341
 SOLUTE CONCENTRATION .0346
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 476.295133
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 495.576663

SPREAD ON OUTPUT: 4.04823172

REGULAR SOLUTION PREDICTIONS OF Wab: 1696.93004

REGULAR SOLUTION PREDICTIONS OF Wab: 1601.69607

SPREAD ON OUTPUT: 5.61213311

SOLUTE OXYGEN METAL LITHIUM - L120

INPUT FROM ADAMS - 7

TEMPERATURE: 570
SOLUTE ACTIVITY COEFF: 10101.0101
SOLUTE CONCENTRATION 9.9E-05
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 670
SOLUTE ACTIVITY COEFF: 2049.18033
SOLUTE CONCENTRATION 4.88E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 770
SOLUTE ACTIVITY COEFF: 602.409638
SOLUTE CONCENTRATION 1.66E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 870
SOLUTE ACTIVITY COEFF: 235.294118
SOLUTE CONCENTRATION 4.25E-03
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 280.489205
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 311.60631
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 339.201038
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 365.315356
SPREAD ON OUTPUT: 30.2422159

REGULAR SOLUTION PREDICTIONS OF Wab: 1740.83172
REGULAR SOLUTION PREDICTIONS OF Wab: 1693.5435
REGULAR SOLUTION PREDICTIONS OF Wab: 1637.66096
REGULAR SOLUTION PREDICTIONS OF Wab: 1586.80806
SPREAD ON OUTPUT: 8.84770549

INPUT FROM ASTM SPEC TECH PUBL

TEMPERATURE: 520
SOLUTE ACTIVITY COEFF: 104166.667

164

SOLUTE CONCENTRATION 9.6E-06
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 570
SOLUTE ACTIVITY COEFF: 48780.4878
SOLUTE CONCENTRATION 2.05E-05
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 670
SOLUTE ACTIVITY COEFF: 15384.6154
SOLUTE CONCENTRATION 6.5E-05
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 273.525021
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 293.790332
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 334.14492
SPREAD ON OUTPUT: 22.1624695

REGULAR SOLUTION PREDICTIONS OF Wab: 1989.67054
REGULAR SOLUTION PREDICTIONS OF Wab: 2037.8179
REGULAR SOLUTION PREDICTIONS OF Wab: 2139.46663
SPREAD ON OUTPUT: 7.52868789

SOLUTE OXYGEN METAL MANGANESE - MnO

INPUT FROM HANSEN

TEMPERATURE: 1670
SOLUTE ACTIVITY COEFF: 1557.6324
SOLUTE CONCENTRATION 6.42E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1770
SOLUTE ACTIVITY COEFF: 1070.66381
SOLUTE CONCENTRATION 9.34E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1870
SOLUTE ACTIVITY COEFF: 763.358779
SOLUTE CONCENTRATION 1.31E-03
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 767.313685
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 801.037218
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 833.289181
SPREAD ON OUTPUT: 8.59824295

REGULAR SOLUTION PREDITIONS OF Wab: 4070.64033
REGULAR SOLUTION PREDITIONS OF Wab: 4096.7562
REGULAR SOLUTION PREDITIONS OF Wab: 4121.41438
SPREAD ON OUTPUT: 1.24732351

INPUT FROM JACOB

TEMPERATURE: 1500
SOLUTE ACTIVITY COEFF: 5586.59218
SOLUTE CONCENTRATION 1.79E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1600
SOLUTE ACTIVITY COEFF: 2336.4486
SOLUTE CONCENTRATION 4.28E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1700
SOLUTE ACTIVITY COEFF: 1084.5987
SOLUTE CONCENTRATION 9.22E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1800
SOLUTE ACTIVITY COEFF: 546.448088
SOLUTE CONCENTRATION 1.83E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1900
SOLUTE ACTIVITY COEFF: 297.619048
SOLUTE CONCENTRATION 3.36E-03
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 723.528023
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 747.11777
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 769.357779
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 789.490718
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 807.685234
SPREAD ON OUTPUT: 11.6315068

REGULAR SOLUTION PREDITIONS OF Wab: 4287.55577
REGULAR SOLUTION PREDITIONS OF Wab: 4113.37141
REGULAR SOLUTION PREDITIONS OF Wab: 3941.93658
REGULAR SOLUTION PREDITIONS OF Wab: 3771.27039
REGULAR SOLUTION PREDITIONS OF Wab: 3608.10704
SPREAD ON OUTPUT: 15.8469947

SOLUTE OXYGEN METAL NEODYMIUM - Nd2O3 - UNSURE S.T. & PHASE
 INPUT FROM HANSEN

TEMPERATURE:	1300
SOLUTE ACTIVITY COEFF:	20
SOLUTE CONCENTRATION	.05
SOLUTE COORDINATION NUMBER:	6
TEMPERATURE:	1400
SOLUTE ACTIVITY COEFF:	10
SOLUTE CONCENTRATION	.1
SOLUTE COORDINATION NUMBER:	6
TEMPERATURE:	1470
SOLUTE ACTIVITY COEFF:	6.66666667
SOLUTE CONCENTRATION	.15
SOLUTE COORDINATION NUMBER:	6
TEMPERATURE:	1540
SOLUTE ACTIVITY COEFF:	5
SOLUTE CONCENTRATION	.2
SOLUTE COORDINATION NUMBER:	6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 470.954814
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 492.617577
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 517.248456
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 550.444731
 SPREAD ON OUTPUT: 16.8784595

REGULAR SOLUTION PREDICTIONS OF Wab: 1429.04451
 REGULAR SOLUTION PREDICTIONS OF Wab: 1317.96938
 REGULAR SOLUTION PREDICTIONS OF Wab: 1278.265
 REGULAR SOLUTION PREDICTIONS OF Wab: 1282.51245
 SPREAD ON OUTPUT: 10.2538485

SOLUTE OXYGEN METAL NICKEL - NiO - (1620-1725)
 INPUT FROM WRIEDT

TEMPERATURE:	1620
SOLUTE ACTIVITY COEFF:	24509.8039
SOLUTE CONCENTRATION	4.08E-05
SOLUTE COORDINATION NUMBER:	6
TEMPERATURE:	1720

SOLUTE ACTIVITY COEFF: 10493.1794
SOLUTE CONCENTRATION 9.53E-05
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 819.581303
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 847.429489
SPREAD ON OUTPUT: 3.39785536

REGULAR SOLUTION PREDICTIONS OF Wab: 5422.65488
REGULAR SOLUTION PREDICTIONS OF Wab: 5274.69767
SPREAD ON OUTPUT: 2.7285015

SOLUTE OXYGEN METAL NICKEL - NiO (1725-2000)
INPUT FROM WRIEDT

TEMPERATURE: 1820
SOLUTE ACTIVITY COEFF: 4926.10838
SOLUTE CONCENTRATION 2.03E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1920
SOLUTE ACTIVITY COEFF: 2506.26566
SOLUTE CONCENTRATION 3.99E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1970
SOLUTE ACTIVITY COEFF: 1831.50183
SOLUTE CONCENTRATION 5.46E-04
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 874.539422
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 900.114574
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 911.307239
SPREAD ON OUTPUT: 4.20424927

REGULAR SOLUTION PREDICTIONS OF Wab: 5126.61855
REGULAR SOLUTION PREDICTIONS OF Wab: 4980.40658
REGULAR SOLUTION PREDICTIONS OF Wab: 4906.75466
SPREAD ON OUTPUT: 4.28867273

INPUT FROM KIMORA

TEMPERATURE: 1730
SOLUTE ACTIVITY COEFF: 93.457944

168

SOLUTE CONCENTRATION .0107
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1830
SOLUTE ACTIVITY COEFF: 42.3728814
SOLUTE CONCENTRATION .0236
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 688.855553
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 693.011477
SPREAD ON OUTPUT: .603308567

REGULAR SOLUTION PREDICTIONS OF Wab: 2656.16129
REGULAR SOLUTION PREDICTIONS OF Wab: 2381.6004
SPREAD ON OUTPUT: 10.3367553

SOLUTE OXYGEN METAL NIOBIUM - Nb2O4

INPUT FROM HANSEN

TEMPERATURE: 2640
SOLUTE ACTIVITY COEFF: 20
SOLUTE CONCENTRATION .05
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2590
SOLUTE ACTIVITY COEFF: 10
SOLUTE CONCENTRATION .1
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2545
SOLUTE ACTIVITY COEFF: 6.66666667
SOLUTE CONCENTRATION .15
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2480
SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 956.400545
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 911.342517
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 895.508381
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 886.430476
SPREAD ON OUTPUT: 7.3159796

REGULAR SOLUTION PREDITIONS OF Wab: 2902.05962
REGULAR SOLUTION PREDITIONS OF Wab: 2438.24336
REGULAR SOLUTION PREDITIONS OF Wab: 2213.05064
REGULAR SOLUTION PREDITIONS OF Wab: 2065.34473
SPREAD ON OUTPUT: 28.831761

SOLUTE OXYGEN METAL PLUTONIUM - PbO2

INPUT FROM HANSEN

TEMPERATURE: 1700
SOLUTE ACTIVITY COEFF: 10
SOLUTE CONCENTRATION .1
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1920
SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 598.178486
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 686.268756
SPREAD ON OUTPUT: 14.726419

REGULAR SOLUTION PREDITIONS OF Wab: 1600.3914
REGULAR SOLUTION PREDITIONS OF Wab: 1598.97656
SPREAD ON OUTPUT: .0884053514

INPUT FROM HANSEN

TEMPERATURE: 1685
SOLUTE ACTIVITY COEFF: 20
SOLUTE CONCENTRATION .05
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1815
SOLUTE ACTIVITY COEFF: 10
SOLUTE CONCENTRATION .1
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1930
SOLUTE ACTIVITY COEFF: 6.66666667
SOLUTE CONCENTRATION .15
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2040

SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 610.429893
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 638.643501
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 679.108517
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 729.160553
SPREAD ON OUTPUT: 19.4503351

REGULAR SOLUTION PREDICTIONS OF Wab: 1852.26154
REGULAR SOLUTION PREDICTIONS OF Wab: 1708.65317
REGULAR SOLUTION PREDICTIONS OF Wab: 1678.2663
REGULAR SOLUTION PREDICTIONS OF Wab: 1698.9126
SPREAD ON OUTPUT: 8.2790112

SOLUTE OXYGEN METAL POTASSIUM - K2O
INPUT FROM ADAMS

TEMPERATURE: 370
SOLUTE ACTIVITY COEFF: 416.666667
SOLUTE CONCENTRATION 2.4E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 470
SOLUTE ACTIVITY COEFF: 149.253731
SOLUTE CONCENTRATION 6.7E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 570
SOLUTE ACTIVITY COEFF: 68.4931507
SOLUTE CONCENTRATION .0146
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 670
SOLUTE ACTIVITY COEFF: 27.027027
SOLUTE CONCENTRATION .037
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 770
SOLUTE ACTIVITY COEFF: 11.4942529
SOLUTE CONCENTRATION .087
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 820
SOLUTE ACTIVITY COEFF: 8.33333333

SOLUTE CONCENTRATION .12
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 160.150463
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 192.432541
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 222.393977
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 247.329424
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 272.012592
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 287.961254
SPREAD ON OUTPUT: 79.8066947

REGULAR SOLUTION PREDICTIONS OF Wab: 742.706838
REGULAR SOLUTION PREDICTIONS OF Wab: 789.666817
REGULAR SOLUTION PREDICTIONS OF Wab: 821.677222
REGULAR SOLUTION PREDICTIONS OF Wab: 788.799032
REGULAR SOLUTION PREDICTIONS OF Wab: 746.989099
REGULAR SOLUTION PREDICTIONS OF Wab: 743.506842
SPREAD ON OUTPUT: .107714577

SOLUTE OXYGEN METAL SCANDIUM - Sc2O3
INPUT FROM KUPRASHVILI - RUSSIAN - CHECKS ONE SOURCE

TEMPERATURE: 1830
SOLUTE ACTIVITY COEFF: 2.94117647
SOLUTE CONCENTRATION .34
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2070
SOLUTE ACTIVITY COEFF: 2.7027027
SOLUTE CONCENTRATION .37
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2270
SOLUTE ACTIVITY COEFF: 2.5
SOLUTE CONCENTRATION .4
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 717.680851
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 835.227816
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 944.29439
SPREAD ON OUTPUT: 31.5758096

REGULAR SOLUTION PREDICTIONS OF Wab: 1500.91004
REGULAR SOLUTION PREDICTIONS OF Wab: 1717.24577

REGULAR SOLUTION PREDITIONS OF Wab: 1913.38897
SPREAD ON OUTPUT: 27.4819227

SOLUTE OXYGEN METAL SILICON - SiO₂ - TWO WIDELY DIFFER SOURCES
INPUT FROM HANSEN

TEMPERATURE: 1650
SOLUTE ACTIVITY COEFF: 4.16666667
SOLUTE CONCENTRATION .24
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1770
SOLUTE ACTIVITY COEFF: 3.33333333
SOLUTE CONCENTRATION .3
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1850
SOLUTE ACTIVITY COEFF: 2.5
SOLUTE CONCENTRATION .4
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 602.29757
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 672.690464
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 769.579128
SPREAD ON OUTPUT: 27.7739055

REGULAR SOLUTION PREDITIONS OF Wab: 1350.09012
REGULAR SOLUTION PREDITIONS OF Wab: 1440.25861
REGULAR SOLUTION PREDITIONS OF Wab: 1559.36987
SPREAD ON OUTPUT: 15.5011686

INPUT FROM ARKHAROV - RUSSIAN

TEMPERATURE: 1688
SOLUTE ACTIVITY COEFF: 25125.6281
SOLUTE CONCENTRATION 3.98E-05
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1873
SOLUTE ACTIVITY COEFF: 1023.54145
SOLUTE CONCENTRATION 9.77E-04
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 853.983481
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 845.289793

SPREAD ON OUTPUT: 1.01801588

REGULAR SOLUTION PREDITIONS OF Wab: 5664.13422

REGULAR SOLUTION PREDITIONS OF Wab: 4307.55486

SPREAD ON OUTPUT: 23.9503393

SOLUTE OXYGEN METAL SODIUM - Na₂O

INPUT FROM ADAMS

TEMPERATURE:	370
SOLUTE ACTIVITY COEFF:	250000
SOLUTE CONCENTRATION	4E-06
SOLUTE COORDINATION NUMBER:	6
TEMPERATURE:	470
SOLUTE ACTIVITY COEFF:	25641.0256
SOLUTE CONCENTRATION	3.9E-05
SOLUTE COORDINATION NUMBER:	6
TEMPERATURE:	570
SOLUTE ACTIVITY COEFF:	5405.40541
SOLUTE CONCENTRATION	1.85E-04
SOLUTE COORDINATION NUMBER:	6
TEMPERATURE:	670
SOLUTE ACTIVITY COEFF:	1869.15888
SOLUTE CONCENTRATION	5.35E-04
SOLUTE COORDINATION NUMBER:	6
TEMPERATURE:	770
SOLUTE ACTIVITY COEFF:	854.700855
SOLUTE CONCENTRATION	1.17E-03
SOLUTE COORDINATION NUMBER:	6
TEMPERATURE:	820
SOLUTE ACTIVITY COEFF:	617.283951
SOLUTE CONCENTRATION	1.62E-03
SOLUTE COORDINATION NUMBER:	6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab:	0	0	198.713984
QUASI-CHEMICAL PREDICTIONS OF Wab:	0	0	238.060292
QUASI-CHEMICAL PREDICTIONS OF Wab:	0	0	274.592052
QUASI-CHEMICAL PREDICTIONS OF Wab:	0	0	310.354705
QUASI-CHEMICAL PREDICTIONS OF Wab:	0	0	345.070594
QUASI-CHEMICAL PREDICTIONS OF Wab:	0	0	362.272199
SPREAD ON OUTPUT: 82.3083569			

REGULAR SOLUTION PREDITIONS OF Wab: 1522.98476
 REGULAR SOLUTION PREDITIONS OF Wab: 1580.25719
 REGULAR SOLUTION PREDITIONS OF Wab: 1623.06486
 REGULAR SOLUTION PREDITIONS OF Wab: 1673.27862
 REGULAR SOLUTION PREDITIONS OF Wab: 1725.46562
 REGULAR SOLUTION PREDITIONS OF Wab: 1750.50801
 SPREAD ON OUTPUT: 14.9392993

INPUT FROM HANSEN

TEMPERATURE: 520
 SOLUTE ACTIVITY COEFF: 4166.66667
 SOLUTE CONCENTRATION 2.4E-04
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 645
 SOLUTE ACTIVITY COEFF: 2000
 SOLUTE CONCENTRATION 5E-04
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 705
 SOLUTE ACTIVITY COEFF: 1000
 SOLUTE CONCENTRATION 1E-03
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 805
 SOLUTE ACTIVITY COEFF: 400
 SOLUTE CONCENTRATION 2.5E-03
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 248.273407
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 299.577826
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 318.168342
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 347.917985
 SPREAD ON OUTPUT: 40.1350189

REGULAR SOLUTION PREDITIONS OF Wab: 1436.00966
 REGULAR SOLUTION PREDITIONS OF Wab: 1625.19656
 REGULAR SOLUTION PREDITIONS OF Wab: 1616.00128
 REGULAR SOLUTION PREDITIONS OF Wab: 1605.27589
 SPREAD ON OUTPUT: 11.7872622

INPUT FROM PARLEE

TEMPERATURE: 1223
SOLUTE ACTIVITY COEFF: 176.678445
SOLUTE CONCENTRATION 5.66E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1523
SOLUTE ACTIVITY COEFF: 45.4545455
SOLUTE CONCENTRATION .022
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 505.552486
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 578.81784
SPREAD ON OUTPUT: 14.4921361

REGULAR SOLUTION PREDICTIONS OF Wab: 2119.61748
REGULAR SOLUTION PREDICTIONS OF Wab: 2012.60383
SPREAD ON OUTPUT: 5.04872471

INPUT FROM ALCOCK

TEMPERATURE: 810
SOLUTE ACTIVITY COEFF: 76923.0769
SOLUTE CONCENTRATION 1.3E-05
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 870
SOLUTE ACTIVITY COEFF: 24390.2439
SOLUTE CONCENTRATION 4.1E-05
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 970
SOLUTE ACTIVITY COEFF: 4830.91788
SOLUTE CONCENTRATION 2.07E-04
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 422.743447
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 440.145515
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 465.506358
SPREAD ON OUTPUT: 10.1155706

REGULAR SOLUTION PREDICTIONS OF Wab: 3017.98525
REGULAR SOLUTION PREDICTIONS OF Wab: 2910.75869
REGULAR SOLUTION PREDICTIONS OF Wab: 2726.06981
SPREAD ON OUTPUT: 9.67252713

INPUT FROM RAPP

TEMPERATURE: 1020
SOLUTE ACTIVITY COEFF: 2061.85567

SOLUTE CONCENTRATION 4.85E-04
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1120
SOLUTE ACTIVITY COEFF: 549.450549
SOLUTE CONCENTRATION 1.82E-03
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1220
SOLUTE ACTIVITY COEFF: 182.149363
SOLUTE CONCENTRATION 5.49E-03
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 474.385725
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 491.238669
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 505.111627
SPREAD ON OUTPUT: 6.47698715

REGULAR SOLUTION PREDICTIONS OF Wab: 2580.29994
REGULAR SOLUTION PREDICTIONS OF Wab: 2348.56102
REGULAR SOLUTION PREDICTIONS OF Wab: 2126.15264
SPREAD ON OUTPUT: 17.6005625

SOLUTE OXYGEN METAL TITANIUM - T10
INPUT FROM HANSEN

TEMPERATURE: 2085
SOLUTE ACTIVITY COEFF: 20
SOLUTE CONCENTRATION .05
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2135
SOLUTE ACTIVITY COEFF: 10
SOLUTE CONCENTRATION .1
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2180
SOLUTE ACTIVITY COEFF: 6.66666667
SOLUTE CONCENTRATION .15
SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2205
SOLUTE ACTIVITY COEFF: 5
SOLUTE CONCENTRATION .2
SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 755.339067
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 751.241804
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 767.075941
 QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 788.136774
 SPREAD ON OUTPUT: 4.3421172

REGULAR SOLUTION PREDICTIONS OF Wab: 2291.96754
 REGULAR SOLUTION PREDICTIONS OF Wab: 2009.90331
 REGULAR SOLUTION PREDICTIONS OF Wab: 1895.6583
 REGULAR SOLUTION PREDICTIONS OF Wab: 1836.32465
 SPREAD ON OUTPUT: 19.879989

SOLUTE OXYGEN METAL URANIUM - UO₂ - S.T. UNSURE
 INPUT FROM HANSEN

TEMPERATURE: 1380
 SOLUTE ACTIVITY COEFF: 120918.984
 SOLUTE CONCENTRATION 8.27E-06
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1470
 SOLUTE ACTIVITY COEFF: 105374.078
 SOLUTE CONCENTRATION 9.49E-06
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1670
 SOLUTE ACTIVITY COEFF: 70921.9858
 SOLUTE CONCENTRATION 1.41E-05
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 1870
 SOLUTE ACTIVITY COEFF: 51282.0513
 SOLUTE CONCENTRATION 1.95E-05
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2070
 SOLUTE ACTIVITY COEFF: 34482.7586
 SOLUTE CONCENTRATION 2.9E-05
 SOLUTE COORDINATION NUMBER: 6

TEMPERATURE: 2270
 SOLUTE ACTIVITY COEFF: 20161.2903
 SOLUTE CONCENTRATION 4.96E-05
 SOLUTE COORDINATION NUMBER: 6

OUTPUT

QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 728.313503
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 773.234194
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 869.618682
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 964.943987
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1057.10632
QUASI-CHEMICAL PREDICTIONS OF Wab: 0 0 1141.63887
SPREAD ON OUTPUT: 56.751024

REGULAR SOLUTION PREDITIONS OF Wab: 5348.41984
REGULAR SOLUTION PREDITIONS OF Wab: 5630.25472
REGULAR SOLUTION PREDITIONS OF Wab: 6177.35672
REGULAR SOLUTION PREDITIONS OF Wab: 6716.43113
REGULAR SOLUTION PREDITIONS OF Wab: 7162.82336
REGULAR SOLUTION PREDITIONS OF Wab: 7451.70762
SPREAD ON OUTPUT: 39.3254053

Surface Tension Theory output

OUTPUT FOR CARBON AND METAL ALUMINUM - NONE??

