A STUDY OF METHODS TO DETERMINE THE DIFFERENCE IN THE DIFFUSION ACTIVATION ENERGY OF A SOLUTE AS COMPARED TO THAT OF SOLVENT SELF-DIFFUSION, AND A NEW RADIUS COMPENSATING MODEL

BY

VLADIMYR IVAN BURACHYNSKY

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ABSTRACT

Four models for the prediction of the activation energy for solid state solute diffusion are tested using a large data base of experimental diffusion results. The models are based on the differences in relative valence, ground state and fermi energies of the solute and solvent. A new procedure extending previous models to include the equilibration of energies and exchange of electrons is reviewed and found to correctly predict the correct sign of the difference between the activation energies for solvent self diffusion and solute self diffusion in over 70 % of the 300+ solvent-solute systems investigated. This model is the most robust ever presented and critical aspects relating to diffusion mechanisms are discussed. The most prominent feature is the incorporation of a radius compensation method that predicts the change in ionic radius of solute ions as a consequence of the redistribution of charge resulting from energy equilibration of solute with solvent.

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LIST OF SYMBOLS

A_O Frequency factor

Q Activation energy (enthalpy)

R Gas Constant

T Temperature

I_P Ionization potential ,where p refers to 1st ,2nd ,3rd etc. valence electron

H_V Heat of sublimation

E_V Electron -volt

E_f Fermi energy

E_{max} Maximum average energy level sum of Eo and Ef

E_O Ground state energy

q_O screening parameter

r_O atomic radius

α solvent energy state that solute must adapt to

β $[\Lambda + \sum_{p=1}^{p=Z} I_p - Q_f + Q_m]$....*intrinsic..solute..element..properties*

γ $\frac{2}{5}k\frac{Z^{\frac{2}{3}}}{r_0^2}$....*energy...term*

Q_f Free atom interaction energy between electrons

Q_m Total mean interaction energy between electron pairs

I_T Transition energy associated with the promotion of an electron from s to p shell

n Charge transfer

N Term includes valence and charge transfer from equilibration formula

U Equivalent to ΔE_O, difference in Ground state energies of solvent and solute

ΔQ Difference in activation energies of solvent and solute

ΔE_O Difference in Ground state energies of solvent and solute

Z Number of high energy , valence electrons

E_0^A Ground state energy of element A, normally the solvent,(superscript A denotes solvent or B denotes solute

k Boltzman Constant

m Mass of an electron

Λ Heat of sublimation

h Planck's Constant

R Gas Constant

Z_L Le Claire (1962) term for valence difference between Solute and Solvent

1.0 INTRODUCTION

1.1 Overview

In the field of solid state diffusion , much experimental effort has been directed at determining the rates of diffusion of dilute impurities in metal solvents. The Smithells Tables now include data for various solute, impurity elements , in over 30 different solvent elements. This record represents over a half century of experimental results. Typically the data on solute diffusion experiments is presented as the two principal variables of the Arrhenius diffusion equation, given here in the classic self-diffusion form for solvent,

$$D = A_o e^{\left(\frac{-Q_o}{RT}\right)}$$ **Equation [1]**

Ao, the frequency factor and Qo, the activation energy term, for self-diffusion. When considering the solute properties in the solvent, the following form of equation 1 is used,

$$D_2 = A_2 e^{\left(\frac{-Q_2}{RT}\right)}$$ **Equation [2]**

Where $\mathbf{A_2}$ is the frequency term for solute diffusion in solvent, and the term $\mathbf{Q_2}$ is the activation energy of the solute. (Note: By convention the subscript 0 will always refer to solvent and the subscript 2 to solute.).

Recent comments suggest the issue of what determines the activation energy of a solute is regarded as a non-issue (Rothman,1993).Yet, no one has been able to predict whether

a solute will diffuse faster or slower in a solvent. It is suggested that the closing of this issue was somewhat premature. If indeed the question of how fast a solute will diffuse cannot be predicted then one must question the merits of the existing theories more closely.

The differences between the activation energies , $\mathbf{Q_0}$ and $\mathbf{Q_2}$, and frequency factors , $\mathbf{A_0}$ and $\mathbf{A_2}$ that have been the focus of intense scrutiny over the previous half century. It was the prime objective to develop a model to describe the interactions between solute and solvent ions in dilute alloys and thus predict the diffusion parameters for any arbitrary solvent solute system. The activation energy (enthalpy) or migration energy has been regarded as a principal means of determining the diffusion coefficient of the solute. Hence if the solute activation energy is lower than that of the solvent self-diffusion , the solute will exhibit fast diffusion, and vice versa.

Extremely high rates of diffusion were regarded as a deviation away from substitutional vacancy diffusion toward interstitial diffusion. The relative values of the solute parameters are thought to be determined by differences in the atomic properties of the two elements and their interactions. The development of a general model was considered of great importance in furthering the understanding the theoretical principles of diffusion in metals and other solid states . The failure of the theory in generating a predictive model of diffusion parameters has resulted in research being directed toward determining specific diffusion parameters for each solvent system. This is a lengthy , expensive and

laborious process as a consequence research has been directed toward a small group of commercially important solvents. This narrowing of the focus has its disadvantages.