INPUT FROM HANSEN

TEMPERATURE: 1070
SOLUTE MAXIMUM SOL: 2.2E-03
METAL SURFACE TENSION: 813

TEMPERATURE: 1270
SOLUTE MAXIMUM SOL: 3.1E-03
METAL SURFACE TENSION: 783

TEMPERATURE: 1370
SOLUTE MAXIMUM SOL: 3.5E-03
METAL SURFACE TENSION: 768

TEMPERATURE: 1470
SOLUTE MAXIMUM SOL: 7.1E-03
METAL SURFACE TENSION: 753

OUTPUT

CALC MAX SOLUBILITY: .178022114
CALC MAX SOLUBILITY: .246497082
CALC MAX SOLUBILITY: .279901839
CALC MAX SOLUBILITY: .312385119

SOLUTE RADIUS N/ECOM: 9.40547641E-09
SOLUTE RADIUS N/ECOM: 1.01445137E-08
SOLUTE RADIUS N/ECOM: 1.05263806E-08
SOLUTE RADIUS N/ECOM: 1.03001728E-08

OUTPUT FOR CARBON AND METAL ANTIMONY - NONE

INPUT FROM HANSEN

TEMPERATURE: 1330
SOLUTE MAXIMUM SOL: 3.36E-03
METAL SURFACE TENSION: 350

TEMPERATURE: 1540
SOLUTE MAXIMUM SOL: 6.91E-03
METAL SURFACE TENSION: 342

TEMPERATURE: 1600

SOLUTE MAXIMUM SOL: 9.56E-03
METAL SURFACE TENSION: 335

OUTPUT

CALC MAX SOLUBILITY: .550053554
CALC MAX SOLUBILITY: .603849582
CALC MAX SOLUBILITY: .621526583

SOLUTE RADIUS N/ECOM: 1.54188894E-08
SOLUTE RADIUS N/ECOM: 1.56862047E-08
SOLUTE RADIUS N/ECOM: 1.56190736E-08

OUTPUT FOR CARBON AND METAL BISMUTH - NONE

INPUT FROM GRIFFITH

TEMPERATURE: 570
SOLUTE MAXIMUM SOL: 2.75E-05
METAL SURFACE TENSION: 362

TEMPERATURE: 670
SOLUTE MAXIMUM SOL: 3.42E-05
METAL SURFACE TENSION: 360

TEMPERATURE: 770
SOLUTE MAXIMUM SOL: 4.01E-05
METAL SURFACE TENSION: 357

TEMPERATURE: 870
SOLUTE MAXIMUM SOL: 4.54E-05
METAL SURFACE TENSION: 353

TEMPERATURE: 970
SOLUTE MAXIMUM SOL: 5.01E-05
METAL SURFACE TENSION: 348

TEMPERATURE: 1070
SOLUTE MAXIMUM SOL: 5.22E-05
METAL SURFACE TENSION: 343

OUTPUT

CALC MAX SOLUBILITY: .236325548
CALC MAX SOLUBILITY: .29509456
CALC MAX SOLUBILITY: .348851637
CALC MAX SOLUBILITY: .397874628
CALC MAX SOLUBILITY: .442684556

CALC MAX SOLUBILITY: .482813377

SOLUTE RADIUS N/ECOM: 1.34768553E-08
SOLUTE RADIUS N/ECOM: 1.44989138E-08
SOLUTE RADIUS N/ECOM: 1.54872242E-08
SOLUTE RADIUS N/ECOM: 1.64533988E-08
SOLUTE RADIUS N/ECOM: 1.74112478E-08
SOLUTE RADIUS N/ECOM: 1.83812947E-08

OUTPUT FOR CARBON AND METAL CERIUM - NONE - S.T. GUESS

INPUT FROM GTE

TEMPERATURE: 870
SOLUTE MAXIMUM SOL: .255
METAL SURFACE TENSION: 1020

TEMPERATURE: 1070
SOLUTE MAXIMUM SOL: .3
METAL SURFACE TENSION: 1000

OUTPUT

CALC MAX SOLUBILITY: .0697363813
CALC MAX SOLUBILITY: .119694376

SOLUTE RADIUS N/ECOM: 3.57805019E-09
SOLUTE RADIUS N/ECOM: 3.76169527E-09

OUTPUT FOR CARBON AND METAL CHROMIUM - NONE - UNSURE S.T. DATA

INPUT FROM HANSEN

TEMPERATURE: 1750
SOLUTE MAXIMUM SOL: .136
METAL SURFACE TENSION: 1720

TEMPERATURE: 1830
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 1700

TEMPERATURE: 1950

SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1680

TEMPERATURE: 2080
SOLUTE MAXIMUM SOL: .3
METAL SURFACE TENSION: 1640

OUTPUT

CALC MAX SOLUBILITY: .107262933
CALC MAX SOLUBILITY: .121231472
CALC MAX SOLUBILITY: .141294685
CALC MAX SOLUBILITY: .166806653

SOLUTE RADIUS N/ECOM: 4.72194106E-09
SOLUTE RADIUS N/ECOM: 4.73622E-09
SOLUTE RADIUS N/ECOM: 4.52984313E-09
SOLUTE RADIUS N/ECOM: 4.09544847E-09

INPUT FROM GTE

TEMPERATURE: 1800
SOLUTE MAXIMUM SOL: .145
METAL SURFACE TENSION: 1705

TEMPERATURE: 1910
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1689

TEMPERATURE: 1990
SOLUTE MAXIMUM SOL: .25
METAL SURFACE TENSION: 1673

OUTPUT

CALC MAX SOLUBILITY: .116306003
CALC MAX SOLUBILITY: .134177337
CALC MAX SOLUBILITY: .148142165

SOLUTE RADIUS N/ECOM: 4.73206829E-09
SOLUTE RADIUS N/ECOM: 4.47118208E-09
SOLUTE RADIUS N/ECOM: 4.255883E-09

OUTPUT FOR CARBON AND METAL COBALT - Co3C - DENSITY IS GUESS

INPUT FROM HANSEN - CHECKS WITH ONE SOURCE
TEMPERATURE: 1620

SOLUTE MAXIMUM SOL: .12
METAL SURFACE TENSION: 1880

TEMPERATURE: 1720
SOLUTE MAXIMUM SOL: .132
METAL SURFACE TENSION: 1855

TEMPERATURE: 1820
SOLUTE MAXIMUM SOL: .143
METAL SURFACE TENSION: 1830

OUTPUT

CALC MAX SOLUBILITY: .0716502962
CALC MAX SOLUBILITY: .0863203477
CALC MAX SOLUBILITY: .101887004

SOLUTE RADIUS N/ECOM: 4.47978208E-09
SOLUTE RADIUS N/ECOM: 4.54133105E-09
SOLUTE RADIUS N/ECOM: 4.60938899E-09

OUTPUT FOR CARBON AND METAL COPPER - NONE

INPUT FROM HANSEN

TEMPERATURE: 1370
SOLUTE MAXIMUM SOL: 5.3E-06
METAL SURFACE TENSION: 1300

TEMPERATURE: 1570
SOLUTE MAXIMUM SOL: 7.94E-06
METAL SURFACE TENSION: 1282

TEMPERATURE: 1770
SOLUTE MAXIMUM SOL: 2.65E-05
METAL SURFACE TENSION: 1265

TEMPERATURE: 1970
SOLUTE MAXIMUM SOL: 1.59E-04
METAL SURFACE TENSION: 1247

OUTPUT

CALC MAX SOLUBILITY: .115862269
CALC MAX SOLUBILITY: .156492968
CALC MAX SOLUBILITY: .197236299
CALC MAX SOLUBILITY: .237451619

SOLUTE RADIUS N/ECOM: 1.18582574E-08
 SOLUTE RADIUS N/ECOM: 1.2568683E-08
 SOLUTE RADIUS N/ECOM: 1.27265706E-08
 SOLUTE RADIUS N/ECOM: 1.23197831E-08

OUTPUT FOR CARBON AND METAL GERMANIUM - NONE - S.T. UNSURE DUE
 TO HIGH TEMPS

INPUT FROM SCARCE

TEMPERATURE: 3000
 SOLUTE MAXIMUM SOL: .0133
 METAL SURFACE TENSION: 330

TEMPERATURE: 3100
 SOLUTE MAXIMUM SOL: .0255
 METAL SURFACE TENSION: 320

TEMPERATURE: 3200
 SOLUTE MAXIMUM SOL: .047
 METAL SURFACE TENSION: 310

TEMPERATURE: 3300
 SOLUTE MAXIMUM SOL: .0833
 METAL SURFACE TENSION: 300

OUTPUT

CALC MAX SOLUBILTY: .778913588
 CALC MAX SOLUBILTY: .790991394
 CALC MAX SOLUBILTY: .802484369
 CALC MAX SOLUBILTY: .813432872

SOLUTE RADIUS N/ECOM: 2.07696163E-08
 SOLUTE RADIUS N/ECOM: 1.97591221E-08
 SOLUTE RADIUS N/ECOM: 1.86195168E-08
 SOLUTE RADIUS N/ECOM: 1.73288493E-08

OUTPUT FOR CARBON AND METAL HAFNIUM - NONE - S.T. UNSURE

INPUT FROM HANSEN

TEMPERATURE: 2480
SOLUTE MAXIMUM SOL: .095
METAL SURFACE TENSION: 1600

TEMPERATURE: 2820
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 1560

TEMPERATURE: 3160
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1530

TEMPERATURE: 3400
SOLUTE MAXIMUM SOL: .25
METAL SURFACE TENSION: 1500

TEMPERATURE: 3685
SOLUTE MAXIMUM SOL: .3
METAL SURFACE TENSION: 1480

OUTPUT

CALC MAX SOLUBILITY: .230979527
CALC MAX SOLUBILITY: .284641434
CALC MAX SOLUBILITY: .33294923
CALC MAX SOLUBILITY: .367110306
CALC MAX SOLUBILITY: .4016145

SOLUTE RADIUS N/ECOM: 6.33054709E-09
SOLUTE RADIUS N/ECOM: 6.13752167E-09
SOLUTE RADIUS N/ECOM: 6.04252315E-09
SOLUTE RADIUS N/ECOM: 5.87496036E-09
SOLUTE RADIUS N/ECOM: 5.73825192E-09

INPUT FROM GTE

TEMPERATURE: 2630
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 1580

TEMPERATURE: 3110
SOLUTE MAXIMUM SOL: .07
METAL SURFACE TENSION: 1535

TEMPERATURE: 3680
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 1480

TEMPERATURE: 4080
SOLUTE MAXIMUM SOL: .3
METAL SURFACE TENSION: 1440

OUTPUT

CALC MAX SOLUBILITY: .255489575
 CALC MAX SOLUBILITY: .325921683
 CALC MAX SOLUBILITY: .401117013
 CALC MAX SOLUBILITY: .448577268

SOLUTE RADIUS N/ECOM: 7.40089451E-09
 SOLUTE RADIUS N/ECOM: 7.69289477E-09
 SOLUTE RADIUS N/ECOM: 7.19819877E-09
 SOLUTE RADIUS N/ECOM: 6.12125621E-09

OUTPUT FOR CARBON AND METAL IRON - Fe₃C

INPUT FROM TURKOGAN

TEMPERATURE: 1570
 SOLUTE MAXIMUM SOL: .1855
 METAL SURFACE TENSION: 1840

TEMPERATURE: 1670
 SOLUTE MAXIMUM SOL: .1948
 METAL SURFACE TENSION: 1820

TEMPERATURE: 1770
 SOLUTE MAXIMUM SOL: .2035
 METAL SURFACE TENSION: 1800

TEMPERATURE: 1870
 SOLUTE MAXIMUM SOL: .2116
 METAL SURFACE TENSION: 1780

OUTPUT

CALC MAX SOLUBILITY: .0698059965
 CALC MAX SOLUBILITY: .0841268478
 CALC MAX SOLUBILITY: .0992702754
 CALC MAX SOLUBILITY: .115084184

SOLUTE RADIUS N/ECOM: 3.97361364E-09
 SOLUTE RADIUS N/ECOM: 4.06039816E-09
 SOLUTE RADIUS N/ECOM: 4.14684185E-09
 SOLUTE RADIUS N/ECOM: 4.23338693E-09

INPUT FROM .GRIGOROVICH - Fe-GRAPHITE EQUIL

TEMPERATURE: 1420
 SOLUTE MAXIMUM SOL: .171
 METAL SURFACE TENSION: 1830

TEMPERATURE: 1710
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1785

TEMPERATURE: 2300
SOLUTE MAXIMUM SOL: .25
METAL SURFACE TENSION: 1725

TEMPERATURE: 2600
SOLUTE MAXIMUM SOL: .3
METAL SURFACE TENSION: 1680

OUTPUT

CALC MAX SOLUBILITY: .0535445944
CALC MAX SOLUBILITY: .0933841283
CALC MAX SOLUBILITY: .182034699
CALC MAX SOLUBILITY: .23045937

SOLUTE RADIUS N/ECOM: 3.87979375E-09
SOLUTE RADIUS N/ECOM: 4.1152805E-09
SOLUTE RADIUS N/ECOM: 4.50588891E-09
SOLUTE RADIUS N/ECOM: 4.52401208E-09

INPUT FROM GIRGOROVICH - Fe₃C-Fe EQUIL

TEMPERATURE: 1420
SOLUTE MAXIMUM SOL: .171
METAL SURFACE TENSION: 1730

TEMPERATURE: 1500
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1745

TEMPERATURE: 1670
SOLUTE MAXIMUM SOL: .25
METAL SURFACE TENSION: 1775

OUTPUT

CALC MAX SOLUBILITY: .0628325556
CALC MAX SOLUBILITY: .0711896616
CALC MAX SOLUBILITY: .0894367283

SOLUTE RADIUS N/ECOM: 3.9903513E-09
SOLUTE RADIUS N/ECOM: 3.89823854E-09
SOLUTE RADIUS N/ECOM: 3.78503735E-09

OUTPUT FOR CARBON AND METAL LITHIUM - NONE

INPUT FROM ADAMS

TEMPERATURE: 570
SOLUTE MAXIMUM SOL: .0105
METAL SURFACE TENSION: 386

TEMPERATURE: 670
SOLUTE MAXIMUM SOL: .017
METAL SURFACE TENSION: 370

TEMPERATURE: 770
SOLUTE MAXIMUM SOL: .0235
METAL SURFACE TENSION: 354

TEMPERATURE: 870
SOLUTE MAXIMUM SOL: .03
METAL SURFACE TENSION: 338

OUTPUT

CALC MAX SOLUBILITY: .214770916
CALC MAX SOLUBILITY: .285258046
CALC MAX SOLUBILITY: .351952554
CALC MAX SOLUBILITY: .413765424

SOLUTE RADIUS N/ECOM: 8.59680605E-09
SOLUTE RADIUS N/ECOM: 9.002421E-09
SOLUTE RADIUS N/ECOM: 9.46643497E-09
SOLUTE RADIUS N/ECOM: 9.95692342E-09

INPUT FROM HANSEN

TEMPERATURE: 680
SOLUTE MAXIMUM SOL: .016
METAL SURFACE TENSION: 372

TEMPERATURE: 830
SOLUTE MAXIMUM SOL: .02
METAL SURFACE TENSION: 346

TEMPERATURE: 970
SOLUTE MAXIMUM SOL: .032
METAL SURFACE TENSION: 322

TEMPERATURE: 1070
SOLUTE MAXIMUM SOL: .052
METAL SURFACE TENSION: 306

TEMPERATURE: 1170
SOLUTE MAXIMUM SOL: .091
METAL SURFACE TENSION: 290

OUTPUT

CALC MAX SOLUBILITY: .288634177
 CALC MAX SOLUBILITY: .387950628
 CALC MAX SOLUBILITY: .470473965
 CALC MAX SOLUBILITY: .522264571
 CALC MAX SOLUBILITY: .569498454

SOLUTE RADIUS N/ECOM: 9.11198243E-09
 SOLUTE RADIUS N/ECOM: 1.01527825E-08
 SOLUTE RADIUS N/ECOM: 1.06720529E-08
 SOLUTE RADIUS N/ECOM: 1.06562488E-08
 SOLUTE RADIUS N/ECOM: 1.03062789E-08

INPUT FROM HANSEN

TEMPERATURE: 1010
 SOLUTE MAXIMUM SOL: .05
 METAL SURFACE TENSION: 316

TEMPERATURE: 1055
 SOLUTE MAXIMUM SOL: .1
 METAL SURFACE TENSION: 309

TEMPERATURE: 1070
 SOLUTE MAXIMUM SOL: .15
 METAL SURFACE TENSION: 306

TEMPERATURE: 1090
 SOLUTE MAXIMUM SOL: .2
 METAL SURFACE TENSION: 303

OUTPUT

CALC MAX SOLUBILITY: .491320232
 CALC MAX SOLUBILITY: .514131755
 CALC MAX SOLUBILITY: .522264571
 CALC MAX SOLUBILITY: .531841125

SOLUTE RADIUS N/ECOM: 1.02553864E-08
 SOLUTE RADIUS N/ECOM: 9.29262086E-09
 SOLUTE RADIUS N/ECOM: 8.53614845E-09
 SOLUTE RADIUS N/ECOM: 7.97466471E-09

OUTPUT FOR CARBON AND METAL MANGANESE - Mn3C - S.T. UNSURE

INPUT FROM HANSEN

TEMPERATURE: 1620
SOLUTE MAXIMUM SOL: .2636
METAL SURFACE TENSION: 1090

TEMPERATURE: 1720
SOLUTE MAXIMUM SOL: .272
METAL SURFACE TENSION: 1070

TEMPERATURE: 1820
SOLUTE MAXIMUM SOL: .2796
METAL SURFACE TENSION: 1050

TEMPERATURE: 1870
SOLUTE MAXIMUM SOL: .2868
METAL SURFACE TENSION: 1040

OUTPUT

CALC MAX SOLUBILITY: .21690522
CALC MAX SOLUBILITY: .243404967
CALC MAX SOLUBILITY: .269704275
CALC MAX SOLUBILITY: .28273523

SOLUTE RADIUS N/ECOM: 4.66546829E-09
SOLUTE RADIUS N/ECOM: 4.79461133E-09
SOLUTE RADIUS N/ECOM: 4.92579693E-09
SOLUTE RADIUS N/ECOM: 4.96664993E-09

INPUT FROM HANSEN

TEMPERATURE: 1500
SOLUTE MAXIMUM SOL: .057
METAL SURFACE TENSION: 1114

TEMPERATURE: 1565
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 1103

TEMPERATURE: 1590
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1096

TEMPERATURE: 1610
SOLUTE MAXIMUM SOL: .25
METAL SURFACE TENSION: 1092

OUTPUT

CALC MAX SOLUBILITY: .185092247
CALC MAX SOLUBILITY: .201720384
CALC MAX SOLUBILITY: .208941305
CALC MAX SOLUBILITY: .214250597

SOLUTE RADIUS N/ECOM: 6.50918022E-09

SOLUTE RADIUS N/ECOM: 5.43751162E-09
SOLUTE RADIUS N/ECOM: 5.06423421E-09
SOLUTE RADIUS N/ECOM: 4.73819283E-09

INPUT FROM HANSEN

TEMPERATURE: 1580
SOLUTE MAXIMUM SOL: .265
METAL SURFACE TENSION: 1094

TEMPERATURE: 1620
SOLUTE MAXIMUM SOL: .272
METAL SURFACE TENSION: 1090

TEMPERATURE: 1720
SOLUTE MAXIMUM SOL: .28
METAL SURFACE TENSION: 1070

TEMPERATURE: 1870
SOLUTE MAXIMUM SOL: .292
METAL SURFACE TENSION: 1040

OUTPUT

CALC MAX SOLUBILITY: .207476706
CALC MAX SOLUBILITY: .21690522
CALC MAX SOLUBILITY: .243404967
CALC MAX SOLUBILITY: .28273523

SOLUTE RADIUS N/ECOM: 4.58993427E-09
SOLUTE RADIUS N/ECOM: 4.61025907E-09
SOLUTE RADIUS N/ECOM: 4.7409357E-09
SOLUTE RADIUS N/ECOM: 4.93079338E-09

OUTPUT FOR CARBON AND METAL MOLYBDENUM - Mo₂C - S.T. UNSURE

INPUT FROM RUDY

TEMPERATURE: 2470
SOLUTE MAXIMUM SOL: .17
METAL SURFACE TENSION: 1065

TEMPERATURE: 2600
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1090

TEMPERATURE: 2700
SOLUTE MAXIMUM SOL: .25

METAL SURFACE TENSION: 1110

OUTPUT

CALC MAX SOLUBILITY: .375546342
CALC MAX SOLUBILITY: .38587368
CALC MAX SOLUBILITY: .393056411

SOLUTE RADIUS N/ECOM: 6.71867489E-09
SOLUTE RADIUS N/ECOM: 6.49372544E-09
SOLUTE RADIUS N/ECOM: 6.08599379E-09

OUTPUT FOR CARBON AND METAL NICKEL - N13C

INPUT FROM HANSEN

TEMPERATURE: 1620
SOLUTE MAXIMUM SOL: .097
METAL SURFACE TENSION: 1800

TEMPERATURE: 1720
SOLUTE MAXIMUM SOL: .104
METAL SURFACE TENSION: 1780

TEMPERATURE: 1820
SOLUTE MAXIMUM SOL: .111
METAL SURFACE TENSION: 1760

TEMPERATURE: 1920
SOLUTE MAXIMUM SOL: .118
METAL SURFACE TENSION: 1740

TEMPERATURE: 2020
SOLUTE MAXIMUM SOL: .124
METAL SURFACE TENSION: 1720

OUTPUT

CALC MAX SOLUBILITY: .0801552768
CALC MAX SOLUBILITY: .0953075868
CALC MAX SOLUBILITY: .111188431
CALC MAX SOLUBILITY: .127649652
CALC MAX SOLUBILITY: .144558299

SOLUTE RADIUS N/ECOM: 4.80248627E-09
SOLUTE RADIUS N/ECOM: 4.90134016E-09
SOLUTE RADIUS N/ECOM: 4.99687888E-09
SOLUTE RADIUS N/ECOM: 5.08942612E-09

SOLUTE RADIUS N/ECOM: 5.18925906E-09

OUTPUT FOR CARBON AND METAL NIOBIUM - NONE - S.T. UNSURE

INPUT FROM KIMURA

TEMPERATURE: 2610
SOLUTE MAXIMUM SOL: .135
METAL SURFACE TENSION: 1994

TEMPERATURE: 2880
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1978

TEMPERATURE: 3110
SOLUTE MAXIMUM SOL: .25
METAL SURFACE TENSION: 1932

TEMPERATURE: 3280
SOLUTE MAXIMUM SOL: .3
METAL SURFACE TENSION: 1898

OUTPUT

CALC MAX SOLUBILITY: .176343251
CALC MAX SOLUBILITY: .21013241
CALC MAX SOLUBILITY: .243887083
CALC MAX SOLUBILITY: .268643209

SOLUTE RADIUS N/ECOM: 5.36568544E-09
SOLUTE RADIUS N/ECOM: 5.07345249E-09
SOLUTE RADIUS N/ECOM: 4.95094094E-09
SOLUTE RADIUS N/ECOM: 4.78057945E-09

OUTPUT FOR CARBON AND METAL PLUTONIUM - NONE

INPUT FROM HANSEN

TEMPERATURE: 1275
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 500

TEMPERATURE: 1420
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 485

TEMPERATURE: 1550
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 475

TEMPERATURE: 1650
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 465

OUTPUT

CALC MAX SOLUBILITY: .410348181
CALC MAX SOLUBILITY: .460335967
CALC MAX SOLUBILITY: .498537012
CALC MAX SOLUBILITY: .527226618

SOLUTE RADIUS N/ECOM: 9.16020036E-09
SOLUTE RADIUS N/ECOM: 8.60527059E-09
SOLUTE RADIUS N/ECOM: 8.24612337E-09
SOLUTE RADIUS N/ECOM: 7.92019717E-09