The development of a general model requires application to all solvents and any model based on a select group of solvents could easily be in error. Typically, the focus has been on the noble metals Copper, Gold and Silver. It never has been stated clearly why these were chosen as the principal focus or why they might be considered typical . It was clear that binary diffusion was not being adequately modelled by the preponderance of so called anomalous diffusion rates observed in experiments, nor was there any more success with ternary systems. The shift in focus toward other areas of diffusion studies does not imply that the issue of what determines diffusion of solutes has been rendered irrelevant. This issue is at the core of all diffusion studies and until it is modelled correctly no significant progress in the field will ever manifest itself. It must be pointed out that inspite of the casual treatment of this issue , still no model exists that can even predict whether a solute will diffuse slower or faster than the solvent self-diffusion rate with any known degree of certainty. Consequently no model can predict, quantitatively , solute diffusion parameters.

Peripheral to the main thrusts of diffusion over the last two decades was work by Hahn and Averback (1986,1987,1988) and earlier by , Owens and Turnbull (1972), Hood (1978) and Warburton and Turnbull(1975). These researchers found a strong link between solute radius and diffusion rates in systems such as lead , titanium and zirconium.

Their general conclusions were that small solutes could take advantage of interstitial diffusion mechanisms and thereby exhibit fast diffusivities and low activation enthalpy. It was not clear whether these studies and their conclusions were extendible to other systems. It was also not evident whether these results corroborated or refuted the prevailing theory of diffusion developed by Le Claire (1962) known as either the relative valence model or the screened coulomb interaction model. It was not an issue with the authors at the time and it might be said that they thought the results simply accounted for anomalous behaviour missed by the dominant models.

The introduction of Le Claire's (1964) amended model relating solute diffusion parameters of homovalent solutes to differences in the ground state energies of the solute and solvent opened the door to many new concepts that were never investigated fully. Since the equilibrium radius of an atom is related to its valence (and thus its Fermi Energy), relative atomic sizes could no longer be dismissed entirely. No attempt has been made to investigate diffusion parameters from the perspective of energy differences over a wide range of solvents nor has any attempt been made to relate these to atomic sizes. This study will attempt to resolve at least some of the issues and will present a model that links the energy, size and diffusion parameters into a basic model .

1.2 BACKGROUND

Several models for the prediction of Activation energies of solutes have been proposed in the past , with mixed results. The largest single problem in verifying these models has always been comparing the theoretical or predictive values of a solvent system with experimental data. Often models were presented with less than a dozen experimental values for diffusion parameters available. Models were necessarily based on the experimental evidence at hand and that was rather limited. New models were developed as more experimental data was accumulated , again with mixed results. No one could in fact verify the validity of sometimes conflicting experimental evidence and the choice of values used to construct models may have been more subjective than anyone really desired.

It is the intention of this dissertation to review some of these earlier efforts and review the ability of the various models to predict diffusion parameters compared with the aggregate of data now available from experimental research. By using data base management system (DBMS) software it was thought possible to conduct hundreds of comparisons between theoretical and experimental values. Of specific interest was one of Le Claire's (1964) last major models based on ground energy states of solute and solvent ions and the work of Varley (1954) dealing with equilibration of energy fields associated with solvent and solute ,in alloys.

The activation energy of solvent self diffusion shows a high degree of correlation with crystal structure and melting point of the atomic species (Cahoon and Sherby ,1992). However, it is not possible to correlate self-diffusion parameters with those of the same species when it is a solute within another atomic species. A general pattern, of impurities adopting the diffusion parameters of the solvent, is more than just coincidental. Unfortunately the solute parameters are rarely if ever identical to those of the solute. This phenomenon of incomplete equilibration is at the core of the problem of how do dilute solutes adapt to the solvent.

Differences in the Q_0 and Q_2 ,

$$\Delta Q = Q_2 - Q_0 \qquad \textbf{Equation [3]}$$

have been variously attributed to differences in atomic radii, atomic volume, ion core charge, first ionization potential , valence and atomic ground state energy. Unfortunately , due to the limited resources, few proposals have been examined and compared with the experimental data.

The successes to date are limited to select groups of solvents , primarily the noble metals Cu, Ag and Au and a small number of the solute elements immediately following these in the atomic table. Attempts to model diffusion in transition elements have not shown any consistent correlation between experimental and predicted values for ΔQ .

1.3 Le Claire Theory (Relative Valence)

One model has been adopted by the discipline as the dominant theory and is regularly quoted in the literature. This is the model proposed by LeClair (1962) often termed the **relative valency model**. The basis of this model is the assumption that the only difference of consequence between a solute and solvent ion on a lattice site is the difference in valence, $\mathbf{Z_L}$(solute valence -solvent valence). This difference totally accounting for differences in solute diffusion.

This model assumes that if the solute valence is greater than that of the solvent then the solute will have a $-\Delta\mathbf{Q}$, that is the solute will require less energy to make a jump to a nearest neighbour vacancy than will a neighbouring solvent atom. The reduction in jump energy required will lead to faster rates of diffusion for the solute than the solvent self-diffusion rate D_0 (thus $D_2 >> D_0$). This model when first described by Leclair (1962) was based largely on two solvents , silver and copper , both of which were taken as having a valence of +1 . The solutes Cd^{+2}, In^{+3}, Sn^{+4} and Sb^{+5} were all found to have a $-\mathbf{Z_L}$ (Le Claire term for charge difference), and $-\Delta\mathbf{Q}$ values when introduced to Ag^{+1}. While the solutes Zn^{+2}, Ga^{+3}, Ge^{+4}, As^{+5}, and Sn^{+4} were also found to have $-\Delta\mathbf{Q}$ when introduced to copper, Cu^{+1}.

The solute is thought to contribute all of its valence electrons to the surrounding sea leaving a positive charged ion core which attracts the negatively charged vacancies , decreasing the energy of activation. A solute with a lower valence than the solvent would

then be expected to have a slightly more negative ion core, repelling vacancies and resulting in a $+\Delta Q$ value for diffusion.

Unfortunately there were problems with the model , notably no means of achieving a $+\Delta Q$ with transition elements was possible unless a new valence designation was adopted specifically for the solute, i.e. Fe^{+2} would have to have a -ve valence in Cu in order to get a $+ Z_L$ and thus $+\Delta Q$ which is typically the result of experimental tests. Furthermore LeClair (1962) acknowledged that even though there might be some grounds upon which to modify transition element valences (Hume-Rothery,1968) he did not address the problem of homovalent , (solutes of same valence as solvent), solutes at that time. Considering these difficulties the model was best suited for noble metal solvents .

The purpose of this project was initially rather vaguely defined as , attempt to find some correlation between ΔQ of solute impurities and some atomic characteristics of the relevant metals. Attempts were made to correlate crystal structure , valence , atomic radii, ionic radii, melting points, boiling points and sublimation energies with ΔQ and all showed marginal relationships at best. An attempt was made to correlate Fermi Energies with ΔQ again with marginal results (Cahoon 1994). An earlier effort by the author to develop a model of diffusion in α-Iron , based on differences in Goldschmidt ionic radii had a surprisingly high degree of qualitative and quantitative agreement with experimental data. This isolated success was based on a modification of work carried out by Cahoon and Sherby (1992). The basis of this modification was intuitive at best and assumed that

regardless of the tendency of the relative valence to favour either a $+\Delta Q$ or $-\Delta Q$ condition , the ultimate deciding factor was the relative differences in ionic radii of the pure elements. Smaller solute ions tended to $-\Delta Q$ and vice versa. Unfortunately the successful correlation fell off markedly in other solvent systems. Lazarus(1954) and Swalin (1957) and other researchers had considered the role of radii in the past but recent researchers have largely ignored them for a number of reasons. These reasons include the difficulty in determining the actual radius values directly. The radius is clearly related to valence and may be a wholly dependant function of the valence . This then brings up the issue of what is the ionization state of a solute under the influence of a solvent? As Le Claire (1962) points out it may well be that size effects are no more than another manifestation of the ion core potential $V(r)$ around the impurity. He regarded radius as an unnecessarily indirect approach to determining differences in activation energies. Recall that the Thomas-Fermi equation for ion core potential is given by

$$V(r) = \alpha \frac{Ze}{r_0} e^{(-qr_0)} \qquad \textbf{Equation [4]}$$

where q the screening factor is given by,

$$q^2 = 4\pi N(E_f) = 4\frac{me^2}{h^2}\left(\frac{3n_0}{\pi}\right)^{\frac{1}{3}} \qquad \textbf{Equation [5]}$$

and $N(E_f)$ is the density of states at mean Fermi Energy , and m,e, n_0 are respectively the mass, charge and number of electrons per unit volume. h is Planck's constant.

E_f can be found from the relationship between valence and radius, where

$$E_f = \frac{3}{5} k \frac{Z^{\frac{2}{3}}}{r_o^2}$$ **Equation [6]**

and $$k = \frac{h^2}{8m}\left(\frac{9}{4\pi^2}\right)^{\frac{2}{3}} = \frac{2\pi^2 m_e e^4}{h^2}$$ **Equation [7]**

Other versions of the Fermi energy equation determine the number of electrons per unit volume of material rather than per atomic volume,

$$\Omega = \frac{4}{3}\pi r^3$$ **Equation [8]**

the discrepancies are based on the variable packing factors typical of different crystal structures. Nevertheless the choice of equation is not considered an issue as long as it is consistently applied.

1.4 Le Claire Theory (Ground State Energy)

LeClair (1964) suggested a model to account for diffusion of homovalent solutes. He concluded that differences in Ground State Energies , E_0 , for the bulk solute and solvent , given by

$$U = \Delta E = \left(E_0^A - E_0^B\right)$$ **Equation [9]**

result in an effective valence difference.The superscripts **A** and **B** indicate solvent and solute species respectively. The core ion potential now becomes in simplest terms,

$$V(r) = U,$$ **Equation [10]**

the difference in potentials within the solute atomic cell of radius R (the Wigner-Seitz sphere) and that of the solvent. U , according to Le Claire (1964) was then correlated directly with ΔQ. (The difference in activation energy between solute and solvent.) A

positive value for U was considered to represent a potential well at the site of the impurity, a basin of attraction for electrons. The increased local density of negative charges was then thought to repel vacancies with their effective "negative charges" (Le Clair 1964) and conversely if U is negative, a potential hump exists at the impurity site with a slightly positive charge making it more attractive to vacancies than the solvent, leading to $-\Delta Q$ values.