OUTPUT FOR CARBON AND METAL RHENIUM - NONE - S.T. UNSURE

INPUT FROM HUGES

TEMPERATURE: 2770
SOLUTE MAXIMUM SOL: .169
METAL SURFACE TENSION: 2780

TEMPERATURE: 2870
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 2760

TEMPERATURE: 2970
SOLUTE MAXIMUM SOL: .23
METAL SURFACE TENSION: 2740

TEMPERATURE: 3040
SOLUTE MAXIMUM SOL: .25
METAL SURFACE TENSION: 2720

OUTPUT

CALC MAX SOLUBILITY: .102324039
CALC MAX SOLUBILITY: .112550524

CALC MAX SOLUBILITY: .123007479
CALC MAX SOLUBILITY: .131031863

SOLUTE RADIUS N/ECOM: 4.41112363E-09
SOLUTE RADIUS N/ECOM: 4.28752736E-09
SOLUTE RADIUS N/ECOM: 4.18308918E-09
SOLUTE RADIUS N/ECOM: 4.12537518E-09

OUTPUT FOR CARBON AND METAL SILVER - NONE

INPUT FROM HANSEN

TEMPERATURE: 1930
SOLUTE MAXIMUM SOL: 1.08E-04
METAL SURFACE TENSION: 800

TEMPERATURE: 2005
SOLUTE MAXIMUM SOL: 2.25E-04
METAL SURFACE TENSION: 787

OUTPUT

CALC MAX SOLUBILITY: .390035565
CALC MAX SOLUBILITY: .410011059

SOLUTE RADIUS N/ECOM: 1.55572486E-08
SOLUTE RADIUS N/ECOM: 1.53312512E-08

OUTPUT FOR CARBON AND METAL SODIUM - NONE

INPUT FROM SALZANO

TEMPERATURE: 850
SOLUTE MAXIMUM SOL: 1.631E-05
METAL SURFACE TENSION: 157.9

TEMPERATURE: 970
SOLUTE MAXIMUM SOL: 3.695E-05
METAL SURFACE TENSION: 146.9

OUTPUT

CALC MAX SOLUBILITY: .655768189
CALC MAX SOLUBILITY: .708936077

SOLUTE RADIUS N/ECOM: 2.5530899E-08
SOLUTE RADIUS N/ECOM: 2.72072698E-08

INPUT FROM HANSEN

TEMPERATURE: 420
SOLUTE MAXIMUM SOL: 6.2E-05
METAL SURFACE TENSION: 197.5

TEMPERATURE: 570
SOLUTE MAXIMUM SOL: 9E-05
METAL SURFACE TENSION: 183.7

TEMPERATURE: 770
SOLUTE MAXIMUM SOL: 1.22E-04
METAL SURFACE TENSION: 165.3

TEMPERATURE: 970
SOLUTE MAXIMUM SOL: 1.44E-04
METAL SURFACE TENSION: 146.9

OUTPUT

CALC MAX SOLUBILITY: .343659548
CALC MAX SOLUBILITY: .480930839
CALC MAX SOLUBILITY: .614088755
CALC MAX SOLUBILITY: .708936077

SOLUTE RADIUS N/ECOM: 1.50435376E-08
SOLUTE RADIUS N/ECOM: 1.78186173E-08
SOLUTE RADIUS N/ECOM: 2.14728955E-08
SOLUTE RADIUS N/ECOM: 2.532937E-08

OUTPUT FOR CARBON AND METAL TANTALUM - NONE

INPUT FROM HANSEN - UNSURE PHASE DIAG

TEMPERATURE: 3070
SOLUTE MAXIMUM SOL: .08
METAL SURFACE TENSION: 2155

TEMPERATURE: 3150
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 2140

TEMPERATURE: 3305
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 2110

TEMPERATURE: 3455
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 2080

OUTPUT

CALC MAX SOLUBILITY: .203024896
CALC MAX SOLUBILITY: .213713905
CALC MAX SOLUBILITY: .234540028
CALC MAX SOLUBILITY: .254756178

SOLUTE RADIUS N/ECOM: 6.28669338E-09
SOLUTE RADIUS N/ECOM: 6.10154218E-09
SOLUTE RADIUS N/ECOM: 5.71314554E-09
SOLUTE RADIUS N/ECOM: 5.41892145E-09

INPUT FROM GTE

TEMPERATURE: 3120
SOLUTE MAXIMUM SOL: .12
METAL SURFACE TENSION: 2146

TEMPERATURE: 3255
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 2120

TEMPERATURE: 3450
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 2080

OUTPUT

CALC MAX SOLUBILITY: .209648532
CALC MAX SOLUBILITY: .227778266
CALC MAX SOLUBILITY: .2542518

SOLUTE RADIUS N/ECOM: 5.81889799E-09
SOLUTE RADIUS N/ECOM: 5.65637702E-09
SOLUTE RADIUS N/ECOM: 5.41499896E-09

OUTPUT FOR CARBON AND METAL TITANIUM - TiC

INPUT FROM GTE

TEMPERATURE: 1920
SOLUTE MAXIMUM SOL: .015
METAL SURFACE TENSION: 1600

TEMPERATURE: 1950
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 1594

TEMPERATURE: 2020
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 1580

TEMPERATURE: 2115
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 1561

TEMPERATURE: 2320
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1520

OUTPUT

CALC MAX SOLUBILITY: .150643046
CALC MAX SOLUBILITY: .156182112
CALC MAX SOLUBILITY: .169204387
CALC MAX SOLUBILITY: .18703853
CALC MAX SOLUBILITY: .225786465

SOLUTE RADIUS N/ECOM: 7.44017933E-09
SOLUTE RADIUS N/ECOM: 6.34465527E-09
SOLUTE RADIUS N/ECOM: 5.68641261E-09
SOLUTE RADIUS N/ECOM: 5.31354689E-09
SOLUTE RADIUS N/ECOM: 5.19448739E-09

INPUT FROM HANSEN

TEMPERATURE: 2110
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 1562

TEMPERATURE: 2210
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 1542

TEMPERATURE: 2350
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 1514

TEMPERATURE: 2490
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1486

OUTPUT

CALC MAX SOLUBILITY: .186096532
CALC MAX SOLUBILITY: .204978847
CALC MAX SOLUBILITY: .231455334
CALC MAX SOLUBILITY: .257805808

SOLUTE RADIUS N/ECOM: 6.66707891E-09
SOLUTE RADIUS N/ECOM: 6.02067491E-09
SOLUTE RADIUS N/ECOM: 5.6872429E-09
SOLUTE RADIUS N/ECOM: 5.4426545E-09

OUTPUT FOR CARBON AND METAL URANIUM - UC2 - S.T. UNSURE

INPUT FROM HANSEN

TEMPERATURE: 1670
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 1455

TEMPERATURE: 1870
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 1425

TEMPERATURE: 2030
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 1401

TEMPERATURE: 2170
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1380

OUTPUT

CALC MAX SOLUBILITY: .138209657
CALC MAX SOLUBILITY: .177127093
CALC MAX SOLUBILITY: .208543214
CALC MAX SOLUBILITY: .235865975

SOLUTE RADIUS N/ECOM: 6.14556225E-09
SOLUTE RADIUS N/ECOM: 5.7610892E-09
SOLUTE RADIUS N/ECOM: 5.49489926E-09
SOLUTE RADIUS N/ECOM: 5.27242999E-09

OUTPUT FOR CARBON AND METAL VANADIUM - NONE - S.T. UNSURE

INPUT FROM STORMS - CHECKED BY ONE SOURCE

TEMPERATURE: 1920
SOLUTE MAXIMUM SOL: .145
METAL SURFACE TENSION: 1980

TEMPERATURE: 2000
SOLUTE MAXIMUM SOL: .167
METAL SURFACE TENSION: 1974

TEMPERATURE: 2120
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1960

TEMPERATURE: 2250
SOLUTE MAXIMUM SOL: .23
METAL SURFACE TENSION: 1937

OUTPUT

CALC MAX SOLUBILITY: .0960974796
CALC MAX SOLUBILITY: .106258309
CALC MAX SOLUBILITY: .122458462
CALC MAX SOLUBILITY: .141503312

SOLUTE RADIUS N/ECOM: 4.53518452E-09
SOLUTE RADIUS N/ECOM: 4.46295373E-09
SOLUTE RADIUS N/ECOM: 4.37280783E-09
SOLUTE RADIUS N/ECOM: 4.33032637E-09

OUTPUT FOR CARBON AND METAL WOLFRAM - WC - S.T. UNSURE

INPUT FROM HANSEN

TEMPERATURE: 3070
SOLUTE MAXIMUM SOL: .4
METAL SURFACE TENSION: 2490

TEMPERATURE: 3350
SOLUTE MAXIMUM SOL: .5
METAL SURFACE TENSION: 2426

OUTPUT

CALC MAX SOLUBILITY: .158455073
CALC MAX SOLUBILITY: .193030301

SOLUTE RADIUS N/ECOM: 3.5226504E-09
SOLUTE RADIUS N/ECOM: 3.24244874E-09

OUTPUT FOR CARBON AND METAL ZIRCONIUM - ZrC - S.T. GUESSED
FROM T1 DATA

INPUT FROM HANSEN

TEMPERATURE: 2100
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 1553

TEMPERATURE: 2270
SOLUTE MAXIMUM SOL: .067
METAL SURFACE TENSION: 1528

TEMPERATURE: 2670
SOLUTE MAXIMUM SOL: .143
METAL SURFACE TENSION: 1468

TEMPERATURE: 3070
SOLUTE MAXIMUM SOL: .276
METAL SURFACE TENSION: 1408

OUTPUT

CALC MAX SOLUBILITY: .186418296
CALC MAX SOLUBILITY: .216763253
CALC MAX SOLUBILITY: .28683433
CALC MAX SOLUBILITY: .352839707

SOLUTE RADIUS N/ECOM: 6.67050636E-09
SOLUTE RADIUS N/ECOM: 6.6414467E-09
SOLUTE RADIUS N/ECOM: 6.23341173E-09
SOLUTE RADIUS N/ECOM: 5.5526501E-09

OUTPUT FOR HYDROGEN AND METAL CALCIUM - CaH₂

INPUT FROM HANSEN

TEMPERATURE: 1235
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 320

TEMPERATURE: 1250
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 319

TEMPERATURE: 1270
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 318

TEMPERATURE: 1320
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 315

OUTPUT

CALC MAX SOLUBILITY: .428483589
CALC MAX SOLUBILITY: .433997657
CALC MAX SOLUBILITY: .440874269
CALC MAX SOLUBILITY: .458158868

SOLUTE RADIUS N/ECOM: 1.12692074E-08
SOLUTE RADIUS N/ECOM: 9.95522072E-09
SOLUTE RADIUS N/ECOM: 9.12260947E-09
SOLUTE RADIUS N/ECOM: 8.60700759E-09

OUTPUT FOR HYDROGEN AND METAL LANTANUM - NONE

INPUT FROM PETERSON - S.T. IFFY

TEMPERATURE: 1200
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 1600

TEMPERATURE: 1210
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 1595

TEMPERATURE: 1220
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 1590

TEMPERATURE: 1240
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1585

TEMPERATURE: 1300
SOLUTE MAXIMUM SOL: .3
METAL SURFACE TENSION: 1575

OUTPUT

CALC MAX SOLUBILITY: .0127642323
CALC MAX SOLUBILITY: .0134127394
CALC MAX SOLUBILITY: .0140827491
CALC MAX SOLUBILITY: .015285342
CALC MAX SOLUBILITY: .0190109928

SOLUTE RADIUS N/ECOM: 4.96781615E-09
SOLUTE RADIUS N/ECOM: 4.38029711E-09
SOLUTE RADIUS N/ECOM: 3.99863844E-09
SOLUTE RADIUS N/ECOM: 3.7189189E-09
SOLUTE RADIUS N/ECOM: 3.30387128E-09

OUTPUT FOR HYDROGEN AND METAL LITHIUM - LiH

INPUT FROM HANSEN

TEMPERATURE: 760
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 352

TEMPERATURE: 920
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 320

TEMPERATURE: 960
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 312

TEMPERATURE: 1090
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 290

OUTPUT

CALC MAX SOLUBILITY: .219827676
CALC MAX SOLUBILITY: .320561721
CALC MAX SOLUBILITY: .345411035
CALC MAX SOLUBILITY: .418858902

SOLUTE RADIUS N/ECOM: 8.42888924E-09
SOLUTE RADIUS N/ECOM: 8.52727272E-09
SOLUTE RADIUS N/ECOM: 8.00735537E-09
SOLUTE RADIUS N/ECOM: 8.15144772E-09

INPUT FROM HUBBERTY

TEMPERATURE: 470
SOLUTE MAXIMUM SOL: 4.1E-04
METAL SURFACE TENSION: 400

TEMPERATURE: 550
SOLUTE MAXIMUM SOL: 2.12E-03
METAL SURFACE TENSION: 386

TEMPERATURE: 650
SOLUTE MAXIMUM SOL: 9.38E-03
METAL SURFACE TENSION: 370

TEMPERATURE: 750
SOLUTE MAXIMUM SOL: .0279
METAL SURFACE TENSION: 354

TEMPERATURE: 870
SOLUTE MAXIMUM SOL: .0741
METAL SURFACE TENSION: 343

OUTPUT

CALC MAX SOLUBILITY: .0618102423
CALC MAX SOLUBILITY: .100708119
CALC MAX SOLUBILITY: .155383689
CALC MAX SOLUBILITY: .213561087
CALC MAX SOLUBILITY: .275398915

SOLUTE RADIUS N/ECOM: 1.00330186E-08
SOLUTE RADIUS N/ECOM: 9.81595019E-09
SOLUTE RADIUS N/ECOM: 9.49203432E-09
SOLUTE RADIUS N/ECOM: 9.12643228E-09
SOLUTE RADIUS N/ECOM: 8.51486854E-09

INPUT FROM ADAMS

TEMPERATURE: 900
SOLUTE MAXIMUM SOL: .117
METAL SURFACE TENSION: 334

TEMPERATURE: 950
SOLUTE MAXIMUM SOL: .188
METAL SURFACE TENSION: 326

OUTPUT

CALC MAX SOLUBILITY: .297053854
CALC MAX SOLUBILITY: .325493894

SOLUTE RADIUS N/ECOM: 7.96900129E-09
SOLUTE RADIUS N/ECOM: 7.3141746E-09

OUTPUT FOR HYDROGEN AND METAL PLUTONIUM - PuH2 - DENSITY DATA
BASED ON URANIUM

INPUT FROM HANSEN

TEMPERATURE: 970
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 545

TEMPERATURE: 1070
SOLUTE MAXIMUM SOL: .075
METAL SURFACE TENSION: 520

OUTPUT

CALC MAX SOLUBILITY: .159177539
CALC MAX SOLUBILITY: .204014774

SOLUTE RADIUS N/ECOM: 7.65283763E-09
SOLUTE RADIUS N/ECOM: 7.65148764E-09

OUTPUT FOR HYDROGEN AND METAL POTASSIUM - NONE

INPUT FROM HUBBERTY

TEMPERATURE: 400
SOLUTE MAXIMUM SOL: 6.61E-06
METAL SURFACE TENSION: 89.19

TEMPERATURE: 500
SOLUTE MAXIMUM SOL: 2.08E-04
METAL SURFACE TENSION: 82.66

TEMPERATURE: 600
SOLUTE MAXIMUM SOL: 2.07E-03
METAL SURFACE TENSION: 76.13

TEMPERATURE: 700
SOLUTE MAXIMUM SOL: .0107
METAL SURFACE TENSION: 69.6

OUTPUT

CALC MAX SOLUBILITY: .482239884
CALC MAX SOLUBILITY: .582320773
CALC MAX SOLUBILITY: .660331052
CALC MAX SOLUBILITY: .72237269

SOLUTE RADIUS N/ECOM: 2.42392722E-08
SOLUTE RADIUS N/ECOM: 2.37337677E-08
SOLUTE RADIUS N/ECOM: 2.31303707E-08
SOLUTE RADIUS N/ECOM: 2.2389101E-08

INPUT FROM ARNIL'DOV - RUSSIAN

TEMPERATURE: 570
SOLUTE MAXIMUM SOL: 1.79E-03
METAL SURFACE TENSION: 78.09

TEMPERATURE: 670
SOLUTE MAXIMUM SOL: .0105
METAL SURFACE TENSION: 71.56

TEMPERATURE: 770
SOLUTE MAXIMUM SOL: .0386
METAL SURFACE TENSION: 65.03

OUTPUT

CALC MAX SOLUBILITY: .638838315
CALC MAX SOLUBILITY: .7051503
CALC MAX SOLUBILITY: .75863344

SOLUTE RADIUS N/ECOM: 2.25201818E-08
SOLUTE RADIUS N/ECOM: 2.16468939E-08
SOLUTE RADIUS N/ECOM: 2.05737855E-08

OUTPUT FOR HYDROGEN AND METAL SODIUM - NaH

INPUT FROM McCLURE

TEMPERATURE: 530
SOLUTE MAXIMUM SOL: 1.899E-04
METAL SURFACE TENSION: 187.4

TEMPERATURE: 630
SOLUTE MAXIMUM SOL: 1.309E-03
METAL SURFACE TENSION: 178.2

OUTPUT

CALC MAX SOLUBILITY: .314580092
CALC MAX SOLUBILITY: .396460847

SOLUTE RADIUS N/ECOM: 1.63155577E-08
SOLUTE RADIUS N/ECOM: 1.6055895E-08

INPUT FROM ADDISON

TEMPERATURE: 520
SOLUTE MAXIMUM SOL: 8.256E-05
METAL SURFACE TENSION: 188.3

TEMPERATURE: 593
SOLUTE MAXIMUM SOL: 1.275E-04
METAL SURFACE TENSION: 181.6

OUTPUT

CALC MAX SOLUBILITY: .305924076
CALC MAX SOLUBILITY: .367270147

SOLUTE RADIUS N/ECOM: 1.68876678E-08
SOLUTE RADIUS N/ECOM: 1.79343623E-08

INPUT FROM HUBBERTY

TEMPERATURE: 400
SOLUTE MAXIMUM SOL: 1.86E-06
METAL SURFACE TENSION: 199.3

TEMPERATURE: 500
SOLUTE MAXIMUM SOL: 6.03E-05
METAL SURFACE TENSION: 190.1

TEMPERATURE: 600
SOLUTE MAXIMUM SOL: 6.11E-04
METAL SURFACE TENSION: 180.9

TEMPERATURE: 700
SOLUTE MAXIMUM SOL: 3.2E-03
METAL SURFACE TENSION: 171.7

OUTPUT

CALC MAX SOLUBILITY: .195989991
CALC MAX SOLUBILITY: .288352943
CALC MAX SOLUBILITY: .373007918

CALC MAX SOLUBILTY: .448301991

SOLUTE RADIUS N/ECOM: 1.70554563E-08
SOLUTE RADIUS N/ECOM: 1.6754253E-08
SOLUTE RADIUS N/ECOM: 1.64197947E-08
SOLUTE RADIUS N/ECOM: 1.60390013E-08

OUTPUT FOR HYDROGEN AND METAL STRONTIUM - SrH2

INPUT FROM HANSEN - SCEWY PHASE DIAG

TEMPERATURE: 1050
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 282

TEMPERATURE: 1065
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 283

TEMPERATURE: 1080
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 285

OUTPUT

CALC MAX SOLUBILTY: .415425564
CALC MAX SOLUBILTY: .419307612
CALC MAX SOLUBILTY: .421837111

SOLUTE RADIUS N/ECOM: 1.10689131E-08
SOLUTE RADIUS N/ECOM: 9.75602297E-09
SOLUTE RADIUS N/ECOM: 8.88628486E-09

OUTPUT FOR HYDROGEN AND METAL URANIUM - UH3 - UNSURE S.T. DATA

INPUT FROM HANSEN

TEMPERATURE: 1400
SOLUTE MAXIMUM SOL: .29
METAL SURFACE TENSION: 1495

TEMPERATURE: 1470

SOLUTE MAXIMUM SOL: .333
METAL SURFACE TENSION: 1485

OUTPUT

CALC MAX SOLUBILITY: .0304161809
CALC MAX SOLUBILITY: .0367283218

SOLUTE RADIUS N/ECOM: 3.56833063E-09
SOLUTE RADIUS N/ECOM: 3.45779081E-09

OUTPUT FOR NITROGEN AND METAL CALCIUM - Ca₃N₂

INPUT FROM HANSEN

TEMPERATURE: 1050
SOLUTE MAXIMUM SOL: .019
METAL SURFACE TENSION: 329

TEMPERATURE: 1110
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 326

TEMPERATURE: 1150
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 324

OUTPUT

CALC MAX SOLUBILITY: .358846533
CALC MAX SOLUBILITY: .382654602
CALC MAX SOLUBILITY: .39791329

SOLUTE RADIUS N/ECOM: 1.17871674E-08
SOLUTE RADIUS N/ECOM: 1.05849198E-08
SOLUTE RADIUS N/ECOM: 9.47474746E-09

OUTPUT FOR NITROGEN AND METAL CHROMIUM - DELTA H DATA FOR CrN₂
- DENSITY DATA FOR CrN - UNSURE S.T.