The importance of Le Claire's second model is twofold; first it is the first model to avoid direct comparisons of the valences, and second it is the only model that compares energy terms which could be used directly to determine **Q** , which is itself an energy term. Le Claire considered only homovalent impurities in his proposal of 1964 but made no mention of any exclusivity in its application . The purpose of this model was to deal with only the homovalent impurities that could not be modelled with the relative valence model.

Le Claire(1964) realised that differences in ground state energy between solvent and solute would also be a factor in heterovalent diffusion but made no attempt to include the effect in his earlier theory (Le Claire, 1962).

In order to make a tractable model many assumptions are often made. In the case of Le Claire's proposals of 1962 and 1964, the solvent was modelled as a lattice of point charges , the ion cores within a field of negative electrons. This model was employed by Corless and March (1962). The solute replacing a solvent atom was simply represented as a

change in the core potential ,Z_e. In effect the background solvent was taken as the zero state.

This model cannot account for local changes in ionic radii. In fact by assuming that the solute and solvent are point charges , it reduces to a problem of simply modelling the differences in charge .

One side effect of neglecting radius , was that only diffusion via a vacancy mechanism could be considered and there was no way to determine if a solute had the potential of using an interstitial diffusion mechanism. The other loss was the fact that differences in activation volume were ignored. Curiously, the success of the Le Claire model was best for the specific series of elements Cu, Ag, and Au where the following elements of increasing valence tend to have proportional radius increments as well. It was as if the model was designed for just such series where one could indeed ignore the effects of radius. This was an extremely encouraging finding that in no way contradicted Le Claire but rather illustrated why success might be restricted from generality. In addition to the previously mentioned shortcomings, was the inability to capture dynamic processes that might influence diffusion.

Hood (1978) fitted equations to existing diffusion data that modelled the relationship between solute atomic radii and diffusion in a-Zr , Cu, and Pb. However they were not intended as a general model nor for use in predicting diffusivities in alternate systems. Again no attempt was made to examine whether the assumption that solute valences chosen were appropriate. The underlying assumption that a solute would have the same

valence or more accurately, ionization state in all solvents was never systematically investigated.

Based on early efforts it became apparent that any model simply based on the valence or Fermi Energy was not very satisfactory in predicting ΔQ qualitatively let alone quantitatively. It appeared that at best 40 to 60 % of the predictions would correlate positively on a qualitative basis , little better than random success. The high rate of error was in part due to the wide variety of methods used to determine solute diffusion coefficients , but experimental error appeared insufficient to account for all errors.

1.5 Energy Equilibration Theories

A re-examination of the earlier assumption of radius irrelevance was undertaken. Jaswon (1954) and Varley (1954) mentioned that in alloys a transfer of charge from solvent to solute was accompanied by a change in radius of the atoms. Specifically, donors of charge shrink while acceptors dilate. The charge redistribution was based in large part on the atomic cell theory of Wigner-Seitz (1933,1934) which assumes that the eigenfunctions of the two atoms will have different amplitudes at the boundary based on their respective ground energy states. As a consequence each eigenfuction will be modified to equilibrate the ground state eigenfunctions thus making it single-valued or self-consistant throughout the alloy or crystal lattice (Varley, 1954).

The equilibration of energy (**Fig.1**) is accomplished through charge transfer and accompanying changes to radius. Solvent atoms have an energy spectrum based on minimum energy, E_o^A and those of solute B based on E_o^B. If electrons from A move

toward the lower unoccupied energy bands of B then the energy of the entire crystal will be lowered.

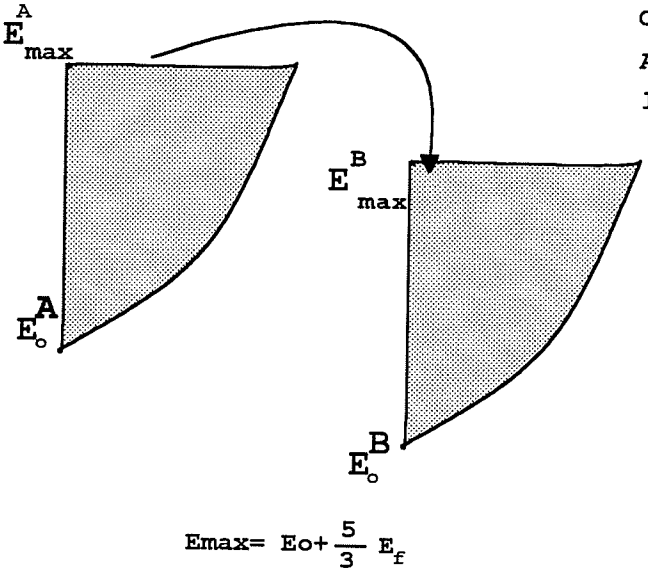


FIGURE 1

Varley (1954) suggests that only the high energy valence electrons actually take part in this exchange or alloying process. Hence the concept of the equilibration of ***Emax*** values. Note since Eo is a function of Ef, the Eo of the solute will also change.

The methods used to calculate the ground state energies , E_0, were derived from the work of Wigner-Seitz (1931, 1933) for a simple monovalent atom,

$$E_0 = -[\Lambda + E_f + I] \qquad \textbf{Equation [11]}$$

where Λ , is the heat of sublimation , and I is the first ionization potential.
Eo has been defined as the energy of the lowest energy electron in the bulk or pure metal , with reference to the energy of an electron in free space which is regarded as zero. In the case of a monovalent metal the energy required to be added in order to sublimate a metal into a state of free atoms would be the difference between ***Eo*** and ***Ef*** such that ignoring all other factors,

$$-(E_o + E_f) = \Lambda + I \qquad \textbf{Equation [12]}$$

Since ***Ef*** , ***Λ*** and ***I*** are known for a large number of elements ***Eo*** can be deduced for many of the pure metals.

In the case of divalent metals in the solid state the interaction energy of the valence electrons must be considered. According to Wigner-Seitz (1933,1934) and Varley (1954) there is a positive contribution to the interaction energy due to Coulomb energy of $1.2e^2/r$ per each possible electron pair in any atomic cell of radius ***r***. Considering the Pauli exclusion principles there will be a negative contribution due to electrons having the same spin of $-.916e^2/r$. An additional factor of $-be^2/r$ must be also included to compensate for the correlation interactions of parallel spin electrons since there is a tendency for electrons of like spin to repel each other slightly. Thus, we obtain an expression for the average interaction energy of an electron pair assuming in this case random mixing of spins,

$\frac{q_o}{r} = \frac{e^2}{r}(0.284 - b)$: where ***b*** **=*b(r)*** (Varley, 1954) **Equation [13]**

The expression for ***Qm*** , the total average interaction energy for a divalent metal , with an atomic cell containing only two valence electrons, becomes ,

$Q_m = \frac{Z(Z-1)}{2} \times \left(\frac{q_o}{r}\right.$ (Varley, 1954) **Equation [14]**

For a trivalent or higher valence atom the first term of the product determines the number of interacting pairs such that for a valence of two there is one pair ,for valence of three there are then three distinct pair interactions.

In the case of the free atom of the given divalent atom the total energy required to remove the electrons is less than would be required if there were no interaction between the electrons. The first ionization potential being less than the second . If no interaction were present the energy required to remove two electrons would simply be 2***Ip.*** The first ionization potential clearly shows the interaction energy contribution of the remaining valence electron. Therefore, the interaction energy of the free atom, ***Qf,*** in the divalent metal is simply the difference between the first and second ionization potentials,

$Q_f = 2I_2 - (I_2 + I_1) = I_2 - I_1$ (Varley, 1954) **Equation [15]**

The solution to total interaction energy of a trivalent metal is essentially the same but for the inclusion of a term to compensate for the ***s-p*** transition that the one electron would

have to undergo in order to be equivalent to I_3. Therefore the expression for the trivalent state must include the promotion energy term , I_T, resulting in ,

$$Q_f = 3I_3 - I_T - \langle I_1 + I_2 + I_3 \rangle \text{ (Varley, 1954)} \qquad \textbf{Equation [16]}$$

and in the case of quadravalent metals there would be two electrons in the p -shell so,

$$Q_f = 4I_4 - 2I_T - \langle I_{1+} I_2 + I_3 + I_4 \rangle. \text{ (Varley, 1954)} \qquad \textbf{Equation [17]}$$

The equation for ***Eo***, in its most general term becomes,

$$E_o = -\tfrac{1}{Z}\langle \Lambda + \sum_{i=1}^{i=Z} I_i + ZE_f - Q_f + Qm \rangle \text{ (Varley, 1954)} \qquad \textbf{Equation [18]}$$

Le Claire (1964) assumes that for homovalent impurities some form of simple charge transfer occurs within an alloy with charge being moved from higher to lower potentials. There is an admission that radius changes will result but are considered irrelevant. In fact, the proposed model of Le Claire presumes that the difference in ***Eo*** values is the only significant factor in determining ΔQ. There was no effort to illuminate the mechanism of equilibration. Difficulties arise with this model when experimental ΔQ values have a contradictory sign when compared with the sign of ***U***. If one considers the actual consequences of equilibration, would additional factors become evident as to the disposition of ΔQ values? Principally are there radius effects that would contradict the general trend of ΔQ ?

The equilibrium radius (Varley, 1954) assumed by a solute ion is related to the ground state energy of the solute such that the

$$\left(\frac{dE_0}{dr}\right)_{r_o} = -\left(\frac{dE_f(Z)}{dr}\right)_{r_0} \qquad \textbf{Equation [19]}$$

Recall that the equation for ***Eo*** contains only two terms that are functions of ***r, Ef*** and the mean interaction term ***Qm*** which is very small.

If charge of amount , ***n*** ,$(n \lesseqgtr 0)$ is transferred from cell ^{A} to cell ^{B} , the new equilibrium radius of the cells will be determined by the relationship,

$$\left(\frac{dE_o}{dr}\right)_{r_o} = -\left(\frac{d\left[E_f(Z+n)\right]}{dr}\right)_{r_o} \qquad \textbf{Equation [20]}$$