INPUT FROM HUMBERT

TEMPERATURE: 1960
SOLUTE MAXIMUM SOL: .172
METAL SURFACE TENSION: 1664

TEMPERATURE: 2000
SOLUTE MAXIMUM SOL: .156
METAL SURFACE TENSION: 1656

TEMPERATURE: 2040
SOLUTE MAXIMUM SOL: .142
METAL SURFACE TENSION: 1648

TEMPERATURE: 2080
SOLUTE MAXIMUM SOL: .129
METAL SURFACE TENSION: 1640

TEMPERATURE: 2130

SOLUTE MAXIMUM SOL: .113
METAL SURFACE TENSION: 1630

OUTPUT

CALC MAX SOLUBILITY: .062233054
CALC MAX SOLUBILITY: .0666534614
CALC MAX SOLUBILITY: .0711960028
CALC MAX SOLUBILITY: .0758555304
CALC MAX SOLUBILITY: .0818366158

SOLUTE RADIUS N/ECOM: 4.77225089E-09
SOLUTE RADIUS N/ECOM: 4.96454324E-09
SOLUTE RADIUS N/ECOM: 5.15171448E-09
SOLUTE RADIUS N/ECOM: 5.34136242E-09
SOLUTE RADIUS N/ECOM: 5.59428039E-09

INPUT FROM HANSEN - 1ST SAMPLE EXPOSED TO AIR - 2ND TO HYDROGEN

TEMPERATURE: 1900
SOLUTE MAXIMUM SOL: .0738
METAL SURFACE TENSION: 1676

TEMPERATURE: 1920
SOLUTE MAXIMUM SOL: .1234
METAL SURFACE TENSION: 1672

OUTPUT

CALC MAX SOLUBILITY: .0558426432
CALC MAX SOLUBILITY: .0579399062

SOLUTE RADIUS N/ECOM: 5.69696332E-09
SOLUTE RADIUS N/ECOM: 5.13724582E-09

OUTPUT FOR NITROGEN AND METAL LITHIUM - L13N - DENISITY DATA

GUESS

INPUT FROM ADAMS

TEMPERATURE: 500
SOLUTE MAXIMUM SOL: 1.25E-03
METAL SURFACE TENSION: 390

TEMPERATURE: 600
SOLUTE MAXIMUM SOL: 5.95E-03
METAL SURFACE TENSION: 374

TEMPERATURE: 700
SOLUTE MAXIMUM SOL: .0182
METAL SURFACE TENSION: 368

OUTPUT

CALC MAX SOLUBILITY: .0779842498
CALC MAX SOLUBILITY: .130182474
CALC MAX SOLUBILITY: .179151631

SOLUTE RADIUS N/ECOM: 9.70228831E-09
SOLUTE RADIUS N/ECOM: 9.50261636E-09
SOLUTE RADIUS N/ECOM: 9.1491775E-09

INPUT FROM ADAMS

TEMPERATURE: 570
SOLUTE MAXIMUM SOL: 7.5E-04
METAL SURFACE TENSION: 386

TEMPERATURE: 670
SOLUTE MAXIMUM SOL: 6.7E-03
METAL SURFACE TENSION: 370

TEMPERATURE: 770
SOLUTE MAXIMUM SOL: .0375
METAL SURFACE TENSION: 354

TEMPERATURE: 870
SOLUTE MAXIMUM SOL: .065
METAL SURFACE TENSION: 338

OUTPUT

CALC MAX SOLUBILITY: .109155262
CALC MAX SOLUBILITY: .164264071
CALC MAX SOLUBILITY: .222298808
CALC MAX SOLUBILITY: .280624795

SOLUTE RADIUS N/ECOM: 1.08032831E-08
SOLUTE RADIUS N/ECOM: 9.97815086E-09
SOLUTE RADIUS N/ECOM: 8.85706763E-09
SOLUTE RADIUS N/ECOM: 8.79090756E-09

INPUT FROM HANSEN

TEMPERATURE: 520
SOLUTE MAXIMUM SOL: 2E-04
METAL SURFACE TENSION: 394

TEMPERATURE: 620
SOLUTE MAXIMUM SOL: 5.9E-03
METAL SURFACE TENSION: 378

TEMPERATURE: 720
SOLUTE MAXIMUM SOL: 6.5E-03
METAL SURFACE TENSION: 362

OUTPUT

CALC MAX SOLUBILITY: .0838870775
CALC MAX SOLUBILITY: .136129046
CALC MAX SOLUBILITY: .193108846

SOLUTE RADIUS N/ECOM: 1.11118199E-08
SOLUTE RADIUS N/ECOM: 9.61635802E-09
SOLUTE RADIUS N/ECOM: 1.04890507E-08

OUTPUT FOR NITROGEN AND METAL MOLYBDENUM - Mo₂N - DENSITY
GUESS - S.T. UNSURE

INPUT FROM HERMAN

TEMPERATURE: 2090
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 985

TEMPERATURE: 2180
SOLUTE MAXIMUM SOL: .25
METAL SURFACE TENSION: 1008

TEMPERATURE: 3250
SOLUTE MAXIMUM SOL: .3
METAL SURFACE TENSION: 1220

OUTPUT

CALC MAX SOLUBILITY: .214056308
CALC MAX SOLUBILITY: .220383874
CALC MAX SOLUBILITY: .292930546

SOLUTE RADIUS N/ECOM: 6.12456891E-09
SOLUTE RADIUS N/ECOM: 5.73864148E-09
SOLUTE RADIUS N/ECOM: 5.93544777E-09

OUTPUT FOR NITROGEN AND METAL SILICON - Si3N4 - DENSITY GUESS

INPUT FROM SCARCE

TEMPERATURE: 2000
SOLUTE MAXIMUM SOL: 7.5E-04
METAL SURFACE TENSION: 700

TEMPERATURE: 2200
SOLUTE MAXIMUM SOL: 2.7E-03
METAL SURFACE TENSION: 680

TEMPERATURE: 2500
SOLUTE MAXIMUM SOL: .0133
METAL SURFACE TENSION: 650

TEMPERATURE: 2700
SOLUTE MAXIMUM SOL: .0313
METAL SURFACE TENSION: 630

TEMPERATURE: 2900
SOLUTE MAXIMUM SOL: .0653
METAL SURFACE TENSION: 610

OUTPUT

CALC MAX SOLUBILITY: .31829045
CALC MAX SOLUBILITY: .363860687
CALC MAX SOLUBILITY: .427237108
CALC MAX SOLUBILITY: .4661751
CALC MAX SOLUBILITY: .502578998

SOLUTE RADIUS N/ECOM: 1.50271963E-08
SOLUTE RADIUS N/ECOM: 1.44977102E-08
SOLUTE RADIUS N/ECOM: 1.35094648E-08
SOLUTE RADIUS N/ECOM: 1.27700481E-08
SOLUTE RADIUS N/ECOM: 1.19371429E-08

OUTPUT FOR NITROGEN AND METAL TITANIUM - TiN

INPUT FROM HANSEN

TEMPERATURE: 2330
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 1518

TEMPERATURE: 2484
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 1486

TEMPERATURE: 2565
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 1472

TEMPERATURE: 2830
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1419

OUTPUT

CALC MAX SOLUBILITY: .118724025
CALC MAX SOLUBILITY: .141323311
CALC MAX SOLUBILITY: .153039098
CALC MAX SOLUBILITY: .193972531

SOLUTE RADIUS N/ECOM: 7.10684687E-09
SOLUTE RADIUS N/ECOM: 6.5021595E-09
SOLUTE RADIUS N/ECOM: 6.02588117E-09
SOLUTE RADIUS N/ECOM: 5.93775833E-09

OUTPUT FOR OXYGEN AND METAL ANTIMONY - Sb2O3

INPUT FROM JACOB

TEMPERATURE: 1000
SOLUTE MAXIMUM SOL: 1.79E-04
METAL SURFACE TENSION: 370

TEMPERATURE: 1100
SOLUTE MAXIMUM SOL: 5.68E-04
METAL SURFACE TENSION: 365

TEMPERATURE: 1175
SOLUTE MAXIMUM SOL: 1.18E-03
METAL SURFACE TENSION: 358

OUTPUT

CALC MAX SOLUBILITY: .298135388
CALC MAX SOLUBILITY: .33779324
CALC MAX SOLUBILITY: .369147252

SOLUTE RADIUS N/ECOM: 1.60044491E-08
SOLUTE RADIUS N/ECOM: 1.57286733E-08
SOLUTE RADIUS N/ECOM: 1.55906038E-08

OUTPUT FOR OXYGEN AND METAL BARIUM - BaO2

INPUT FROM HANSEN

TEMPERATURE: 1000
SOLUTE MAXIMUM SOL: .167
METAL SURFACE TENSION: 255

TEMPERATURE: 1170
SOLUTE MAXIMUM SOL: .211
METAL SURFACE TENSION: 250

TEMPERATURE: 1370
SOLUTE MAXIMUM SOL: .277
METAL SURFACE TENSION: 245

TEMPERATURE: 1520
SOLUTE MAXIMUM SOL: .318
METAL SURFACE TENSION: 237

OUTPUT

CALC MAX SOLUBILITY: .434281657
CALC MAX SOLUBILITY: .497134049
CALC MAX SOLUBILITY: .557145038
CALC MAX SOLUBILITY: .60050071

SOLUTE RADIUS N/ECOM: 8.78033063E-09
SOLUTE RADIUS N/ECOM: 8.94327844E-09
SOLUTE RADIUS N/ECOM: 8.87971006E-09
SOLUTE RADIUS N/ECOM: 8.98394739E-09

OUTPUT FOR OXYGEN AND METAL BISMUTH - BiO

INPUT FROM GRIFFITH

TEMPERATURE: 670
SOLUTE MAXIMUM SOL: 3.32E-05
METAL SURFACE TENSION: 360

TEMPERATURE: 770
SOLUTE MAXIMUM SOL: 1.51E-04
METAL SURFACE TENSION: 357

TEMPERATURE: 870
SOLUTE MAXIMUM SOL: 4.73E-04
METAL SURFACE TENSION: 353

TEMPERATURE: 970
SOLUTE MAXIMUM SOL: 1.23E-03
METAL SURFACE TENSION: 348

TEMPERATURE: 1020
SOLUTE MAXIMUM SOL: 1.83E-03
METAL SURFACE TENSION: 346

OUTPUT

CALC MAX SOLUBILITY: .17248214
CALC MAX SOLUBILITY: .219483917
CALC MAX SOLUBILITY: .265237297
CALC MAX SOLUBILITY: .309297132
CALC MAX SOLUBILITY: .329718085

SOLUTE RADIUS N/ECOM: 1.45198194E-08
SOLUTE RADIUS N/ECOM: 1.44375104E-08
SOLUTE RADIUS N/ECOM: 1.43968803E-08
SOLUTE RADIUS N/ECOM: 1.43232327E-08
SOLUTE RADIUS N/ECOM: 1.42867751E-08

OUTPUT FOR OXYGEN AND METAL CALCIUM - DELTA H FOR CaO -
DENSITY FOR CaO2

INPUT FROM HANSEN

TEMPERATURE: 1110
SOLUTE MAXIMUM SOL: 1.5E-03
METAL SURFACE TENSION: 326

TEMPERATURE: 1620
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 300

OUTPUT

CALC MAX SOLUBILITY: .382654602
CALC MAX SOLUBILITY: .545687126

SOLUTE RADIUS N/ECOM: 1.55944207E-08
SOLUTE RADIUS N/ECOM: 1.16865981E-08

OUTPUT FOR OXYGEN AND METAL CESIUM - Cs2O

INPUT FROM ADAMS

TEMPERATURE: 320
SOLUTE MAXIMUM SOL: .197
METAL SURFACE TENSION: 67.75

TEMPERATURE: 420
SOLUTE MAXIMUM SOL: .227
METAL SURFACE TENSION: 63.05

TEMPERATURE: 520
SOLUTE MAXIMUM SOL: .256
METAL SURFACE TENSION: 58.35

TEMPERATURE: 620
SOLUTE MAXIMUM SOL: .268
METAL SURFACE TENSION: 53.65

TEMPERATURE: 720

SOLUTE MAXIMUM SOL: .304
METAL SURFACE TENSION: 48.95

OUTPUT

CALC MAX SOLUBILITY: .500325541
CALC MAX SOLUBILITY: .612005459
CALC MAX SOLUBILITY: .692792318
CALC MAX SOLUBILITY: .753495362
CALC MAX SOLUBILITY: .800618201

SOLUTE RADIUS N/ECOM: 9.18058744E-09
SOLUTE RADIUS N/ECOM: 1.04161576E-08
SOLUTE RADIUS N/ECOM: 1.1549024E-08
SOLUTE RADIUS N/ECOM: 1.2928527E-08
SOLUTE RADIUS N/ECOM: 1.38700967E-08

OUTPUT FOR OXYGEN AND METAL CHROMIUM - Cr2O3

INPUT FROM HANSEN - CHECKS ONE SOURCE

TEMPERATURE: 2100
SOLUTE MAXIMUM SOL: .02
METAL SURFACE TENSION: 1610

TEMPERATURE: 2173
SOLUTE MAXIMUM SOL: .03
METAL SURFACE TENSION: 1600

TEMPERATURE: 2373
SOLUTE MAXIMUM SOL: .04
METAL SURFACE TENSION: 1590

TEMPERATURE: 2473
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 1580

OUTPUT

CALC MAX SOLUBILITY: .0814604775
CALC MAX SOLUBILITY: .0899642126
CALC MAX SOLUBILITY: .111739947
CALC MAX SOLUBILITY: .123719979

SOLUTE RADIUS N/ECOM: 7.48653386E-09
SOLUTE RADIUS N/ECOM: 7.2325886E-09
SOLUTE RADIUS N/ECOM: 7.2641667E-09
SOLUTE RADIUS N/ECOM: 7.17659433E-09

OUTPUT FOR OXYGEN AND METAL COBALT - CoO

INPUT FROM HANSEN

TEMPERATURE: 1720
SOLUTE MAXIMUM SOL: 8.47E-03
METAL SURFACE TENSION: 1855

TEMPERATURE: 1760
SOLUTE MAXIMUM SOL: .02
METAL SURFACE TENSION: 1845

TEMPERATURE: 1820
SOLUTE MAXIMUM SOL: .04
METAL SURFACE TENSION: 1830

OUTPUT

CALC MAX SOLUBILITY: .0293766981
CALC MAX SOLUBILITY: .0324259074
CALC MAX SOLUBILITY: .0372984734

SOLUTE RADIUS N/ECOM: 6.97092786E-09
SOLUTE RADIUS N/ECOM: 6.40239158E-09
SOLUTE RADIUS N/ECOM: 5.92987644E-09

INPUT FROM HANSEN - FROM RUSSIAN

TEMPERATURE: 1820
SOLUTE MAXIMUM SOL: 7E-03
METAL SURFACE TENSION: 1830

TEMPERATURE: 1920
SOLUTE MAXIMUM SOL: .01
METAL SURFACE TENSION: 1810

OUTPUT

CALC MAX SOLUBILITY: .0372984734
CALC MAX SOLUBILITY: .0458014329

SOLUTE RADIUS N/ECOM: 7.36232755E-09
SOLUTE RADIUS N/ECOM: 7.32516738E-09

OUTPUT FOR OXYGEN AND METAL COPPER - Cu₂O

INPUT FROM PARLEE

TEMPERATURE: 1223
SOLUTE MAXIMUM SOL: 6.99E-03
METAL SURFACE TENSION: 1310

OUTPUT

CALC MAX SOLUBILITY: .0300916688

SOLUTE RADIUS N/ECOM: 7.13419739E-09

HERE OUTPUT FOR OXYGEN AND METAL COPPER - Cu₂O - DIFF DELTA H USED

INPUT FROM HANSEN

TEMPERATURE: 1373
SOLUTE MAXIMUM SOL: .023
METAL SURFACE TENSION: 1290

TEMPERATURE: 1473
SOLUTE MAXIMUM SOL: .067
METAL SURFACE TENSION: 1280

OUTPUT

CALC MAX SOLUBILITY: .0462772682
CALC MAX SOLUBILITY: .0582931772

SOLUTE RADIUS N/ECOM: 6.64086525E-09
SOLUTE RADIUS N/ECOM: 5.84531378E-09

OUTPUT FOR OXYGEN AND METAL GALLIUM - Ga₂O₃

INPUT FROM ALCOCK

TEMPERATURE: 1050
SOLUTE MAXIMUM SOL: 1.72E-05
METAL SURFACE TENSION: 642.5

TEMPERATURE: 1150
SOLUTE MAXIMUM SOL: 7.02E-05
METAL SURFACE TENSION: 632.4

TEMPERATURE: 1250
SOLUTE MAXIMUM SOL: 2.29E-04
METAL SURFACE TENSION: 622.3

TEMPERATURE: 1350
SOLUTE MAXIMUM SOL: 6.27E-04
METAL SURFACE TENSION: 612.2

OUTPUT

CALC MAX SOLUBILITY: .135140914
CALC MAX SOLUBILITY: .165518421
CALC MAX SOLUBILITY: .196252998
CALC MAX SOLUBILITY: .226896477

SOLUTE RADIUS N/ECOM: 1.40331989E-08
SOLUTE RADIUS N/ECOM: 1.38216484E-08
SOLUTE RADIUS N/ECOM: 1.35989958E-08
SOLUTE RADIUS N/ECOM: 1.33650867E-08

INPUT FROM STEVENSON

TEMPERATURE: 1023
SOLUTE MAXIMUM SOL: 6.59E-05
METAL SURFACE TENSION: 645

TEMPERATURE: 1123
SOLUTE MAXIMUM SOL: 1.8E-04
METAL SURFACE TENSION: 635

TEMPERATURE: 1223
SOLUTE MAXIMUM SOL: 4.16E-04
METAL SURFACE TENSION: 625

TEMPERATURE: 1323
SOLUTE MAXIMUM SOL: 6.02E-04
METAL SURFACE TENSION: 615

OUTPUT

CALC MAX SOLUBILITY: .127166971
CALC MAX SOLUBILITY: .157317295
CALC MAX SOLUBILITY: .187961057
CALC MAX SOLUBILITY: .218612516

SOLUTE RADIUS N/ECOM: 1.2950759E-08

SOLUTE RADIUS N/ECOM: 1.29420881E-08
SOLUTE RADIUS N/ECOM: 1.2935435E-08
SOLUTE RADIUS N/ECOM: 1.32369747E-08

OUTPUT FOR OXYGEN AND METAL GERMANIUM GeO₂

INPUT FROM JACOB

TEMPERATURE: 1230
SOLUTE MAXIMUM SOL: 9.55E-04
METAL SURFACE TENSION: 670

TEMPERATURE: 1330
SOLUTE MAXIMUM SOL: 2.37E-03
METAL SURFACE TENSION: 600

TEMPERATURE: 1400
SOLUTE MAXIMUM SOL: 4.16E-03
METAL SURFACE TENSION: 550

OUTPUT

CALC MAX SOLUBILITY: .168356365
CALC MAX SOLUBILITY: .228649965
CALC MAX SOLUBILITY: .276659041

SOLUTE RADIUS N/ECOM: 1.18415789E-08
SOLUTE RADIUS N/ECOM: 1.21318461E-08
SOLUTE RADIUS N/ECOM: 1.23806968E-08

OUTPUT FOR OXYGEN AND METAL HAFNIUM - HfO₂ - S.T. UNSURE

INPUT FROM KARNILOV - RUSSIAN

TEMPERATURE: 2570
SOLUTE MAXIMUM SOL: .3
METAL SURFACE TENSION: 1590

TEMPERATURE: 2670
SOLUTE MAXIMUM SOL: .35
METAL SURFACE TENSION: 1580

TEMPERATURE: 2770
SOLUTE MAXIMUM SOL: .4
METAL SURFACE TENSION: 1570

TEMPERATURE: 2860
SOLUTE MAXIMUM SOL: .45
METAL SURFACE TENSION: 1560

TEMPERATURE: 2950
SOLUTE MAXIMUM SOL: .5
METAL SURFACE TENSION: 1550

OUTPUT

CALC MAX SOLUBILITY: .132180321
CALC MAX SOLUBILITY: .144345132
CALC MAX SOLUBILITY: .156630671
CALC MAX SOLUBILITY: .167949861
CALC MAX SOLUBILITY: .179321971

SOLUTE RADIUS N/ECOM: 4.62338141E-09
SOLUTE RADIUS N/ECOM: 4.41436593E-09
SOLUTE RADIUS N/ECOM: 4.2139569E-09
SOLUTE RADIUS N/ECOM: 4.00999337E-09
SOLUTE RADIUS N/ECOM: 3.80663532E-09