According to Varley (1954) if the $\frac{dE_o}{dr}$ is assumed to be constant in the region r = r_o and the direct dependence of ***Eo*** on ***n*** is small and can be neglected, then

$$\left(\frac{dE_o}{dr}\right)_{r_0} = \left(\frac{dE_o}{dr}\right)_{r} \qquad \textbf{Equation [21]}$$

where ***r*** is the new equilibrium radius. Therefore according to Varley (1954) the relationship

$$\left(\frac{d\left[E_f(Z+n)\right]}{r}\right)_{r} = \left(\frac{d\left[E_f(Z)\right]}{r}\right)_{r_0}, \qquad \textbf{Equation [22]}$$

will now be valid. It follows then that since ,

$$[E_f(Z)] = \tfrac{3}{5}k\frac{Z^{\frac{2}{3}}}{r_o^2} \ldots\ldots\ldots then \ldots\ldots [E_f(Z+n)] = \tfrac{3}{5}k\frac{(Z+n)^{\frac{2}{3}}}{r^2}, \qquad \textbf{Equation [23]}$$

Radius is then related to charge transfer n , by the relationship (Varley, 1954),

$$r = r_0\left(1 + \frac{n}{Z}\right)^{\frac{2}{9}} \qquad \textbf{Equation [24]}$$

which is found by solving **Equation [22]** .

In **Equation [24]** , **r** is the new radius , ***n*** the charge transfer and ***Z*** the original valence , i.e. a gain **+n** increases the radius, a loss of charge, **-n** reduces the radius. **Z** can be misleading while it is referred to as valence it actually is the number of valence electrons, not the ionization state which is the number of valence electrons given up. The difference is subtle but important.

The issue here was not whether Le Claire's theorem was appropriate but whether the addition of a method of accounting for the solute radius based on Varley's methods was possible and whether it could account accurately for what were previously referred to as anomalous activation energies. Furthermore, all the values used previously in determining the differences in core potential are based on the bulk material properties. Equilibrium between the electrons of solvent and solute atoms was not at issue. Le Claire's success in correlating U , with ΔQ, was deemed sufficient in 1962 and appears to have been left as it was presented. So taking these factors into account improvements are expected.

Jaswon (1963) and Hume-Rothery(1968) have both separately remarked that solubility of alloy elements is a function of the relative sizes of the two atomic cells and that valence was a significant determining factor in achieving solubility. Jaswon (1954) also

indicates that under certain circumstances a solute ion may shrink sufficiently to attempt to occupy a site adjacent to a solvent atom such that the total volume occupied by the pair is substantially less than bulk volume would suggest. By extension it seemed possible for vacancy space to be increased or diminished as a consequence of these changes in dimensions. Whether or not this phenomenon has any relationship to anomalous solute diffusion rates was not apparent but considered worth investigating.

2.0 OBJECTIVES

The focus of this project was to determine if a general model predicting , $\Delta \mathbf{Q}$ for solute diffusion , qualitatively, was possible to implement. Also the evaluation of the existing models was to be used as a comparison . Le Claire's models (1962,1964) were to be the starting points , primarily due to their ease of implementation, requiring little more than bulk valence and E_0 values. A modification to this model was made to conform to Varley's assumption that only the highest level electrons are actually engaged in transfer of charge. So rather than Eo values , the Emax values were used. This model , to be called the Modified Le Claire Model (M.L.C.), and the original Relative Valence (R.V.M.) and Homovalent models ,would be compared with a data base of experimental solute diffusion parameters and evaluated as to their conformity with the empirical values.

Recall that Le Clair (1964) was originally restricted in the number of solvent systems evaluated and extension to heterovalent systems was not attempted. It was decided to complete the assessment of this model by extending it to the heterovalent systems and broadening the scope to include a larger data base. As much of this model is compatible, even integral to the second model ,the Radius Compensating Model (R.C.M.) , it was quite conveniently accomplished.

The R.C.M. is an attempt to modify the energy difference approach by considering the radius adaptations of solutes . The four models would be tested for a number of solvent systems for qualitative correlation with experimental ΔQ data extracted from the literature and the results tabulated . The four models would be scored in a simple

manner relating the number of correct guesses for the sign of ΔQ versus the actual reported experimental values. If the Radius Compensation Model was indeed valid, an increase in the percentage of correct guesses was to be expected over that of the Modified Le Claire Model and the Relative Valence Model. If success of a model was found to be consistent for a wide variety of solvent systems , it was to be regarded as a sign of general applicability for that model.

If a model was found to have some general application, then a further investigation of the significance would be initiated , with respect to the underlying diffusion mechanisms and the possible extension to quantitative analysis of solute activation energy and frequency factors. No attempt was to be made regarding quantitative estimates of solute diffusion within this dissertation. This was felt appropriate since no experimental proof of any kind of general success had been demonstrated for any model . It was considered prudent to confirm the models experimentally before proceeding to construct a quantitative model.

Ultimately should this work reveal the existence or validity of a general model then there is great hope for the development of quantitative determination of diffusion parameters. The comparison of the three models would in some measure determine the direction for subsequent improvements .

The emphasis on the R.C.M. was due in part to a belief that it would serve as the basis for computer simulation studies of diffusion mechanisms.

3.0 METHODOLOGY

3.1 Compilation of diffusion data

The twenty solvent systems chosen for evaluation have well established values within the body of literature and represent some of the most common and extensively investigated solvents. The solvent systems used for model testing are given in Table 1.

TABLE 1 Solvent Systems Evaluated

α-Iron	**Beryllium**	**Silver**	**Cobalt**	**Gold**
γ-Iron	**Zinc**	**Nickel**	**Magnesium**	**Tungsten**
Molybdenum	**Copper**	**Tin**	**γ-Uranium**	**Aluminum**
Niobium	**Lithium**	**Lead**	**Praseodymium**	**β-Thorium**

To begin the project it was necessary to compile all the available data on the self-diffusion of the elements into a data base. Since this data is representative of the bulk state of the elements it was incorporated into a master data base which included basic physical properties and the ionization potentials for all the elements (TABLE 2). For the purpose of this study the gases and many of the heavier elements were later excluded since either they were of no practical interest or the atomic data was not complete. Where several allotropes were recognised for a element they were included when sufficient data existed. The data presented in **Table 2** includes the self diffusion values for activation energies , and D_o for each element where available (Cahoon and Sherby,1992). The entire contents of the atomic data table, 78 atomic identities (elements and allotropes) , were then run against one of the twenty solvent elements. This in effect produced over

1500 solvent -solute systems for evaluation. Experimental data used to evaluate the performance of the models was however limited to 324 systems. Evaluation of the model performance was based on the experimental data and for some solvents this may represent less than 10 solutes. Several systems had experimental data on as many as 25 solutes.

Table 2 also includes the values for atomic parameters taken from various sources. These include; Goldschmidt ionic radius, atomic radius and interatomic distances (taken as being equivalent), valence (Flinn and Trojan, 1990) , Heats of sublimation and ionization potentials (Kaye and Laby, ****). The Fermi energy values and subsequent calculations of Emax and Eo are based on these extracted values. The master table in spreadsheet form is converted to a relational data base allowing the element data to be sorted and converted back into an ASCII data base (Appendix see **iter.dat**). This extracted data is then used by a C++ program (Appendix see **iter.cpp**) for the various iterative processes used to equilibrate the Emax values and determine the charge transfer and equilibrium radius of the solute. The program was set up to process the entire data base of 78 solutes within a particular solvent system. This was more convenient than trying to reconfigure the data base to the empirical data. Additionally it was interesting to review some of the predictions for solutes for which no impurity diffusion data exists and compare with known solutes. The output of the program **iter.cpp** was merged with the existing table of impurity diffusion parameters of solutes in a particular solvent system **,Tables 3-23**. These tables include the published diffusion data for the various solutes examined within each solvent system and basic atomic information. The predictions as to

solute activation energy are made on the basis of the various relevant factors, discussed later, and compared with the empirical results.

The output of the program iter.cpp included the new adaptive equilibrium radius for each solute within a particular solvent, also the charge transfer required for equilibration of the solute , either positive or negative was determined and presented . Since charge transfer is typically a fractional quantity, an attempt to predict the next full integer value of charge transfer and the dependent radius was also determined. For example if Charge transfer was determined to be n= - .5 with a radius of .98 Angstroms then the next full charge value would be n=-1.0 and a new smaller radius would be determined. Since the transfer of charge is by electrons , the fractional charges relate only to some statistical average and not to actual ionization states possible.

The most significant feature of this procedure is the enormous number of calculations performed for each solute within a given system. It was found to be more efficient to process all the elements as solvents than to attempt to perform calculations for one solute at a time.

The model of Le Claire and proposed radius adaptation procedures was to be tested against a wide variety of solvent systems for which experimental impurity diffusion parameters were available. This type of information pertaining specifically to Activation Energies and Frequency Factors is available in Smithells Metals Reference Book (1967).

Augmentations of this data base from other sources (Fricke,1972, Hirano **** , Mrowec ,1980) increased the data base size significantly.

This results in 324 solvent-solute system pairs for which experimental data exists for the solute impurity diffusion parameters (see appendix for tables 3-22). The predictions generated according to the models are checked against these values and the accuracy determined. Note that each solvent system includes itself as a potential solute. This technique was employed to check the accuracy of the output. It was assumed that the models should return null values for any solute with atomic parameters identical to that of the solvent.

Typically the diffusion data (both self and impurity) is quite variable due to the variation in experimental technique and wherever possible several values may be listed along with references. The tables on impurity data a are cross referenced to the atomic data in a relational database by indexing the element . This allows for complex investigations of interrelationships between the solutes and the various solvents. Included in the master atomic table in addition to self-diffusion data, was atomic radius , ionic radius valence, and heats of sublimation. The variables specific to each element such as the Fermi Energy, Emax, sum of ionization potentials correlation and interaction potentials were determined for each element through the use of supplementary computer code and application specific routines. Some data , principally the heats of sublimation or higher ionization potentials,

was unavailable for the radioactive elements and these elements were excluded from the main body of the table.

Elements were sorted on the basis of valence for ease of review. Subsequent sorts were conducted to organise, in descending order, the elements as to Eo and Emax values. Graphical results (Figure 2) were produced to aid in visualising relationships between energies , radius, and any other variable of potential interest. The use of a computer data base was primarily to streamline energy calculations and to control the rather extensive volume of material generated. Data was extremely easy to extract , in an ASCII format, from the basic tables and exported for use by supplementary C++ programs and vice versa. This in effect suggests that atomic elements could become a data type according to Object Oriented Programming techniques, permitting sophisticated programming approaches to quantum mechanics problems.