OUTPUT FOR OXYGEN AND METAL INDIUM - In2O3

INPUT FROM JACOB

TEMPERATURE: 920
SOLUTE MAXIMUM SOL: 3.92E-04
METAL SURFACE TENSION: 570

TEMPERATURE: 1000
SOLUTE MAXIMUM SOL: 1.01E-03
METAL SURFACE TENSION: 500

TEMPERATURE: 1100
SOLUTE MAXIMUM SOL: 2.71E-03
METAL SURFACE TENSION: 486

OUTPUT

CALC MAX SOLUBILITY: .131796885
CALC MAX SOLUBILITY: .194871358
CALC MAX SOLUBILITY: .235719503

SOLUTE RADIUS N/ECOM: 1.17927624E-08
SOLUTE RADIUS N/ECOM: 1.23098805E-08
SOLUTE RADIUS N/ECOM: 1.21222983E-08

OUTPUT FOR OXYGEN AND METAL IRON Fe(.947)O...WUSTITE

INPUT FROM WRIDT - CHECKS ONE SOURCE

TEMPERATURE: 1820
SOLUTE MAXIMUM SOL: 6.28E-03
METAL SURFACE TENSION: 1795

TEMPERATURE: 1920
SOLUTE MAXIMUM SOL: 9.77E-03
METAL SURFACE TENSION: 1785

TEMPERATURE: 1970
SOLUTE MAXIMUM SOL: .0119
METAL SURFACE TENSION: 1780

OUTPUT

CALC MAX SOLUBILITY: .0397199269
CALC MAX SOLUBILITY: .0477942015
CALC MAX SOLUBILITY: .0520593745

SOLUTE RADIUS N/ECOM: 7.51462534E-09
SOLUTE RADIUS N/ECOM: 7.39489738E-09
SOLUTE RADIUS N/ECOM: 7.33952575E-09

OUTPUT FOR OXYGEN AND METAL LEAD - PbO

INPUT FROM RAPP

TEMPERATURE: 1050
SOLUTE MAXIMUM SOL: 3.44E-04
METAL SURFACE TENSION: 420

TEMPERATURE: 1150
SOLUTE MAXIMUM SOL: 1E-03
METAL SURFACE TENSION: 415

OUTPUT

CALC MAX SOLUBILITY: .270270353

CALC MAX SOLUBILITY: .307173218

SOLUTE RADIUS N/ECOM: 1.47984137E-08

SOLUTE RADIUS N/ECOM: 1.45002913E-08

INPUT FROM HANSEN

TEMPERATURE: 670

SOLUTE MAXIMUM SOL: 1.3E-04

METAL SURFACE TENSION: 445

TEMPERATURE: 770

SOLUTE MAXIMUM SOL: 2.6E-04

METAL SURFACE TENSION: 440

TEMPERATURE: 870

SOLUTE MAXIMUM SOL: 5.8E-04

METAL SURFACE TENSION: 435

TEMPERATURE: 970

SOLUTE MAXIMUM SOL: 1.17E-03

METAL SURFACE TENSION: 430

TEMPERATURE: 1070

SOLUTE MAXIMUM SOL: 2.33E-03

METAL SURFACE TENSION: 425

OUTPUT

CALC MAX SOLUBILITY: .113901893

CALC MAX SOLUBILITY: .154270697

CALC MAX SOLUBILITY: .194871358

CALC MAX SOLUBILITY: .234580578

CALC MAX SOLUBILITY: .272760282

SOLUTE RADIUS N/ECOM: 1.216475E-08

SOLUTE RADIUS N/ECOM: 1.25966901E-08

SOLUTE RADIUS N/ECOM: 1.27952526E-08

SOLUTE RADIUS N/ECOM: 1.29333516E-08

SOLUTE RADIUS N/ECOM: 1.29474644E-08

INPUT FROM HANSEN

TEMPERATURE: 870

SOLUTE MAXIMUM SOL: 2E-04

METAL SURFACE TENSION: 435

TEMPERATURE: 970

SOLUTE MAXIMUM SOL: 6E-04

METAL SURFACE TENSION: 430

TEMPERATURE: 1030
SOLUTE MAXIMUM SOL: 1E-03
METAL SURFACE TENSION: 427

OUTPUT

CALC MAX SOLUBILITY: .194871358
CALC MAX SOLUBILITY: .234580578
CALC MAX SOLUBILITY: .257698244

SOLUTE RADIUS N/ECOM: 1.36787569E-08
SOLUTE RADIUS N/ECOM: 1.35579941E-08
SOLUTE RADIUS N/ECOM: 1.35287145E-08

INPUT FROM ALCOCK

TEMPERATURE: 780
SOLUTE MAXIMUM SOL: 7.4E-05
METAL SURFACE TENSION: 439

TEMPERATURE: 870
SOLUTE MAXIMUM SOL: 3.18E-04
METAL SURFACE TENSION: 435

TEMPERATURE: 970
SOLUTE MAXIMUM SOL: 1.36E-03
METAL SURFACE TENSION: 430

OUTPUT

CALC MAX SOLUBILITY: .158675993
CALC MAX SOLUBILITY: .194871358
CALC MAX SOLUBILITY: .234580578

SOLUTE RADIUS N/ECOM: 1.36245349E-08
SOLUTE RADIUS N/ECOM: 1.33011629E-08
SOLUTE RADIUS N/ECOM: 1.27883906E-08

INPUT FROM CHARLE - GERMAN

TEMPERATURE: 1000
SOLUTE MAXIMUM SOL: 1.73E-03
METAL SURFACE TENSION: 428

TEMPERATURE: 1100
SOLUTE MAXIMUM SOL: 5.01E-03
METAL SURFACE TENSION: 423

TEMPERATURE: 1143
SOLUTE MAXIMUM SOL: 7.47E-03
METAL SURFACE TENSION: 421

OUTPUT

CALC MAX SOLUBILITY: .246617731
CALC MAX SOLUBILITY: .284283499
CALC MAX SOLUBILITY: .299769366

SOLUTE RADIUS N/ECOM: 1.27754897E-08
SOLUTE RADIUS N/ECOM: 1.22997597E-08
SOLUTE RADIUS N/ECOM: 1.20843782E-08

OUTPUT FOR OXYGEN AND METAL LEAD - PbO - NEW DELTA H

INPUT FROM RAPP

TEMPERATURE: 1250
SOLUTE MAXIMUM SOL: 2.45E-03
METAL SURFACE TENSION: 410

TEMPERATURE: 1350
SOLUTE MAXIMUM SOL: 5.47E-03
METAL SURFACE TENSION: 405

OUTPUT

CALC MAX SOLUBILITY: .342038266
CALC MAX SOLUBILITY: .374842484

SOLUTE RADIUS N/ECOM: 1.41887432E-08
SOLUTE RADIUS N/ECOM: 1.38095052E-08

INPUT FROM HANSEN

TEMPERATURE: 1170
SOLUTE MAXIMUM SOL: 4.94E-03
METAL SURFACE TENSION: 420

OUTPUT

CALC MAX SOLUBILITY: .309083268

SOLUTE RADIUS N/ECOM: 1.27472022E-08

INPUT FROM CHARLE - GERMAN

TEMPERATURE: 1240
SOLUTE MAXIMUM SOL: .0187
METAL SURFACE TENSION: 416

TEMPERATURE: 1340
SOLUTE MAXIMUM SOL: .0346

METAL SURFACE TENSION: 411

OUTPUT

CALC MAX SOLUBILITY: .333767332

CALC MAX SOLUBILITY: .366697635

SOLUTE RADIUS N/ECOM: 1.14142447E-08

SOLUTE RADIUS N/ECOM: 1.09758083E-08

OUTPUT FOR OXYGEN AND METAL LITHIUM - L120

INPUT FROM ADAMS - 7

TEMPERATURE: 570

SOLUTE MAXIMUM SOL: 9.9E-05

METAL SURFACE TENSION: 386

TEMPERATURE: 670

SOLUTE MAXIMUM SOL: 4.88E-04

METAL SURFACE TENSION: 370

TEMPERATURE: 770

SOLUTE MAXIMUM SOL: 1.66E-03

METAL SURFACE TENSION: 354

TEMPERATURE: 870

SOLUTE MAXIMUM SOL: 4.25E-03

METAL SURFACE TENSION: 338

OUTPUT

CALC MAX SOLUBILITY: .109155262

CALC MAX SOLUBILITY: .164264071

CALC MAX SOLUBILITY: .222298808

CALC MAX SOLUBILITY: .280624795

SOLUTE RADIUS N/ECOM: 1.22293063E-08

SOLUTE RADIUS N/ECOM: 1.23153116E-08

SOLUTE RADIUS N/ECOM: 1.23665602E-08

SOLUTE RADIUS N/ECOM: 1.24255104E-08

INPUT FROM ASTM SPEC TECH PUBL

TEMPERATURE: 520

SOLUTE MAXIMUM SOL: 9.6E-06

METAL SURFACE TENSION: 394

TEMPERATURE: 570
SOLUTE MAXIMUM SOL: 2.05E-05
METAL SURFACE TENSION: 386

TEMPERATURE: 670
SOLUTE MAXIMUM SOL: 6.5E-05
METAL SURFACE TENSION: 370

OUTPUT

CALC MAX SOLUBILITY: .0838870775
CALC MAX SOLUBILITY: .109155262
CALC MAX SOLUBILITY: .164264071

SOLUTE RADIUS N/ECOM: 1.29419101E-08
SOLUTE RADIUS N/ECOM: 1.32324483E-08
SOLUTE RADIUS N/ECOM: 1.38478944E-08

OUTPUT FOR OXYGEN AND METAL MANGANESE - MnO

INPUT FROM HANSEN

TEMPERATURE: 1670
SOLUTE MAXIMUM SOL: 6.42E-04
METAL SURFACE TENSION: 1080

TEMPERATURE: 1770
SOLUTE MAXIMUM SOL: 9.34E-04
METAL SURFACE TENSION: 1060

TEMPERATURE: 1870
SOLUTE MAXIMUM SOL: 1.31E-03
METAL SURFACE TENSION: 1040

OUTPUT

CALC MAX SOLUBILITY: .120600948
CALC MAX SOLUBILITY: .141027142
CALC MAX SOLUBILITY: .16217619

SOLUTE RADIUS N/ECOM: 1.11737939E-08
SOLUTE RADIUS N/ECOM: 1.13115308E-08
SOLUTE RADIUS N/ECOM: 1.14497828E-08

INPUT FROM JACOB

TEMPERATURE: 1500
SOLUTE MAXIMUM SOL: 1.79E-04

METAL SURFACE TENSION: 1114

TEMPERATURE: 1600
 SOLUTE MAXIMUM SOL: 4.28E-04
 METAL SURFACE TENSION: 1094

TEMPERATURE: 1700
 SOLUTE MAXIMUM SOL: 9.22E-04
 METAL SURFACE TENSION: 1074

TEMPERATURE: 1800
 SOLUTE MAXIMUM SOL: 1.83E-03
 METAL SURFACE TENSION: 1054

TEMPERATURE: 1900
 SOLUTE MAXIMUM SOL: 3.36E-03
 METAL SURFACE TENSION: 1034

OUTPUT

CALC MAX SOLUBILITY: .0881128092
 CALC MAX SOLUBILITY: .106839146
 CALC MAX SOLUBILITY: .126641406
 CALC MAX SOLUBILITY: .147304497
 CALC MAX SOLUBILITY: .168634638

SOLUTE RADIUS N/ECOM: 1.12965187E-08
 SOLUTE RADIUS N/ECOM: 1.11625768E-08
 SOLUTE RADIUS N/ECOM: 1.10233132E-08
 SOLUTE RADIUS N/ECOM: 1.08739697E-08
 SOLUTE RADIUS N/ECOM: 1.07220499E-08

OUTPUT FOR OXYGEN AND METAL NEODYNIUM - Nd2O3 - UNSURE S.T. &
 PHASE

INPUT FROM HANSEN

TEMPERATURE: 1300
 SOLUTE MAXIMUM SOL: .05
 METAL SURFACE TENSION: 688

TEMPERATURE: 1400
 SOLUTE MAXIMUM SOL: .1
 METAL SURFACE TENSION: 678

TEMPERATURE: 1470
 SOLUTE MAXIMUM SOL: .15
 METAL SURFACE TENSION: 668

TEMPERATURE: 1540
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 658

OUTPUT

CALC MAX SOLUBILITY: .177102865
CALC MAX SOLUBILITY: .205149384
CALC MAX SOLUBILITY: .226199724
CALC MAX SOLUBILITY: .24720508

SOLUTE RADIUS N/ECOM: 7.88519322E-09
SOLUTE RADIUS N/ECOM: 7.2267062E-09
SOLUTE RADIUS N/ECOM: 6.77175473E-09
SOLUTE RADIUS N/ECOM: 6.43232399E-09

OUTPUT FOR OXYGEN AND METAL NICKEL - N10 - (1620-1725)

INPUT FROM WRIEDT

TEMPERATURE: 1620
SOLUTE MAXIMUM SOL: 4.08E-05
METAL SURFACE TENSION: 1800

TEMPERATURE: 1720
SOLUTE MAXIMUM SOL: 9.53E-05
METAL SURFACE TENSION: 1780

OUTPUT

CALC MAX SOLUBILITY: .0264035455
CALC MAX SOLUBILITY: .0338800124

SOLUTE RADIUS N/ECOM: 9.99567406E-09
SOLUTE RADIUS N/ECOM: 9.91305396E-09

OUTPUT FOR OXYGEN AND METAL NICKEL - N10 (1725-2000)

INPUT FROM WRIEDT

TEMPERATURE: 1820

SOLUTE MAXIMUM SOL: 2.03E-04
METAL SURFACE TENSION: 1760

TEMPERATURE: 1920
SOLUTE MAXIMUM SOL: 3.99E-04
METAL SURFACE TENSION: 1740

TEMPERATURE: 1970
SOLUTE MAXIMUM SOL: 5.46E-04
METAL SURFACE TENSION: 1730

OUTPUT

CALC MAX SOLUBILITY: .0422985836
CALC MAX SOLUBILITY: .0516022064
CALC MAX SOLUBILITY: .0565655932

SOLUTE RADIUS N/ECOM: 9.82722893E-09
SOLUTE RADIUS N/ECOM: 9.7396765E-09
SOLUTE RADIUS N/ECOM: 9.69386586E-09

INPUT FROM KIMORA

TEMPERATURE: 1730
SOLUTE MAXIMUM SOL: .0107
METAL SURFACE TENSION: 1778

TEMPERATURE: 1830
SOLUTE MAXIMUM SOL: .0236
METAL SURFACE TENSION: 1758

OUTPUT

CALC MAX SOLUBILITY: .034680328
CALC MAX SOLUBILITY: .0431901492

SOLUTE RADIUS N/ECOM: 6.96385033E-09
SOLUTE RADIUS N/ECOM: 6.54504834E-09

OUTPUT FOR OXYGEN AND METAL NIOBIUM - Nb2O4

INPUT FROM HANSEN

TEMPERATURE: 2640
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 1990

TEMPERATURE: 2590

SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 2000

TEMPERATURE: 2545
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 2009

TEMPERATURE: 2480
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 2021

OUTPUT

CALC MAX SOLUBILITY: .0849652463
CALC MAX SOLUBILITY: .0799992164
CALC MAX SOLUBILITY: .0756252806
CALC MAX SOLUBILITY: .0695670867

SOLUTE RADIUS N/ECOM: 6.6070913E-09
SOLUTE RADIUS N/ECOM: 5.72303118E-09
SOLUTE RADIUS N/ECOM: 5.13788889E-09
SOLUTE RADIUS N/ECOM: 4.65761065E-09

OUTPUT FOR OXYGEN AND METAL PLUTONIUM - PbO2

INPUT FROM HANSEN

TEMPERATURE: 1700
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 460

TEMPERATURE: 1920
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 445

OUTPUT

CALC MAX SOLUBILITY: .412694172
CALC MAX SOLUBILITY: .468563667

SOLUTE RADIUS N/ECOM: 9.66800292E-09
SOLUTE RADIUS N/ECOM: 8.73355594E-09

INPUT FROM HANSEN

TEMPERATURE: 1685
SOLUTE MAXIMUM SOL: .05
METAL SURFACE TENSION: 462

TEMPERATURE: 1815
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 450

TEMPERATURE: 1930
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 443

TEMPERATURE: 2040
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 437

OUTPUT

CALC MAX SOLUBILITY: .407868881
CALC MAX SOLUBILITY: .444435694
CALC MAX SOLUBILITY: .472004889
CALC MAX SOLUBILITY: .496255995

SOLUTE RADIUS N/ECOM: 1.0955037E-08
SOLUTE RADIUS N/ECOM: 1.01000445E-08
SOLUTE RADIUS N/ECOM: 9.52812782E-09
SOLUTE RADIUS N/ECOM: 9.08437101E-09

OUTPUT FOR OXYGEN AND METAL POTASSIUM - K2O

INPUT FROM ADAMS

TEMPERATURE: 370
SOLUTE MAXIMUM SOL: 2.4E-03
METAL SURFACE TENSION: 91.15

TEMPERATURE: 470
SOLUTE MAXIMUM SOL: 6.7E-03
METAL SURFACE TENSION: 84.62

TEMPERATURE: 570
SOLUTE MAXIMUM SOL: .0146
METAL SURFACE TENSION: 78.09

TEMPERATURE: 670
SOLUTE MAXIMUM SOL: .037
METAL SURFACE TENSION: 71.56

TEMPERATURE: 770
SOLUTE MAXIMUM SOL: .087
METAL SURFACE TENSION: 65.03

TEMPERATURE: 820
SOLUTE MAXIMUM SOL: .12
METAL SURFACE TENSION: 61.76

OUTPUT

CALC MAX SOLUBILITY: .446742146
CALC MAX SOLUBILITY: .554943588
CALC MAX SOLUBILITY: .638838315
CALC MAX SOLUBILITY: .7051503
CALC MAX SOLUBILITY: .75863344
CALC MAX SOLUBILITY: .781649039

SOLUTE RADIUS N/ECOM: 1.64001149E-08
SOLUTE RADIUS N/ECOM: 1.74753525E-08
SOLUTE RADIUS N/ECOM: 1.84088028E-08
SOLUTE RADIUS N/ECOM: 1.84134167E-08
SOLUTE RADIUS N/ECOM: 1.78209605E-08
SOLUTE RADIUS N/ECOM: 1.75845633E-08

OUTPUT FOR OXYGEN AND METAL SCANDIUM - Sc203

INPUT FROM KUPRASHVILI - RUSSIAN - CHECKS ONE SOURCE

TEMPERATURE: 1830
SOLUTE MAXIMUM SOL: .34
METAL SURFACE TENSION: 1600

TEMPERATURE: 2070
SOLUTE MAXIMUM SOL: .37
METAL SURFACE TENSION: 1560

TEMPERATURE: 2270
SOLUTE MAXIMUM SOL: .4
METAL SURFACE TENSION: 1520

OUTPUT

CALC MAX SOLUBILITY: .057283469
CALC MAX SOLUBILITY: .0850110274
CALC MAX SOLUBILITY: .111898826

SOLUTE RADIUS N/ECOM: 3.68147072E-09
SOLUTE RADIUS N/ECOM: 3.80675173E-09
SOLUTE RADIUS N/ECOM: 3.87695862E-09

OUTPUT FOR OXYGEN AND METAL SILICON - SiO₂ - TWO WIDELY DIFFER
SOURCES

INPUT FROM HANSEN

TEMPERATURE: 1650
SOLUTE MAXIMUM SOL: .24
METAL SURFACE TENSION: 735

TEMPERATURE: 1770
SOLUTE MAXIMUM SOL: .3
METAL SURFACE TENSION: 723

TEMPERATURE: 1850
SOLUTE MAXIMUM SOL: .4
METAL SURFACE TENSION: 711

OUTPUT

CALC MAX SOLUBILITY: .232932478
CALC MAX SOLUBILITY: .262881631
CALC MAX SOLUBILITY: .28448919

SOLUTE RADIUS N/ECOM: 5.93213981E-09
SOLUTE RADIUS N/ECOM: 5.68995991E-09
SOLUTE RADIUS N/ECOM: 5.11742038E-09

INPUT FROM ARKHAROV - RUSSIAN

TEMPERATURE: 1688
SOLUTE MAXIMUM SOL: 3.98E-05
METAL SURFACE TENSION: 732

TEMPERATURE: 1873
SOLUTE MAXIMUM SOL: 9.77E-04
METAL SURFACE TENSION: 708

OUTPUT

CALC MAX SOLUBILITY: .242102604
CALC MAX SOLUBILITY: .290432322

SOLUTE RADIUS N/ECOM: 1.60196867E-08
SOLUTE RADIUS N/ECOM: 1.41916974E-08

OUTPUT FOR OXYGEN AND METAL SODIUM - Na₂O

INPUT FROM ADAMS

TEMPERATURE:	370
SOLUTE MAXIMUM SOL:	4E-06
METAL SURFACE TENSION:	202.1
TEMPERATURE:	470
SOLUTE MAXIMUM SOL:	3.9E-05
METAL SURFACE TENSION:	192.9
TEMPERATURE:	570
SOLUTE MAXIMUM SOL:	1.85E-04
METAL SURFACE TENSION:	183.7
TEMPERATURE:	670
SOLUTE MAXIMUM SOL:	5.35E-04
METAL SURFACE TENSION:	174.5
TEMPERATURE:	770
SOLUTE MAXIMUM SOL:	1.17E-03
METAL SURFACE TENSION:	165.3
TEMPERATURE:	820
SOLUTE MAXIMUM SOL:	1.62E-03
METAL SURFACE TENSION:	156.1

OUTPUT

CALC MAX SOLUBILITY:	.167531969
CALC MAX SOLUBILITY:	.261209459
CALC MAX SOLUBILITY:	.34849695
CALC MAX SOLUBILITY:	.426611855
CALC MAX SOLUBILITY:	.495510484
CALC MAX SOLUBILITY:	.53651831
SOLUTE RADIUS N/ECOM:	1.58096757E-08
SOLUTE RADIUS N/ECOM:	1.64831766E-08
SOLUTE RADIUS N/ECOM:	1.71156376E-08
SOLUTE RADIUS N/ECOM:	1.78243656E-08
SOLUTE RADIUS N/ECOM:	1.85852489E-08
SOLUTE RADIUS N/ECOM:	1.92546908E-08

INPUT FROM HANSEN

TEMPERATURE:	520
SOLUTE MAXIMUM SOL:	2.4E-04
METAL SURFACE TENSION:	188.3
TEMPERATURE:	645
SOLUTE MAXIMUM SOL:	5E-04

METAL SURFACE TENSION: 176.8

TEMPERATURE: 705
SOLUTE MAXIMUM SOL: 1E-03
METAL SURFACE TENSION: 171.9

TEMPERATURE: 805
SOLUTE MAXIMUM SOL: 2.5E-03
METAL SURFACE TENSION: 162.1

OUTPUT

CALC MAX SOLUBILITY: .305924076
CALC MAX SOLUBILITY: .407969548
CALC MAX SOLUBILITY: .450441938
CALC MAX SOLUBILITY: .517556948

SOLUTE RADIUS N/ECOM: 1.59004477E-08
SOLUTE RADIUS N/ECOM: 1.74523812E-08
SOLUTE RADIUS N/ECOM: 1.76404019E-08
SOLUTE RADIUS N/ECOM: 1.80782469E-08

OUTPUT FOR OXYGEN AND METAL TIN - SnO2

INPUT FROM PARLEE

TEMPERATURE: 1223
SOLUTE MAXIMUM SOL: 5.66E-03
METAL SURFACE TENSION: 470

TEMPERATURE: 1523
SOLUTE MAXIMUM SOL: .022
METAL SURFACE TENSION: 440

OUTPUT

CALC MAX SOLUBILITY: .284510988
CALC MAX SOLUBILITY: .388697241

SOLUTE RADIUS N/ECOM: 1.21611544E-08
SOLUTE RADIUS N/ECOM: 1.20462463E-08

INPUT FROM ALCOCK

TEMPERATURE: 810
SOLUTE MAXIMUM SOL: 1.3E-05
METAL SURFACE TENSION: 525

TEMPERATURE: 870
SOLUTE MAXIMUM SOL: 4.1E-05
METAL SURFACE TENSION: 519

TEMPERATURE: 970
SOLUTE MAXIMUM SOL: 2.07E-04
METAL SURFACE TENSION: 509

OUTPUT

CALC MAX SOLUBILITY: .120033641
CALC MAX SOLUBILITY: .142100597
CALC MAX SOLUBILITY: .179722116

SOLUTE RADIUS N/ECOM: 1.38080813E-08
SOLUTE RADIUS N/ECOM: 1.36383456E-08
SOLUTE RADIUS N/ECOM: 1.33253849E-08

INPUT FROM RAPP

TEMPERATURE: 1020
SOLUTE MAXIMUM SOL: 4.85E-04
METAL SURFACE TENSION: 504

TEMPERATURE: 1120
SOLUTE MAXIMUM SOL: 1.82E-03
METAL SURFACE TENSION: 494

TEMPERATURE: 1220
SOLUTE MAXIMUM SOL: 5.49E-03
METAL SURFACE TENSION: 484

OUTPUT

CALC MAX SOLUBILITY: .198657021
CALC MAX SOLUBILITY: .236295952
CALC MAX SOLUBILITY: .27318434

SOLUTE RADIUS N/ECOM: 1.30247447E-08
SOLUTE RADIUS N/ECOM: 1.25344819E-08
SOLUTE RADIUS N/ECOM: 1.20044915E-08

OUTPUT FOR OXYGEN AND METAL TITANIUM - T10

INPUT FROM HANSEN

TEMPERATURE: 2085
SOLUTE MAXIMUM SOL: .05

METAL SURFACE TENSION: 1568

TEMPERATURE: 2135
SOLUTE MAXIMUM SOL: .1
METAL SURFACE TENSION: 1558

TEMPERATURE: 2180
SOLUTE MAXIMUM SOL: .15
METAL SURFACE TENSION: 1548

TEMPERATURE: 2205
SOLUTE MAXIMUM SOL: .2
METAL SURFACE TENSION: 1541

OUTPUT

CALC MAX SOLUBILITY: .085452841
CALC MAX SOLUBILITY: .0919174643
CALC MAX SOLUBILITY: .0980193585
CALC MAX SOLUBILITY: .101685204

SOLUTE RADIUS N/ECOM: 6.61477206E-09
SOLUTE RADIUS N/ECOM: 5.88716816E-09
SOLUTE RADIUS N/ECOM: 5.41718356E-09
SOLUTE RADIUS N/ECOM: 5.02948451E-09

OUTPUT FOR OXYGEN AND METAL URANIUM - UO₂ - S.T. UNSURE

INPUT FROM HANSEN

TEMPERATURE: 1380
SOLUTE MAXIMUM SOL: 8.27E-06
METAL SURFACE TENSION: 1500

TEMPERATURE: 1470
SOLUTE MAXIMUM SOL: 9.49E-06
METAL SURFACE TENSION: 1485

TEMPERATURE: 1670
SOLUTE MAXIMUM SOL: 1.41E-05
METAL SURFACE TENSION: 1455

TEMPERATURE: 1870
SOLUTE MAXIMUM SOL: 1.95E-05
METAL SURFACE TENSION: 1425

TEMPERATURE: 2070
SOLUTE MAXIMUM SOL: 2.9E-05

METAL SURFACE TENSION: 1395

TEMPERATURE: 2270
SOLUTE MAXIMUM SOL: 4.96E-05
METAL SURFACE TENSION: 1365

OUTPUT

CALC MAX SOLUBILITY: .0285741907
CALC MAX SOLUBILITY: .0367283218
CALC MAX SOLUBILITY: .0578595802
CALC MAX SOLUBILITY: .0827047384
CALC MAX SOLUBILITY: .110332597
CALC MAX SOLUBILITY: .139900832

SOLUTE RADIUS N/ECOM: 1.08748581E-08
SOLUTE RADIUS N/ECOM: 1.12139018E-08
SOLUTE RADIUS N/ECOM: 1.18665315E-08
SOLUTE RADIUS N/ECOM: 1.25029777E-08
SOLUTE RADIUS N/ECOM: 1.30497592E-08
SOLUTE RADIUS N/ECOM: 1.34555084E-08

Appendix B Experimental Data

This appendix contains the experimental data used to analyze the theoretical equations. The appendix contains solute activity coefficient data, solute maximum solubility data, and solute solubility ratio data (concentration over the square root of pressure).

The data is grouped by metals which are in alphabetical order. An example of a data entry will best serve to explain the format used:

```
j=*          Parlee  TMS AIME 1976 Vol 227 p245
7   0         0       0
```

1000 °K - 6.754 Ksol

1000 °K - 1.34E-3 Xmax

1000 °K - .01 Xsol - 1.24E-4 ACSOL

The j=* signifies the solute. If the * is 1 the solute is Hydrogen, 2 for Carbon, 3 for Nitrogen, and 4 for Oxygen. Parlee is the author of the book or article. TMS AIME is the magazine (Transactions of the Metal Society of AIME). 1976 is the year of publication, Vol 227 is the volume of the magazine, and p245 is the page number of the article.

The second row contains information in the form of four numbers which are keys. The first number tells what kind of experimental

technique was used to measure solubility data. The second number tells what kind of experimental technique was used to measure activity coefficient data. The third number tells the convention of the activity coefficient. The fourth number tells if there is anything special about the entry. The keys are explained below.

The third, fourth, and fifth lines contain data. °K signifies degrees Kelvin for all three lines. Ksol signifies solubility ratio data in units of atom fraction divided by the square root of atmospheres. Xmax signifies maximum solubility data in units of atom fraction. ACSOL is activity coefficient data. ACSOL is unit less. Xsol is solubility data for the ACSOL activity coefficient data.

Explanation of Solubility Experiment Key

- 0 - No solubility data given
- 1 - Hot volume technique
- 2 - Quenching technique
- 3 - Incipient melting of solids of known content
- 4 - Henries law technique, specific to Parlee article
- 5 - Calculation scheme, specific to Otsuka
- 6 - Melting technique, specific to Scarce
- 7 - Technique not reported
- 8 - Henries law technique, specific to Rapp
- 9 - Evolution of gas during melting of a solid sample
- 10 - EMF technique

Explination of Activity Coefficient Experiment Key

- 0 - No activity coefficient data given
- 1 - EMF technique
- 2 - Ploting of pressure verses solubility data, specific to Kor
- 3 - Computed from free energy and solubility ratio data
- 4 - Equilibrium of Hydrogen and Methane vapor, specific to
Turkdogan

Explination of Activity Coefficient Convention Key

- 0 - No activity coefficient data given
- 1 - Activity Coefficient equals one at solute infinite dilution

Explination of Unusual Data Key

- 0 - Nothing unusual about the data
- 1 - Solubility data given at one atmosphere only
- 2 - unsure of units of data
- 3 - sample exposed to Hydrogen, specific to Nitrogen data
measurements
- 4 - activity coefficient data generated by Otsuka and fellow
workers
- 5 - Unusual phase diagram, may not apply well to theory of

surface

tension theory

6 - Something strange about article, but unable to put a finger on it

9 - Unsure of activity coefficient convention

A few non-standard abbreviations were used for titles. They are:

IAN Metal - Izv Akad Nauk SSSR, Metal

TMS AIME - Trans Metal Soc AIME

Hansen (1) - "Constitution of Binary Phase Alloys"

Hansen (2) - "Constitution of Binary Phase Alloys, 1st Supplement"

Hansen (3) - "Constitution of Binary Phase Alloys, 2nd Supplement"

GTE - "The Handbook of Binary Phase Diagrams" Volume 1 &

ALUMINUM

j = 1 Hansen (2) - 39

7 0 0 1

970 °K - 1.51E-5 ksol

1070 2.96

1170 5.25

1270 8.46

j = 1 Bircumshaw, Trans Faraday Society 1935 Vol131 p51

1 0 0 1

970 °K - 1.567E-6 ksol

1070 5.574E-6

1170 1.057E-5

1270 2.004E-5

j = 2 Hansen (3) - 18

2 0 0 0

1070 °K - .0022 Xmax - 813 dyne/cm

1270 .0031 783.5

1370 .0035 768.5

ALUMINUM

j = 1 Hansen (2) - 39
7 0 0 1

970 `K - 1.51E-5 ksol
1070 2.96
1170 5.25
1270 8.46

j = 1 Bircumshaw, Trans Faraday Society 1935 Vol131 p51
1 0 0 1

970 `K - 1.567E-6 ksol
1070 5.574E-6
1170 1.057E-5
1270 2.004E-5

j = 2 Hansen (3) - 18
2 0 0 0

1070 `K - .0022 Xmax - 813 dyne/cm
1270 .0031 783.5
1370 .0035 768.5
1470 .0071 753.5

ANTIMONY

j = 2 Hansen (1) - 378
7 0 0 0

1330 `K - .00336 Xmax - 350 dyne/cm
1540 .00691 342
1600 .00956 335

j = 4 Stevenson J Electrochem Soc 1981 vol 130 p47
5 1 1 9 has Bismuth, Gallium & Indium data also

ACSOL = 5.97E5 * exp(-25020/T) T = 1023-1223 `K
Xsol = 3.96E-2 * exp(-2503/T)

1023 °K - .00338 Xsol - .0000143 ACSOL
 1123 .00420 .000126
 1223 .00504 .000778

j = 4 Otsuka Metal Trans 1979 Vol 10B p565
 0 6 1 4 has Lead data also

970 °K - .01 Xsol - 5.34E-5 ACSOL
 1070 .01 2.63E-4
 1100 .01 5.25E-4

j = 4 Otsuka Metal Trans 1981 Vol 12B p616
 0 6 1 6

agrees with Otsuka data above

j = 4 Otsuka Metal Trans 1981 Vol 12B p455
 0 6 1 4

1073 °K - .01 Xsol - 1.19E-4 ACSOL

j = 4 Stevenson J Chem Thermo 1972 Vol 11 p627
 6 1 3 0 article has Bismuth data also

1073 °K - .0210 Xsol - 0.97E-4 ACSOL
 1123 .0327 1.31
 1173 .0446 1.68
 1223 .0868 1.95

NOTE - NOT USED - incorrect reference state for
 regular solution and quasi-chemical model

j = 4 Jacob Z Metallk 1979 Vol 70 p366
 6 0 0 0

$\text{Log}(X_{\text{max}}) = -5500/T + 1.754$ $T = 1000-1175$ °K

1000 °K - .000179 Xmax - 370 dyne/cm
 1100 .000568 365
 1175 .00118 358

BARIUM

j = 1 Franzen J Less Common Metals 1978 p65
1 0 0 0

1008 °K - 6.789 ksol
1053 4.783
1113 2.895
1188 1.944
1223 1.627

j = 4 Hansen (2) - 152
7 0 0 0

1000 °K - .167 Xmax - 255 dyne/cm
1170 .211 250
1370 .277 245
1520 .318 237

BISMUTH

j = 2 Griffith J American Chemical Society 1953 Vol 75 p1832
2 0 0 0

570 °K - 2.75E-5 Xmax - 362 dyne/cm
670 3.42 360
770 4.01 357
870 4.54 353
970 5.01 348
1070 5.22 343

j = 4 Same article and Technique as above

Log(Wt Frac) = -3400/T - 0.53 T = 670-1020 °K
Equation written in units of weight
fraction. Data below in atom fraction.

670 °K - 3.322E-5 Xmax - 360 dyne/cm
770 1.515E-4 357
870 4.729E-4 353
970 1.231E-3 348
1070 1.828E-3 346

j = 4 Fitzner Z Metalk 1980 Vol 71 p178

0 1 1 0

$\ln(\text{ACSOL}) = -125315 / (RT) + 13.87 / R$ T = 950-1150 `K

NOT USED - no data on solubility of Oxygen found or recorded ???

j = 4 Stevenson J Electrochem Soc 1981 Vol 130 p47
5 1 1 9 has Antimony, Gallium and Indium data also

$\text{ACSOL} = 157.59 * \exp(-11488/T)$ T = 1023-1273`K

$\text{Xsol} = 0.34 * \exp(-6406/T)$

1023 `K - .000649 Xsol - .00209 ACSOL

1148 .00128 .00608

1273 .00222 .019

j = 4 Otsuka Metal Trans 1981 Vol 12B p427
0 6 1 4 article has Germanium data also

970 `K - .01 Xsol - 1.80E-3 ACSOL

1070 .01 5.85E-3

1170 .01 1.55E-2

j = 4 Stevenson J Cehm Thermo 1972 Vol 11 p627
6 1 3 0 article has Antimony data also

1073 `K - 1.54E-4 Xsol - .250 ACSOL

1123 1.93 .416

1173 2.63 .466

1223 3.42 .683

NOT USED - reference state not in agreement with that
of the regular solution and quasi-chemical

CALCIUM

j = 1 Hansen (2) - 241
7 0 0 0

1235 `K - .05 Xmax - 320 dyne/cm

1250 .10 319

1270 .15 318

1320 .20 315

j = 3 Hansen (1) - 403

7 0 0 0

1050 `K - .019 Xmax - 329 dyne/cm

1110 .05 326

1150 .10 324

j = 4 Hansen (2) - 244

7 0 0 0

1110 `K - .0015 Xmax - 326 dyne/cm

1620 .10 300

CERIUM

j = 2 GTE

7 0 0 2

870 `K - .355 Xmax - 1020 dyne/cm

1170 .300 1000

NOTE - surface tension data almost total guess

CESIUM

j = 4 Adams J Less Common Metals 1975 Vol 42 p1

7 0 0 0 also has Lithium data

320 `K - .197 Xmax - 67.75 dyne/cm

420 .227 63.05

520 .256 58.35

620 .268 53.65

720 .304 48.95

CHROMIUM

j = 1 Weinstein Trans Metal Soc AIME 1963 Vol 227 p285

1 0 0 1 has Cobalt, Iron, and Nickel data

2180 °K - 3.3E-3 ksol

Might contains Gibbs free energy data

j = 2 Hansen (1) - 352
7 0 0 0 unsure of surface tension data

1750 °K - .136 Xmax - 1720 dyne/cm
1830 .150 1700
1950 .200 1680
2010 .250 1660
2080 .300 1640

j = 2 GTE
7 0 0 0 unsure of surface tension data

1800 °K - .145 Xmax - 1705 dyne/cm
1850 .170 1695
1910 .200 1689
1990 .250 1673

j = 3 Humberty Trans Metal Soc AIME 1960 Vol 218 p1076
1 0 0 0 has Iron & Nickel data also
unsure surface tension data

1960 °K - .172 Xmax - 1664 dyne/cm
2000 .156 1656
2040 .142 1648
2080 .129 1640
2130 .113 1630

j = 3 Hansen (1) - 539
3 0 0 0 unsure surface tension data

1900 °K - .0738 Xmax - 1676 dyne/cm sample exposed to air
1920 .1234 1672 sample exposed to Hydrogen

j = 3 Kalinyuk I.A.N. Metal 1974 Vol 1 p18
0 0 0 0

$\log(X_{\max}) = 0.5 * \log(\text{pressure in Pascal}) - 4.69 + 2950/T$
T = 1973-2488 °K

NOT PROCESSED - found late
Might have Gibbs free energy data

j = 4 Hansen (1) - 547
0 0 0 0

2100	`K - .02	Xmax - 1610	dyne/cm
2173	.03	1600	
2373	.04	1590	
2473	.05	1580	

Believe heat of formation data also given.
Checks with Trans Metal Soc Vol 203 p253

COBALT

j = 1	Weinstein	Trans Metal Soc AIME	1963	Vol 227	p285
1 0	0	1	has Chromium, Iron, & Nickel data		

1870	`K - .00128	ksol
1970	.00148	
2070	.00172	

Might contain Gibbs free energy data.
Checks with Busch Trans Metal Soc AIME 1960 Vol 218 p490

j = 2	Hansen (2) - 211
2 0	0 0

$\log (X_{\max}) = -1093.8/T - .245$ $T = 1620-1820^{\circ}\text{K}$

1620	`K - .120	Xmax - 1880	dyne/cm
1720	.132	1855	
1820	.143	1830	

Checks with Turkdogan J Iron Steel Inst (London)
1956 Vol 182 p274

j = 3	Pehlke	Trans Metal Soc AIME	1966	Vol 236	p28

Either lost data or above is useless reference

j = 4	Hansen (1) - 487
7 0	0 0

1720	`K - .00847	Xmax - 1855	dyne/cm
1760	.020	1845	
1820	.040	1830	

j = 4	Hansen (2) - 327

7 0 0 4

1820 `K - .0070 Xmax - 1830 dyne/cm
 1870 .0088 1820
 1920 .0103 1810

Taken by Hansen from Russian Source

COPPER

j = 1 Parlee Metal Trans 1970 Vol 1 p5377
 7 0 0 1 also has Nickel data

1923 `K - 9.0E-4 ksol

j = 1 Hansen (1) - 587
 1 0 0 0

1400 `K - 3.43E-4 ksol
 1510 4.57
 1619 5.11
 1690 6.86

Checks with Bever Trans Metal Soc AIME 1942 ?????
 Bever also has Tin data.

j = 1 Degtyaren I.A.N. Metal 1970 Vol 4 p42
 1 0 1 1

Solubility predictions; as far as I can tell (article translated
 from Russian), the data from this article is extremely different
 the other three sources. The data from this source was NOT USED.

j = 2 Hansen (1) - 353
 2 0 0 0

1370 `K - 5.30E-6 Xmax - 1300 dyne/cm
 1570 7.94E-6 1282
 1770 2.65E-5 1265
 1970 1.59E-4 1247

j = 4 Otsuka Metal Trans 1981 Vol 12B p501
 0 1 1 4

1370 `K - .01 Xsol - .1323 ACSOL
 1470 .01 .2047

1550 .01 .2816
Checks with:

Fitzner	Metal Tech	1973		p273
Wilder	Trans Metal Soc AIME	1966	Vol 236	p1035
Jacob	Trans Inst Mining & Metal	1971	Vol 80	pC32
Kalkarni	Metal Trans	1973	Vol 4	p1713

j = 4 Rapp Metal Trans 1973 Vol 4 p61
7 0 0 1

NOT USED - data contained within did not correspond well with
other data found.

j = 4 Hansen (1) - 487
0 0 0 0

1373 `K - .023 Xmax - 1290 dyne/cm
1473 .067 1280

j = 4 Parlee High Temp Sci 1982 Vol 15 p55
7 0 0 0

1223`K - .00699 Xmax - 1310 dyne/cm

ERBIUM

j = 4 Hansen (2) - 402
7 0 0 5

1800 `K - .20 Xmax
1900 .25
2150 .30

NOT USED - screwy phase diagram and a total lack of
surface tension data.

GALLIUM

j = 4 Alcock J Less Common Metals 1977 Vol 53 p211
2 0 0 0

$\log (X_{\max}) = -7380/T + 2.264$ $T = 1050-1400$ `K

$$\log (ksol) = -11514/T + 1.474 \quad T = 1050-1400 \text{ } ^\circ\text{K}$$

1050	$^\circ\text{K}$	- 2.89E-10	ksol	- 1.72E-5	Xmax	- 642.5	dyne/cm
1150		2.60E-9		7.02E-5		632.4	
1250		1.64E-8		2.29E-4		622.3	
1350		7.91E-8		6.27E-4		612.2	

j = 4 Stevenson J Electrochem Soc 1980 Vol 130 p47
 5 1 1 4 has Antimony, Bismuth & Indium data

$$\begin{aligned} \text{ACSOL} &= 27450 * \exp (-30943/T) & T &= 1023-1273 \text{ } ^\circ\text{K} \\ \text{Xsol} &= 5.26 * \exp (-22528/T) \end{aligned}$$

1023	$^\circ\text{K}$	- 6.59E-5	Xsol	- 2.006E-9	ACSOL
1123		1.80E-4		2.965E-8	
1223		4.16E-4		2.822E-8	
1273		6.02E-4		7.622E-8	

GERMANIUM

j = 1 Petrushevski Izv V.U.Z. Chern Metal 1976 Vol 6 p5
 0 0 0 4

$$\log (Xsol) = 0.5 \log (\text{Hydrogen pressure in Pascal}) - 750/T - 4.97$$

$$T = 1770-1970 \text{ } ^\circ\text{K}$$

1770	$^\circ\text{K}$	- 3.73E-4	ksol
1870		3.82	
1970		3.89	

Might contain Gibbs free energy data.

j = 2 Scarce J Chem Phys 1957 Vol 30 p1551
 6 0 0 0 has Silicon data also
 surface tension data unsure due to high temp

$$\log (Xmax) = -26316/T + 6.895 \quad T = 3000-3400 \text{ } ^\circ\text{K}$$

3000	$^\circ\text{K}$	- .0133	Xmax	- 330	dyne/cm
3100		.0255		320	
3200		.0470		310	
3300		.0833		300	

j = 4 Otsuka Met Trans 1981 Vol 12B p427
 0 1 1 0

1230	$^\circ\text{K}$	- .01	Xsol	- 4.58E-5	ACSOL
1330		.01		2.66E-4	

j = 4 Jacob Metal Trans 1977 Vol 8B p669
 2 0 0 0

$\log (X_{\max}) = -6470/T + 2.24$ T = 1233-1400 °K

1230 °K	- 9.55E-4	Xmax - 670 dyne/cm
1330	2.37E-3	600
1400	4.16E-3	550

HAFNIUM

j = 2 Hansen (3) - 145
 7 0 0 5 surface tension data unsure

2480 °K	- .095	Xmax - 1600 dyne/cm
2820	.15	1560
3160	.20	1530
3400	.25	1500
3685	.30	1480

j = 2 GTE
 7 0 0 5 surface tension data unsure

2630 °K	- .05	Xmax - 1580 dyne/cm
3110	.07	1535
3680	.15	1480
4080	.30	1440

j = 4 Karnilov I.A.N. Neorg Mater 1965 Vol 1 p1778
 7 0 0 0

2570 °K	- .30	Xmax - 1590 dyne/cm
2670	.35	1580
2770	.40	1570
2860	.45	1560
2950	.50	1550

INDIUM

j = 4 Otsuka Metal Trans 1980 Vol 11B p313
 0 1 1 4

970 `K - .01 Xsol - 1.53E-7 ACSOL
 1070 .01 1.19E-6
 1170 .01 6.48E-6

j = 4 Otsuka Metal Trans 1981 Vol 12B p455
 0 1 1 4

1070 `K - .01 - 2.62E-2

NOT USED - does not compare well with other data

j = 4 Stevenson J Electrochem Soc 1980 Vol 130 p47
 5 1 1 9 has Antimony, Bismuth, & Gallium data

ACSOL = 54.598 exp (-19213/T) T = 1023-1273 `K
 Xsol = 3.287 exp (-9443/T)

1050 `K - 4.08E-4 Xsol - 6.17E-7 ACSOL
 1150 8.93E-4 3.03E-6
 1250 1.72E-3 1.15E-5

j = 4 Jacob J Less Common Metal 1977 Vol 52 p279
 2 0 0 0

log (Xmax) = -4726/T + 1.73 T = 920-1100 `K

920 `K - 3.92E-4 Xmax - 510 dyne/cm
 1000 1.01E-3 500
 1100 2.71E-3 486

IRON

j = 1 Weinstein 1963 Vol 227 p285
 1 0 0 1 has Chromium, Cobalt, & Nickel data also

1810 `K - 1.25E-3 ksol
 1910 1.43
 2000 1.60
 2100 1.77

Checks with:

Busch	Trans Metal Soc AIME	1960	Vol 218	p490
Gunji	Trans Natl Res Inst for Metals	1964	Vol 6	p202
Parlee	Metal Trans	1970	Vol 1	p5377
Pehlke	Metal Trans	1974	Vol 5	p399

j = 1 Lakomski Dokl Akad Nauk S.S.S.R 1960 Vol 147 p628
 1 0 0 2

1950 °K - 1.924E-3 ksol
 2300 1.83
 2580 1.31
 2730 1.06

j = 2 Turkogan Acta Metal 1956 Vol 4 p396
 7 0 0 0

$\log (X_{\max}) = -560/T - 0.375$ $T = 1570-1870^{\circ}\text{K}$

1570 °K - 0.1855 $X_{\max}$ - 1840 dyne/cm
 1670 0.1948 1820
 1770 0.2035 1800
 1870 0.2116 1780

Has interesting ideas on the calculation of Carbon activity.
 Did not investigate the ideas.

j = 2 Grigorovich I.A.N. Neorg Mater 1963 Vol 1 p1764
 7 0 0 0

1420 °K - .171 $X_{\max}$ - 1870 dyne/cm
 1710 .200 1812
 2300 .250 1694
 2600 .300 1634

Above for graphite - Iron equilibrium conditions

1420 °K - .171 $X_{\max}$ - 1870 dyne/cm
 1500 .200 1854
 1670 .250 1820

Above for Fe₃C - Fe equilibrium conditions

j = 3 Busch Tran Metal Soc AIME 1960 Vol 218 p490
 1 0 0 1 has Hydrogen-Iron data which checks with
 four other sources (above)
 also has Cobalt data

1870 °K - 1.576E-3 ksol

j = 3 Parlee Trans Metal Soc AIME 1958 p86
 1 0 0 1

1770 °K - 1.70E-3 ksol
 1870 1.75
 1970 1.81
 2070 1.87

2170 1.93

Checks with

Humberty Trans Metal Soc AIME 1960 Vol 218 p1076
 Pehlke Trans Metal Soc AIME 1960 Vol 218 p1088

j = 3 Dodd Trans Metal Soc 1961 Vol 221 p233
 2 0 0 1

1820 °K - 1.60E-3 ksol

j = 3 Chem Abstracts 1975 abstract #100266h
 7 0 0 1

1700 °K - 1.05E-3 ksol

1800 1.28

1900 1.53

j = 3 Uda Trans Natl Res Inst Metals 1968 Vol 10 p21
 2 0 0 0

2470 °K - 2.145E-3 ksol

j = 4 Wriedt Trans Metal Soc AIME 1955 p477
 7 0 0 0 Nickel data also

1820 °K - 6.28E-3 Xmax - 1795 dyne/cm

1870 8.03E-3 1790 dyne/cm

1920 9.77E-3 1785 dyne/cm

1970 1.19E-2 1780 dyne/cm

Checks with ????? Ian Otd Tekhn Nauk 1957 Vol 8 p120

LANTATHANUM

j = 1 Peterson J Phys Chem 1966 Vol 70 p2980
 1 0 0 0 surface tension data very unsure

1200 °K - .05 Xmax - 1600 dyne/cm

1210 .10 1595

1220 .15 1590

1240 .20 1585

1300 .30 1575

1350 .40 1565

LEAD

j = 1 Opei Trans Metal Soc AIME 1951 p244

Either bad reference or lost data

j = 4 Otsuka Metal Trans 1979 Vol 10B p565
0 1 1 4 has Antimony data also

1070	°K	-	.01	Xsol	-	9.42E-4	ACSOL
1170			.01			2.92E-3	
1270			.01			7.38E-3	
1320			.01			1.13E-2	

j = 4 Rapp High Temp Science 1972 Vol 4 p437
8 0 0 0

$\log (X_{\max}) = -5600/T + 1.87$ T = 1050-1350 °K

1050	°K	-	3.44E-4	Xmax	-	420	dyne/cm
1150			1.00E-3			415	
1250			2.45E-3			410	
1350			5.47E-3			405	

j = 4 Alcock Trans Faraday Soc 1964 Vol 60 p822
10 0 0 0

780	°K	-	7.40E-5	Xmax	-	439	dyne/cm
870			3.18E-4			435	
970			1.36E-3			430	

j = 4 Hansen (3) - 563
7 0 0 0

670	°K	-	1.30E-4	Xmax	-	445	dyne/cm
770			2.60E-4			440	
870			5.80E-4			435	
970			1.17E-3			430	
1070			2.33E-3			425	
1170			4.94E-3			420	

j = 4 Hansen (1) - 1065
3 0 0 5

870	°K	-	2.00E-4	Xmax	-	435	dyne/cm
970			4.00E-4			430	
1030			1.00E-3			427	

j = 4 Charle Z Phys Chem 1976 Vol 99 p199
0 0 0 0 in German

$$\log (X_{sol}) = 0.5 \log (\text{pressure in Pascal}) + 6260/T - 5.33$$

T = 1000-1340 °K

$$\log (X_{max}) = -5060/T + 2.30 \quad T = 1000-1143 \text{ °K}$$

$$\log (X_{max}) = -4450/T + 1.86 \quad T = 1143-1340 \text{ °K}$$

1000 °K	- 2.08E-1	ksol	- 1.73E-3	Xmax	- 428	dyne/cm
1100	1.18E-1		5.01E-3		423	
1143	::::::::::		7.47E-3		421	
1143	::::::::::		9.26E-3		421	
1200	7.33E-2		::::::::::		:::	
1240	::::::::::		1.87E-2		416	
1300	4.91E-3		::::::::::		:::	
1340	::::::::::		3.46E-2		411	

Might have Gibbs free energy data

LITHIUM

j = 1 Hansen (2) - 498
7 0 0 0

760 °K	- .05	Xmax	- 352	dyne/cm
920	.10		320	
960	.15		312	
1090	.20		290	

j = 1 Hubbersty J Less Common Metal 1979 Vol 49 p253
7 0 0 0 has Potassium & Sodium data also

$$\log (X_{max}) = -2308/T + 1.523 \quad (\text{for Hydrogen}) \quad T = 470-820 \text{ °K}$$

$$\log (X_{max}) = -2873/T + 2.321 \quad (\text{for Dueterium}) \quad T = 550-750 \text{ °K}$$

	Hydrogen	Dueterium	
470 °K	- 4.10E-4	Xmax	- :::::::::: Xmax - 400 dyne/cm
550	2.12E-3	1.25E-3	386
650	9.38E-3	7.96E-3	370
750	2.79E-2	3.09E-2	354
870	7.41E-2	::::::::::	343

j = 1 & 3 Adams J Less Common Metals 1975 Vol 42 p325
8 0 0 0 has Potassium & Sodium data also

$$\log (X_{max}) = -2308/T + 1.523 \quad (\text{for Hydrogen}) \quad T = 520-775 \text{ °K}$$

$$\log (X_{max}) = -2036/T + 1.168 \quad (\text{for Nitrogen}) \quad T = 470-705 \text{ °K}$$

Hydrogen data duplicates Hubbersty data above. For Nitrogen:

500	$\text{K} - 1.25\text{E-}3$	$X_{\text{max}} - 390$	dyne/cm
600	$5.95\text{E-}3$	374	
700	$1.82\text{E-}2$	358	

j = 1, 2, 3, & 4 Adams J Less Common Metal 1975 Vol 42 pl
7 0 0 0

Hydrogen
900 $\text{K} - 1.17\text{E-}1$ $X_{\text{max}} - 334$ dyne/cm
950 $1.88\text{E-}1$ 326

	Carbon	Nitrogen	Oxygen	
570 $\text{K} - 1.05\text{E-}2$	$X_{\text{max}} - 7.50\text{E-}4$	$X_{\text{max}} - 9.90\text{E-}5$	$X_{\text{max}} - 386$	dyne/cm
670	$1.70\text{E-}2$	$6.70\text{E-}3$	$4.88\text{E-}4$	370
770	$2.35\text{E-}2$	$3.75\text{E-}2$	$1.66\text{E-}3$	354
870	$3.00\text{E-}2$	$6.50\text{E-}2$	$4.25\text{E-}3$	338
970	::::::	$1.15\text{E-}1$	::::::	322
1000	::::::	$2.10\text{E-}1$	::::::	319

j = 2 Hansen (2) - 219
7 0 0 0

680 $\text{K} - 1.16\text{E-}2$	$X_{\text{max}} - 373$	dyne/cm
830	2.00	346
970	3.20	322
1070	5.20	306
1170	9.12	290

j = 2 & 3 Hansen (2) - 582
7 0 0 0

Carbon
1010 $\text{K} - 5.00\text{E-}2$ $X_{\text{max}} - 316$ dyne/cm
1055 $1.00\text{E-}1$ 309
1070 $1.50\text{E-}1$ 306
1090 $2.00\text{E-}1$ 303

Nitrogen
520 $\text{K} - 2.00\text{E-}4$ $X_{\text{max}} - 394$ dyne/cm
620 $8.00\text{E-}4$ 378
720 $6.50\text{E-}3$ 362

j = 4 Astm Special Tech Publication 1960 Vol 272 pl95
2 0 0 0

520	$\text{`K} - 9.60\text{E-}6$	$X_{\text{max}} - 394$	dyne/cm
570	$2.05\text{E-}5$	-	386
620	$3.74\text{E-}5$		378
670	$6.50\text{E-}5$		370

MAGNESIUM

$j = 1$	Hansen (2) - 500
7 0	0 0

950	$\text{`K} - 1.00\text{E-}3$	ksol
1000	$1.30\text{E-}3$	
1050	$1.37\text{E-}3$	

MANGANESE

$j = 1$	Hansen (1) - 785
1 0	0 1

1530	$\text{`K} - 2.94\text{E-}3$	ksol

$j = 1$	Levin	Tran	Ural	Politech	Inst	1974	Vol	231	p86
0 0	0		1						

$\log(X_{\text{sol}}) = 0.5 * \log(\text{pressure in Pascal}) - 1590/T - 4.40$
 $T = 1623-1718 \text{ `K}$

1620	$\text{`K} - 3.78\text{E-}4$	ksol
1720	$4.00\text{E-}4$	

$j = 2$	Hansen (3) - 148
2 0	0 0 unsure of surface tension data

$\log(X_{\text{max}}) = -375.8/T - 0.347$ $T = 1620-1870 \text{ `K}$

1620	$\text{`K} - .2636$	$X_{\text{max}} - 1090$	dyne/cm
1720	$.2720$		1070
1820	$.2796$		1050
1870	$.2866$		1040

$j = 2$	Hansen (1) - 368
7 0	0 0

1500	`K - .057	Xmax - 1114	dyne/cm
1565	.150	1103	
1590	.200	1096	
1610	.250	1092	

j = 2	Hansen (2) - 220
2 0	0 0

1580	`K - .265	Xmax - 1094
1620	.272	1090
1720	.280	1070
1870	.292	1040

j = 3	Kor Metal Trans 1978	Vol 9B	p97
2 2	1 9		

$\log (ksol) = -2071/T + 0.16$

1570	`K - 6.93E-2	ksol
1670	8.32	
1770	9.77	

1570	`K - .02	Xsol - 1.09	ACSOL
1570	.06	1.30	
1570	.10	1.55	
1670	.02	1.13	
1670	.06	1.43	
1670	.10	1.82	
1770	.02	1.16	
1770	.06	1.54	
1770	.10	2.06	

ACSOL data NOT USED - unsure of reference state

j = 3	Goken Trans Metal Soc 1961	Vol 221	p200
2 0	0 1		

Not sure exactly what is measured

j = 4	Hansen (3) - 503
2 0	0 0

1670	`K - 6.42E-4	Xmax - 1080	dyne/cm
1770	9.34E-4	1060	
1870	1.31E-3	1040	

j = 4 Jacob Metal Trans 1981 Vol 12B p675
8 0 0 0

$\log (X_{\max}) = -9070/T + 2.3$ T = 1500-1900 °K

1500 °K	- 1.79E-4	Xmax - 1114 dyne/cm
1600	4.28E-4	1094
1700	9.22E-4	1074
1800	1.82E-3	1054
1900	3.36E-3	1034

MOLYBDENUM

j = 2 Rudy Trans Metal Soc AIME 1967 Vol 239 p 1247
3 0 0 0 unsure surface tension data

2470 °K	- .17	Xmax - 1065 dyne/cm
2600	.20	1090
2700	.25	1110

j = 3 Herman J Less Common Metal 1978 Vol 58 p85
0 0 0 0

2200 °K	- 7.57E-3	ksol
2400	8.08	
2600	8.54	
2800	8.96	

2090 °K	- .20	Xmax - 985 dyne/cm
2180	.25	1008
3250	.30	1200

j = 3 Domke Scripta Metal 1974 Vol 8 p289
2 0 0 1

2920 °K - 8.42 ksol

NOTE -

Herman; above, stated that quenching was an unsatisfactory technique for the Nitrogen-Molbdenum system as it gave a "spongy" solid. Herman used some kind of calculation technique.
Domke; above, used quenching. He quenched in liquid Nitrogen. Herman did not specify his quenching agent.
The data of Domke Dokl Akad Nauk SSSR 1969 Vol 184 p398 was ignored as it did not agree with the data of Herman and Domke.

j = 4 Kozina I.A.N. SSSR Metal 1970 Vol 1 p56
7 0 0 0

3000 `K - 1.71 ksol

ksol driven a calculation scheme which was not understood.

NEODYNUM

j = 4 Hansen (2) - 653
7 0 0 5 unsure surface tension data

1300 `K - .05 Xmax - 688 dyne/cm
1400 .10 678
1470 .15 668
1540 .20 658

NICKEL

j = 1 Parlee Metal Trans 1970 Vol 1 p5377
7 0 0 1 has Silver data also

1923 `K - 2.54E-3 ksol

j = 1 Weinstein Trans Metal Soc AIME 1963 Vol 227 p285
1 0 0 1 has Chromium, Cobalt, & Iron data also

1800 `K - 2.27E-3 ksol
1900 2.43
2000 2.60

Checks with Busch Trans Metal Soc AIME 1960 Vol 218 p60

j = 2 Hansen (3) - 151
2 0 0 2

$\log (X_{\max}) = -895.7/T - 0.462$

1620 `K - .097 Xmax - 1800 dyne/cm
1720 .104 1780
1820 .111 1760
1920 .118 1740
2020 .124 1720

j = 3 Humberty Trans Metal Soc AIME 1960 Vol 218 p1076
1 0 0 1 has Chromium & Iron data also

1870 `K - 2.10E-5 ksol

believe metal exposed to Hydrogen during experimental runs

j = 4 Wriedt Trans Metal Soc AIME 1955 p477
2 0 0 0 has Iron data also

1620 `K - 4.08E-5 Xmax - 1800 dyne/cm

1720 9.53E-5 1780

1820 2.03E-4 1760

1920 3.99E-4 1740

1970 5.46E-4 1730

j = 4 Kemori J Chem Thermo 1981 Vol 13 p 313
2 1 1 4

$\ln(X_{\max}) = -25080/T + 9.960$ $T = 1722-1859$ `K

1730 `K - .0107 Xmax - 1776 dyne/cm

1830 .0236 1736

Note large difference between Wriedt and Kemori results. Why ???

1730 `K - .01 Xsol - .247 ACSOL

1830 .01 .324

NIOBIUM

j = 1 Lokomski Dokl Akad Nauk SSSR 1965 Vol 165 p1091
2 0 0 2

2900 `K - .0115 ksol

3000 .0110

3100 .0106

Duplicated in Lakomski I.A.N. Metal 1968 Vol 4 p28

j = 2 Kimura Trans Japan Inst Metal 1961 Vol 2 p98
3 0 0 0 unsure of surface tension data

2610 `K - .135 Xmax - 1994 dyne/cm

2880 .200 1978

3110 .250 1932

3280 .300 1898

Checks with GTE

j = 3 Revyakin I.A.N. Metal 1968 p28
7 0 0 0 has Tantalum & Vanadium data also

2800 `K - .733 ksol

j = 4 Hansen (2) - 263
3 0 0 5

2640 °K - .05 Xmax - 1990 dyne/cm
2590 .10 2000
2545 .15 2009
2480 .20 2021

PALLADIUM

j = 1 Kalinyuk Zh Fiz Khim 1980 vol 54 p2815
2 0 0 0

1870 °K - 9.40E-3 ksol
2363 7.52

PLUTONIUM

j = 1 Hansen (2) - 504
7 0 0 0

970 °K - .050 Xmax - 535 dyne/cm
1070 .075 520

j = 2 Hansen (2) - 225
7 0 0 0

1275 °K - .05 Xmax - 500 dyne/cm
1420 .10 485
1550 .15 475
1650 .20 465

j = 4 Hansen (2) - 689
7 0 0 0

1685 °K - .05 Xmax - 462 dyne/cm
1815 .10 450
1930 .15 443
2040 .20 437

j = 4 Hansen (3) - 568

7 0 0 0

1700 °K - .10 X_{mx} - 460
 1920 .20 445

POTASSIUM

j = 1 Hubbersty J Less Common Metal 1979 Vol 49 p253
 7 0 0 0 has Lithium & Sodium data also

$\log (X_{\max}) = -2994/T + 2.305$ T = 400-700 °K

400 °K - 6.61E-6 X_{max} - 89.19 dyne/cm
 500 2.08E-4 82.66
 600 2.07E-3 76.13
 700 1.07E-2 69.60

j = 1 Arnildov I.A.N. Metal ????
 1 0 0 0

$\log (X_{\max} \text{ in weight frac}) = -2930/T + 0.8$ T = 600-770 °K
 $\log (\text{saturation pressure in mm Hg}) = -5860/T + 11.3$

570 °K - 1.79E-3 X_{max} - 78.09 dyne/cm
 670 1.05E-2 71.56
 770 3.86E-2 65.03

Proposes a value for k_{sol} which is constant over a temperature range.

320 to 720 °K - 14.2 Weight % Hydrogen / (pressure in mm Hg) ^{1/2}

j = 4 Adams J Less Common Metal 1975 Vol 42 p325
 7 0 0 0

370 °K - 2.40E-3 X_{max} - 91.15 dyne/cm
 470 6.70E-3 84.62
 570 1.46E-2 78.09
 670 3.70E-2 71.56
 770 8.80E-2 65.03
 820 1.20E-1 61.76

j = 4 Leffler J Phys Chem 1964 Vol 68 p2882
 9 0 0 0

775 °K - .640 X_{max}
 875 .636
 975 .632

NOT USED - data is strange.

RHENIUM

j = 2 Hughes J Less Common Metal 1959 Vol 1 p 377
2 0 0 0 unsure of surface tension

2770 `K - .169 Xmax - 2780 dyne/cm
2870 .20 2769
2970 .23 2740
3040 .25 2720

SCANDIUM

j = 4 Kuprashvili I.A.N. Neorg Mater 1969 Vol 5 p2123
3 0 0 0 surface tension data is guess

1830 `K - .34 Xmax - 1600 dyne/cm
2070 .37 1560
2270 .43 1520
Checks with GTE.

SILICON

j = 1 Kostina I.A.N. Neorg Mater 1970 Vol 6 p117
1 0 0 1

1800 `K - 1.99E-2 ksol
1900 2.93
2000 4.16
2100 5.71
2200 7.62

j = 2 Laplev Izv Vuz Chern Metal 1974 Vol 8 p13
0 0 0 0 in Russian

delta Gibbs free energy (j/mole) = -115520 + 37.30 * T 1688-2270 `K

j = 3 Scarce J Chem Phys 1957 Vol 30 p1551
6 0 0 0

2000 `K - 7.50E-4 Xmax - 700 dyne/cm
2200 2.70E-3 680

2500	1.33E-2	650
2700	3.13E-2	630
2900	6.53E-2	610

j = 4 Hansen (3) - 572
7 0 0 0

1650	°K - .24	Xmax - 735	dyne/cm
1770	.30	723	
1850	.40	711	

j = 4 Arkharow Ukr Khim Zhur 1974 Vol 40 p129
0 0 0 0 in Russian

1688	°K - 3.98E-5	Xmax - 732	dyne/cm
1873	9.77E-4	708	

SILVER

j = 1 Parlee Metal Trans 1970 Vol 1 p5377
7 0 0 1 has Nickel data also

1282	°K - 2.37E-5	ksol
1587	8.41E-5	
1973	2.04E-4	

j = 2 Hansen (1) - 11
7 0 0 0

1930	°K - 1.08E-4	Xmax - 800.2	dyne/cm
2005	2.25	787.1	

j = 4 Otsuka Metal Trans 1981 Vol 12B p501
0 1 0 9

1270	°K - .01	Xsol - 47.67	ACSOL
1370	.01	53.11	
1470	.01	58.64	

NOT USED - unsure of standard state

j = 4 Hansen (1) - 37
7 0 0 1

1210	°K - 2.15E-2	ksol
1540	1.68E-2	
1825	1.35E-2	

2130 1.01E-2

2440 3.37E-3

Checks with Parlee Trans Metal Soc AIME 1965 Vol 233 p1918

SODIUM

j = 1 McClure J Phys Chem 1965 Vol 69 p 3542
 1 0 0 0

 $\log(\text{weight percent}) = -2800/T + 2.20 \quad T = 475-630 \text{ } ^\circ\text{K}$
475 $^\circ\text{K}$ - 4.92E-5 Xmax - 183.2 dyne/cm

530 1.90E-4 187.4

630 1.31E-3 178.2

j = 1 Addison J Cehm Soc London 1965 p116
 1 0 0 0

 $\log(\text{weight percent}) = -5021/T + 6.211 \quad T = 520-593 \text{ } ^\circ\text{K}$
520 $^\circ\text{K}$ - 8.26E-5 Xmax - 188.3 dyne/cm

570 5.80E-4 183.7

593 1.28E-4 181.7

j = 1 Hubbersty J Less Common Metal 1979 Vol 49 p253
 7 0 0 0 has Lithium & Potassium data also

 $\log(X_{\text{max}}) = -3019/T + 1.818 \quad T = 400-700 \text{ } ^\circ\text{K}$
400 $^\circ\text{K}$ - 1.86E-6 Xmax - 199.3 dyne/cm

500 6.03E-5 190.1

600 6.11E-4 180.9

700 3.20E-3 171.7

j = 1 Williams J Phys Chem 1957 Vol 61 p379
 1 0 0 0

600 $^\circ\text{K}$ - 1.60E-3 Xmax - 180.9 dyne/cm

660 1.00E-2 175.4

720 4.00E-2 169.9

j = 2 Salzano Nuclear Tech 1972 Vol 13 p289
 7 0 0 0

 $\log(\text{weight fraction}) = -2440/T - 2.30 \quad T = 850-970 \text{ } ^\circ\text{K}$
850 $^\circ\text{K}$ - 1.61E-5 Xmax - 150 dyne/cm

970 3.70 147

j = 2 Hansen (2) - 222
7 0 0 0

420 °K - 6.20E-5 Xmax - 197.5 dyne/cm
570 9.00E-5 183.7
770 1.22E-4 165.3
970 1.44E-4 146.9

j = 4 Hansen (2) - 248
7 0 0 0

520 °K - 2.40E-4 Xmax - 188.3 dyne/cm
645 5.00E-4 176.9
750 1.50E-3 167.1
805 2.50E-3 162.1

j = 4 Adams J Less Common Metal 1975 Vol 42 p325
7 0 0 0 has Lithium & Potassium data also

370 °K - 4.06E-6 Xmax - 202.1 dyne/cm
470 3.90E-5 192.9
570 1.85E-4 183.7
670 5.34E-4 174.5
770 1.17E-3 165.3
820 1.62E-3 156.1

STRONTIUM

j = 1 Peterson J Less Common Metal 1980 Vol 72 p251
1 0 0 0

1070 °K - 2.61 ksol
1170 1.52

j = 1 Hansen (3) - 409
7 0 0 5

1050 °K - .05 Xmax - 282 dyne/cm
1065 .10 283
1095 .20 287

TANTALUM

j = 2 GTE
7 0 0 0

3120 `K - .12 Xmax - 2146 dyne/cm
3255 .15 2120
3450 .20 2080

j = 2 Hansen (1) - 381
3 0 0 5

3070 `K - .08 Xmax - 2155 dyne/cm
3150 .10 2140
3305 .15 2110
3455 .20 2080

j = 3 Revyakin I.A.N. Metal 1968 p28
7 0 0 0 has Niobium and Vanadium data

3310 `K - .383 ksol

TELLURIUM

j = 4 Otsuka Metal Trans 1980 Vol 11B p119
0 1 1 4

760 `K - .01 Xsol - 9.34E-3 ACSOL
820 .01 2.69E-2

THALLIUM

j = 4 Otsuka Metal Trans 1980 Vol 11b p313
0 1 1 4

973 °K - .01 Xsol - 1.66E-3 Acsol
1073 .01 4.79E-3
1173 .01 1.15E-2

THORIUM

j = 2 Hansen (2) - 231
7 0 0 5

1900 °K - .07 Xmax
2010 .10
2270 .15
2490 .20

NOT USED - phase diagram is unusual, surface tension data is
non-existent

TIN

j = 1 Parlee Metal Trans 1970 Vol 1 p5377
7 0 0 1 has Nickel & Silver data also

1282 °K - 4.58E-6 ksol
1587 4.30E-5
1923 2.23E-4

j = 1 Bever Trans Metal Soc Aime 1942 ?????
1 0 0 1

1273 °K - 4.24E-6 ksol
1373 9.54E-6
1473 2.17E-5
1573 3.76E-5

j = 1 Hansen (1) - 796
7 0 0 1

670 `K - 4.66E-5 ksol
 830 6.04E-5
 980 7.42E-5
 1070 9.86E-5
 1170 1.48E-4
 1280 1.55E-4

j = 4 Alcock Trans Faraday Soc 1965 Vol 61 p443
 EMF 0 0 0

810 `K - 1.30E-5 Xmax - 525 dyne/cm
 870 4.10E-5 519
 970 2.07E-4 509

j = 4 Rapp Metal Trans 1072 Vol 3 p3239
 8 0 0 0

log (Xmax) = -15098/T + 9.775 T = 1020-1220 `K
 log (ksol) = 20131/T - 2.825

1020 `K - 4.85E-4 Xmax - 504 dyne/cm
 1120 1.82E-3 494
 1220 5.49E-3 484

ksol values NOT USED as they are huge

j = 4 Parlee High Temp Sci 1982 Vol 15 p55
 7 0 0 0

1223 `K - 5.66E-3 Xmax - 470 dyne/cm
 1523 2.20E-2 440

j = 4 Otsuka Metal Trans 1981 Vol 12B p427
 0 1 1 4

970 `K - .01 Xsol - 4.03E-7 ACSOL
 1070 .01 3.07E-6
 1170 .01 1.66E-5

Checks with Fitzner Z Metallk 1981 p512

j = 4 Nover Trans Inst Min Met C 1972 Vol 81 pC63

Found late NOT PROCESSED. Has max solubility and Gibbs free
 energy data.

TITANIUM

j = 2 GTE
7 0 0 5

1920 °K - .015 Xmax - 1600 dyne/cm
1950 .050 1594
2020 .100 1580
2115 .150 1561
2320 .200 1520

j = 2 Hansen (1) - 384
7 0 0 0

2110 °K - .05 Xmax - 1562 dyne/cm
2210 .10 1542
2350 .15 1514
2490 .20 1486

j = 3 Levinski I.A.N. Neorg Mater 1974 Vol 10 p1628
7 0 0 1

2280 °K - 5.070 ksol
2430 4.285
2610 4.194
2750 2.712

j = 3 Hansen (1) - 990
7 0 0 5

2330 °K - .05 Xmax - 1518 dyne/cm
2484 .10 1486
2565 .15 1472
2830 .20 1419

j = 4 Hansen (1) - 1069
3 0 0 5

2085 °K - .05 Xmax - 1568 dyne/cm
2135 .10 1558
2180 .15 1548
2205 .20 1541

Kornilov Dokl Akad Nauk SSSR 1963 Vol 150 p313 verifies
the phase diagram proposed in Hansen. Kornilov shows more
information than Hansen in the solid regions.

URANIUM

j = 1 Hansen (1) - 803
7 0 0 1 unsure surface tension data

1400 `K - 6.66E-3 ksol - .290 Xmax - 1498 dyne/cm
1470 6.91 .333 1485

j = 2 Hansen (1) - ???
7 0 0 0 unsure surface tension data

1670 `K - .05 Xmax - 1455 dyne/cm
1870 .10 1425
2030 .15 1401
2170 .20 1380

j = 3 Hansen (3) - 534
7 0 0 1

2270 `K - .05 ksol
2465 .10
2640 .15
2740 .20

j = 4 Hansen (2) - 700
7 0 0 0 unsure surface tension data

1380 `K - 8.27E-6 Xmax - 1500 dyne/cm
1470 9.49E-6 1485
1670 1.41E-5 1455
1870 1.95E-5 1425
2070 2.90E-5 1395
2270 4.96E-5 1365

VANADIUM

j = 2 Storms High Temp Science 1973 Vol 5 p276
7 0 0 0

1920 `K - .145 Xmax - 1980 dyne/cm
2000 .167 Xmax - 1974
2120 .200 1960
2250 .230 1937

Checks with GTE

j = 3 Revyakin I.A.N. Metal 1968 p28
 7 0 0 0 has Niobium & Tantalum data also

2200 °K - 1.72 ksol

WOLFRAM

j = 2 Hansen (3) - 237
 2 0 0 5 unsure surface tension data

3070 °K - .40 Xmax - 2490 dyne/cm
 3350 .50 2426

ZIRCONIUM

j = 2 Hansen (1) - 239
 7 0 0 0

2100 °K - .050 Xmax - 1553 dyne/cm
 2270 .067 1528
 2670 .143 1468
 3070 .276 1408

j = 3 Levinski Zh Fiz Khim 1974 Vol 48 p845
 7 0 0 1

2170 °K - 85.7 ksol
 2270 73.4
 2390 43.6

Data taken from phase diagram given for system pressure
 equals one PSIA.

j = 4 Hansen (1) - 709
 7 0 0 5 surface tension data guessed from Titanium data

2173 °K - .41 Xmax - 1543 dyne/cm
 2470 .48 1498
 2670 .54 1468

YTTRIUM

j = 2 Carlson Trans Metal Soc AIME 1968 Vol 242 p846
 3 0 0 0

1800	`K - .025	Xmax - 1718	dyne/cm
1820	.050	1715	
1850	.075	1712	
1890	.100	1706	
2016	.150	1688	
2170	.200	1662	

j = 4 Hansen (2) - 707
 7 0 0 5 surface tension data guessed from Hafnium data

1720	`K - .454	Xmax - 1730	dyne/cm
2220	.500	1655	

Appendix C Experimental Techniques

This appendix contains a review on the various experimental techniques encountered during data gathering. This appendix is not intended as a critique on the experimental techniques. It is intended as a brief introduction to the experimental techniques most commonly used.

Hot Volume Method

A popular method of measuring solubility data during the 1920's - 1970's was the Sieverts or hot volume method. The technique is simple in theory: melt a sample of metal in the presence of a pure gas and determine gas absorption by monitoring changes in gas pressure.

The problems of the hot volume method are well reviewed by Gunji (26). One problem is absorption of liquid metal by the crucible and absorption of metal gas by the experimental chamber wall. Another crucible/chamber material related problem is chemical reaction between crucible/chamber material and liquid metal, gaseous metal, or any metal-solute complex. If absorption and reaction data are available, these problems can be minimized.

To equate pressure to molar amounts requires a volume factor, in this case the volume of the reaction chamber. The volume must be known at experimental temperatures with the liquid metal in the chamber. This volume is known as the "hot volume". The hot volume is recorded by pumping known amounts of inert gas into the chamber and recording

the pressure. A problem in recording the hot volume is that there are fixed heat sources in the reaction chamber. This will lead to thermal gradients. If the chamber is inefficiently designed there could exist dead spaces or areas of the chamber which are significantly below the average temperature of the chamber. Gunji measured the hot volume of an efficiently designed chamber using Argon and Helium. The hot volume measured using Argon was 1-2% smaller than the that measured using Helium. Argon has a larger thermal conductivity. Care should be taken to avoid dead spots within the reaction chamber and to use an inert gas of the same relative thermal conductivity as the experimental gas. Lastly the assumption of insolubility of the inert gas in the liquid metal should be accounted for if false.

During experimental runs the liquid metal will be free to vaporize. This will cause an array of problems from reaction between gaseous metal and solute gas to depletion of the liquid metal. But time must be allowed for the gas absorption to achieve equilibrium.

A similar method involves melting of pure metal-solute complex and measuring the gas evolved. When melted, the sample will dissociate into a saturated liquid metal-solute solution and liquid metal-solute complex. An equilibrium will be reached where the pressure of the solute gas is equal to the dissociation pressure of the metal-solute complex. At this point if gas is withdrawn from the reaction chamber, metal-solute complex will dissociate to re-establish equilibrium. When gas is withdrawn from the chamber and the pressure does not return to the metal-solute complex dissociation pressure, all complexes have dissociated into a saturated solution of liquid metal and solute. With

knowledge of the amount of gas withdrawn, the hot volume of the chamber, and the amount of metal-solute complex put in the chamber the maximum solubility of the solute can be calculated.

Quenching Technique

Quenching involves equilibrating a pure liquid metal sample with a pure solute gas. The resulting metal-solute solution is rapidly frozen or quenched. The resulting solid is then analyzed to determine the solute concentration. The various techniques for analyzing the solid solutions will not be reviewed here.

While liquid, the metal can react with the crucible material. To avoid contamination resulting from reactions of metal or metal-solute complex with the crucible it is wise to grind off the outer layer of the solid sample obtained from quenching. The solid sample should be split and analyzed across its width. This will insure that time was allowed for the entire sample to reach equilibrium.

A unique problem with the quenching technique is the evolution of solute from the sample during solidification. Herman (27) states that quenching is unsatisfactory for Molybdenum-Nitrogen systems. Herman states the Molybdenum-Nitrogen produce a spongy solid when quenched. Domke (17) conducted quenching experiments on the Molybdenum-Nitrogen systems. His results compare favorable with the

results of Herman which were generated from a calculation scheme.

Domke quenched in liquid Nitrogen, insuring a rapid solidification.

Herman did report his quenching method.

The quenching technique can be use for measuring the solubility of Carbon in liquid metals. Melt the metal in a graphite crucible. Allow time for the graphite to dissolve into the liquid metal.

To avoid quenching and analyzing the entire sample a portion of the liquid metal-solute solution can withdrawn by a syringe, and quenched therein. The syringe material is then dissolved away by a chemical reagent.

Uda (110) found that the solubility of Nitrogen in quenched Iron was significantly higher for arc melted samples as opposed to sample levitated in Nitrogen gas streams. Uda attributed the higher solubility to an activation of the Nitrogen molecule when exposed to the welding arc.

Melting Technique

The melting technique involves the melting of a sample. The sample is made by mixing a known quantity of powdered metal and powdered metal-solute, then compressing the mixture into a solid pellet.

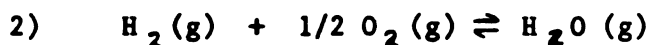
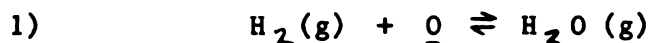
The temperature at which the pellet begins to melt and pellet

composition marks a point on the solidus line of the solute-metal phase diagram. The temperature at which the entire pellet melts and the pellet composition marks a point on the liquidus line of the solute-metal phase diagram. A unique advantage is that this technique can be run backwards and forwards repeatedly.

A related technique calls for optically fixing the line of liquid-solid interface in a partially melted pellet. The pellet is then quenched. The two portions are physically separated and analyzed. This allows for determination of solidus and liquidus points of the phase diagram.

Water Vapor Calculation Scheme

The following calculation scheme was found in Tankins (106) and Jacob (38). If Hydrogen and Oxygen gas are present over a liquid metal-Oxygen solution the following reactions must be at equilibrium:



Where $\underline{\text{O}}$ refers to the Oxygen dissolved in the liquid metal. The

equilibrium constants corresponding to the above reactions:

$$3) \quad K = [P_{H_2O}] / \{ [P_{H_2}] [\gamma(O) X(O)] \} = K' / \gamma(O)$$

$$4) \quad K^* = [P_{H_2O}] / \{ [P_{H_2}] [P_{O_2}]^{1/2} \}$$

Where P_{H_2O} is the partial pressure of water vapor, $\gamma(O)$, $X(O)$ are the activity coefficient and concentration the Oxygen dissolved in the liquid metal.

The equilibrium constant K^* is a well defined quantity. If the partial pressures of Hydrogen and water vapor and the concentration of Oxygen dissolved in the liquid metal are known Henry's law constant can be calculated:

$$5) \quad K_{\text{henry}} = K^* / K' = X(O) / [P_{O_2}]^{1/2}$$

No mention was made of the effect of Hydrogen or water vapor dissolved in the liquid solution.

Electromotive Force Technique

A battery is composed of a liquid solution with electrodes at opposite ends, when the electrodes are connected via a conducting material a electrical circuit is completed. The solution and the electrodes must be of a certain type. The solution usually contains a least two ions. One ion transferring electrons to one electrode, the other ion transferring electrons away from the other electrode. Thus a current flows. If an external voltage or electromotive force (EMF) is applied to the battery, the current can be made to run in the opposite direction, thus "charging" the battery. The battery principle is the basic principle used in the EMF technique.

A typical apparatus for electromotive force experiments is shown in Figure 17. The electrodes are the liquid metal-solute solution and the Platinum surrounding the cell holding the liquid solution. The cell wall is made of an electrolyte pourous to the solute. At the Platinum electrode solute in the gas will convert to ionic form. The ion will migrate across the electrolyte wall to the liquid solution. There the ion will convert to a non-charged solute species. Thus a circuit is completed, and of course the circuit can run in reverse.

The solute concentration is assumed uniform in both the liquid solution and in the gas surrounding and within the pourous Platinum electrode. The solute chemical potential is therefore uniform within the liquid solution and the gas. Any gradient in the solute chemical potential is thus assumed wholely contained within the electrolyte cell wall.

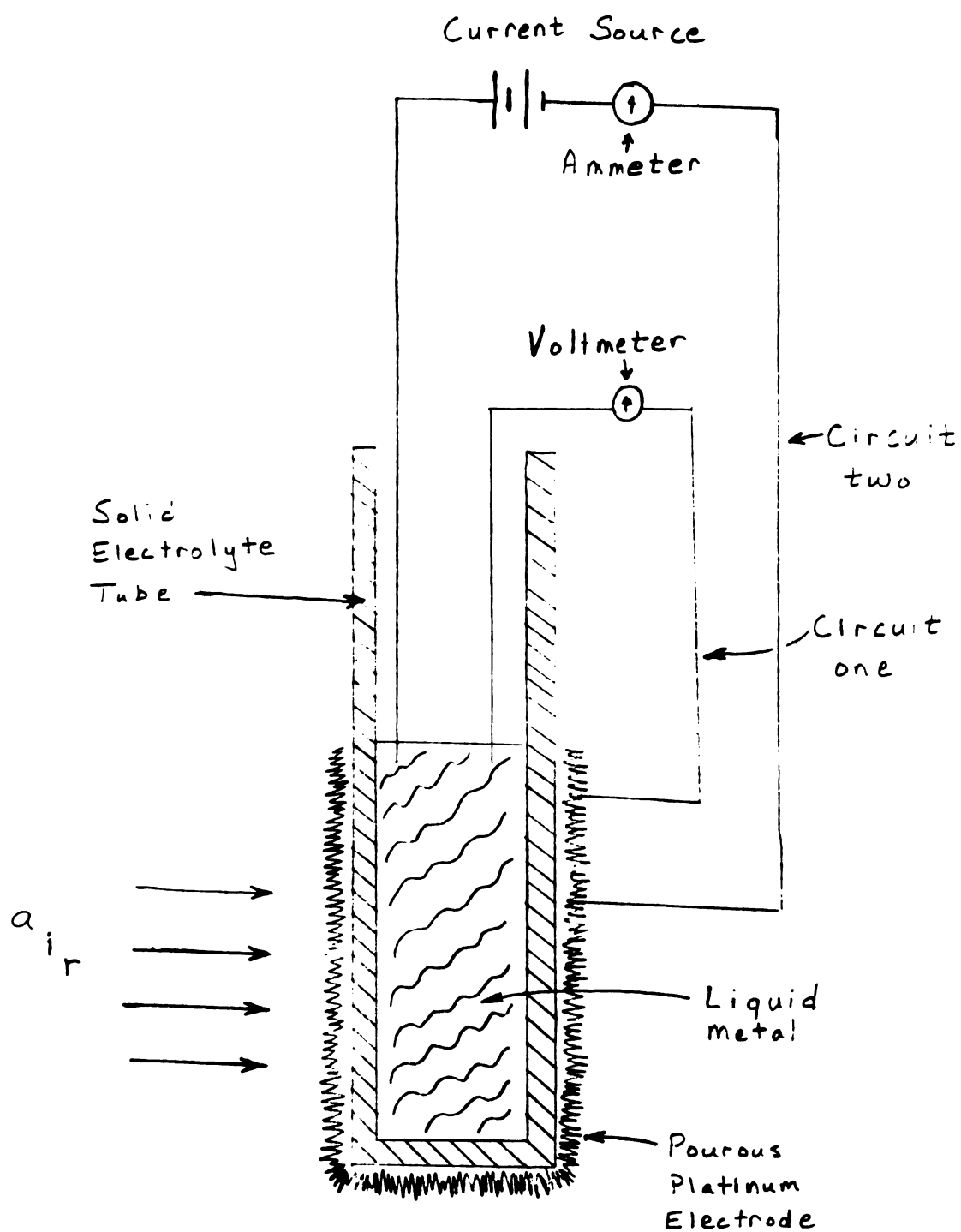
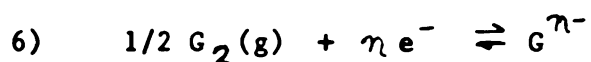
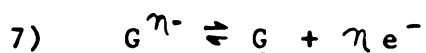


Figure 17
Electrochemical Cell

Experiments are conducted by applying an external EMF to the experimental cell which will pump electrons into the Platinum electrode. At the Platinum electrode the gaseous solute (G) undergoes the following reaction:

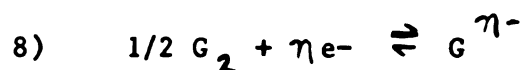


Where η is the valence number of the solute. The solute ion ($G^{\eta-}$) diffuses through the cell wall to the liquid solution. There the following reaction occurs to complete the electrical circuit:

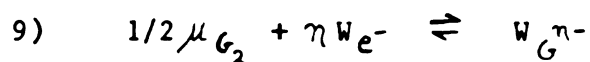


Where $\underline{G}$ is the solute in the liquid solution. By pumping electrons into the Platinum electrode, solute is pumped into the liquid solution. Reversing the direction of electron motion pumps solute out of the liquid solution. The following sections will show how this technique can be used to measure the activity of the solute in liquid solution.

The following derivation of mathematics used to describe a EMF cell is based on work found in Rapp (87). Within the cell wall the following equilibrium equation should hold at all points:



Equation 8 generates the equation:



Where μ_{G_2} is the chemical potential of the solute within the cell wall. W_{e^-} and $W_{G^{\eta-}}$ are the electrochemical potential of the excess electrons and of the solute ions within the cell wall.

Electrochemical potential can be expressed:

$$10) \quad W_i = \mu_i + Z_i F \phi$$

Where μ_i is the chemical potential, Z_i is the valance number, F is Faradays constant, and ϕ is the local electric potential.

The current flow due to ion diffusion (I_{ion}) is given by Wagner (112):

$$11) \quad I_{ion} = \sigma_{ion} A / (2F) * (d w_G n / dx)$$

Where the term ($\sigma_{ion} A$) will be shown to be related to current flow resistance. Equation 11 and 9 can be combined to yield:

$$12) \quad (1/2) d\mu_G^2 + n d w_{e^-} = \frac{2 I_{ion} F}{\sigma_{ion} A} dx$$

Integrating equation 12 from $X=0$ to $X=1$, or from the outer surface of the cell wall to the inner surface:

$$13) \quad 1/2 [\mu_G''^2 - \mu_G^2] + n[w_{e^-}'' - w_{e^-}] = \frac{2 I_{ion} \Omega_{ion} F}{\sigma_{ion} A}$$

Note that variables with double prime superscript refer to conditions at the outer surface of the cell wall while non-prime variables refer to conditions at the inside surface of the cell wall. Ω_{ion} is expressed:

$$14) \quad \Omega_{ion} = (1/A) \int_{X=0}^{X=1} dx / \sigma_{ion}$$

Combining equations 13 and 10:

$$15) \quad -n[\mu_{e^-}'' + z_{e^-} F \phi'' - \mu_{e^-} - z_{e^-} F \phi] = \\ (1/2) [\mu_{G_2}'' - \mu_{G_2}] - 2 \text{ Ion } \Omega \text{ ion } F$$

Where μ_{e^-} is the chemical potential of excess electrons. If we make the assumption:

$$16) \quad \mu_{e^-}'' = \mu_{e^-}$$

Equation 15 reduces to: (Note that $z_{e^-} = -1$)

$$17) \quad \phi'' - \phi = (1 / (2 n F)) * [\mu_{G_2}'' - \mu_{G_2}] - \text{Ion } \Omega \text{ ion}$$

Where ϕ is electrical potential. $\phi'' - \phi$ is thus the electromotive force applied to the experimental cell. Equation 17 can thus be written:

$$18) \quad \mathcal{E} = E - \text{Ion } \Omega \text{ ion}$$

Where $\mathcal{E}$ is external EMF applied to the cell and E is the internal EMF, measurable if a voltmeter were attached to the Platinun electrode and to the liquid metal solution (circuit 1 of Figure 17). If the applied EMF is zero it can be seen:

$$19) \quad \Omega_{\text{ion}} = R_{\text{cell}}$$

Where R_{cell} is the resistance of the electrolyte cell wall to ionic motion. The resistivity should be independent of the solute activity.

The chemical potential of a diatomic substance (G_2) is defined:

$$20) \quad \mu_{G_2} = \mu_{G_2}^{\circ} + 2RT \ln a(G)$$

Where $\mu_{G_2}^{\circ}$ is the chemical potential at a chosen reference state. $a(G)$ is the activity of the substance relative to the reference state. If the reference state of the solute at the inner and outer surfaces of the cell wall are chosen to be the same, equations 17, 18, 19, and 20 combine to yield:

$$21) \quad \mathcal{E} = (RT / (\eta F)) \ln (a(G)'' / a(G)) - I_{ion} R_{cell}$$

Choosing the reference state to be pure gaseous solute at one atmosphere pressure:

$$22) \quad \mathcal{E} = (RT / (\eta F)) \ln (P_{G_2}''^{1/2} / a(G)) - I_{ion} R_{cell}$$

As stated earlier, when the cell internal EMF equals the applied EMF, the ionic current goes to zero. Thus at steady state, equation 22 transforms to:

$$23) \quad \mathcal{E} = (RT / (\eta F)) \ln (P_{G_2}''^{1/2} / a(G))$$

The activity of the solute can be calculated from equation 23 when the applied EMF and the partial pressure of the solute in the gas phase is known at steady state.

When an EMF is applied to the cell, an ionic current will flow to drive the cell internal EMF to equal the applied EMF. When the internal EMF equals the applied EMF equilibrium is achieved and the current falls to zero. The total quantity of electric charge (Q_{ion}) which flows while waiting for steady state is:

$$24) \quad Q_{ion} = \int_0^T I_{ion} dt = \eta F N_G$$

Where T is the time required for the internal and applied EMFs to reach equilibrium, while N_G is the number of solute molecules transferred.

The concentration of the solute in the liquid solution after current has flowed can be expressed:

$$25) \quad C_2 = (C_1 M_T + N_G) / (M_T + N_G)$$

Where C_1 and C_2 are the concentrations of the solute in the liquid solution before and after current flow. M_T is the total moles of liquid solution before current flow. If solute concentrations are low, equation 25 can be expressed:

$$26) \quad C_2 - C_1 = N_G / M_L = Q_{ion} / (\eta F M_L)$$

Where M_L is the moles of liquid metal solution. This allows the calculation of the solute concentration after applying an external EMF to the cell.

As the applied EMF is raised the solute concentration rises in the liquid solution. When the solute reaches its maximum solubility, the internal EMF will have reached its maximum value. If the applied EMF is increased above this maximum internal EMF, the ionic current will not fall to zero. Solute will continue to be pumped into the liquid solution where it will produce solute gas or precipitate. Thus the maximum solubility can be measured by raising the applied EMF until the current does not fall to zero.

The above discussion hold exactly for an ideal electrochemical cell. A real cell requires certain corrections. The following review is based on Otsuka (70).

An ideal electrolyte cell wall should be permeable to solute ions, should be a non-conductor, and should not release or entrap solute ions. If the electrolyte is conductive to electricity, a conductive current (I_c) must be subtracted from the measured current to obtain a true ionic current (I_{ion}). The conductive current is measurable. When the internal EMF reaches equilibrium with the applied EMF, the current does not fall to zero. This steady state current is the conductive current. Subtracting the conductive current from the

measured current yields the true ionic current.

If the electrolyte cell wall releases or entraps solute ions this must be accounted for. Otsuka measured a true ionic current for experimental runs designed to pump solute out of a pure liquid metal. Otsuka concluded that the ionic current generated was a result of pumping solute ions out of the electrolyte wall. It was assumed that these solute ions would move from the cell wall into the liquid solution during a pump in experiments. Thus the quantity of electricity obtained from the pump out experiments on a pure liquid metal is subtracted from the measured quantity of electricity flow (Q_{ion} in equation 26) for normal experimental runs. It was found that this "false" ionic current is proportional to the applied EMF.

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