3.2 Determination of the Mean Fermi Energy , E_f, and Ground State Energy, E_0 .

The important variables to be determined in the development of the various models was , E_o, the ground state energy. The formula for which, was given earlier in its most basic form for monovalent elements. A more general form taken from Varley (1954), and capable of handling polyvalent atoms, was used throughout this study,

$$E_o = -\frac{1}{Z}\langle \Lambda + \sum_{i=1}^{i=Z} Ip_i + ZE_f - Q_m + Q_f \rangle \qquad \textbf{Equation [25]}$$

where , Z is the valence , Λ the heat of sublimation , $\sum_{Z=1}^{i=Z} Ip_i$, is just the sum of ionization potentials up to the value of Z, the valence.

$$E_f = \frac{3}{5} k \frac{z^{\frac{2}{3}}}{r_o^2}$$ for the bulk element **Equation [26]**

where $$k = \frac{h^2}{8m}\left(\frac{9}{4\pi^2}\right)^{\frac{2}{3}}$$ ***h***, is Planck's constant and ***m*** the mass of the electron .

Since $$k = 2.25 \times 10^{-39} \frac{(Joules \times \sec)^2}{kg}$$, r_o =***metres*** , and ***Z*** is dimensionless

the units for the expression ***Ef*** are in Joules /mole.

$$E_f = \left(\frac{3}{5}\right) \times 2.25 \times 10^{-38} \frac{(Joules \times \sec)^2}{kg} \times \frac{(Z)^{\frac{2}{3}}}{r_o^2} \times \frac{1}{m^2} = \frac{\left(Joules^2 \times \sec^2\right)}{kg \times m^2} = \frac{J^2}{m} \times \frac{s^2}{kg \times m}$$

$$= \frac{J^2}{m} \times \frac{1}{N} = \frac{J^2}{J} = Joules$$ **Equation [27]**

It was decided that working in units of electron Volts and Angstroms would be more convenient , so the following conversion modifications were made ,

$$E_f = \left(\frac{3}{5}\right) \times 2.25 \times 10^{-38} \times \frac{(Joules \times \sec)^2}{kg} \times \frac{1}{10^{-20}} \times \frac{1}{A^2} \times \frac{1}{1.602 \times 10^{-19}} \times \frac{eVolts}{Joules} = \left(\frac{eVolts}{atom}\right)$$

Equation [28]

where $$1 \frac{eVolt}{atom} = 1.602 \times 10^{-19} \frac{Joules}{mole}$$

3.3 Energy Equilibration

It was assumed that the statement of Varley (1954) , that only the high energy electrons take part in the charge exchange process was correct. Then it follows that the solvent

Emax becomes the base to which the solute is expected to adapt through a mechanism of charge transfer and radius compensation.

For the purposes of this project, the Fermi energy component which includes radius and valence was considered to be the most significant route toward equilibration. In effect it will be assumed that only the Ef value of the solute Emax can be altered in order to equilibrate with the Solvent Emax value. The Ef value then becomes a function of the charge transfer and equilibrium radius and hence the Emax value .

$$E^{A}_{\max} \equiv E^{B}_{\max} = -E^{B}_{o} + k\frac{(Z+n)^{\frac{2}{3}}}{\left[r_o\left(1+\frac{n}{Z}\right)^{\frac{2}{9}}\right]^2} \qquad \textbf{Equation [29]}$$

The assumption is that the only possible mechanisms for equilibration are the transfer of charge and the change in the equilibrium radius by the solute.

since ,

$$E^{B}_{0} = -\frac{1}{(Z)}\left[\Lambda^{B} + \Sigma I^{B}_{i} + (Z)\frac{3}{5}k\frac{(Z)^{\frac{2}{3}}}{[r_0]^2} - Q_f + Q_m\right], \qquad \textbf{Equation [30]}$$

then,

$$E^{A}_{\max} \equiv E^{B}_{\max} = -\frac{1}{(Z+n)}\left[\Lambda^{B} + \Sigma I_i + (Z+n)\frac{3}{5}k\frac{(Z+n)^{\frac{2}{3}}}{\left[r_0\left(1+\frac{n}{Z}\right)^{\frac{2}{9}}\right]^2} - Q_f + Q_m\right] + k\frac{(Z+n)^{\frac{2}{3}}}{\left[r_0\left(1+\frac{n}{Z}\right)^{\frac{2}{9}}\right]^2}$$

Equation [31]

3.4 Polynomial Solution

The solution to **Eq.31** is a polynomial of the form,

$$\alpha + \beta N + \gamma N^{\frac{-2}{9}} = 0 \qquad \textbf{Equation [32]}$$

where $\alpha = E_{\max}$ of the solvent,

and β is the term $[\Lambda + \Sigma I_i - Q_f + Q_m]$ for the solute

and $\gamma = -\frac{2}{5} k \frac{Z^{\frac{4}{9}}}{r_o^2}$

Since no closed form solution is possible for Eq.31 an iterative solution is employed to solve for N which includes only the number of valence electrons and the charge transfer variable n.

3.5 Determination of Charge Transfer

The solution of the previous polynomial yields a value for N from which the value of charge transfer can be derived once a value for the number of valence electrons is inserted, where

$$N = \frac{1}{(Z+n)} \quad \text{or} \quad n = \frac{1}{N} - Z \qquad \textbf{Equation [33]}$$

The term ($Z+n$) is the new effective valence of the solute ion. This term provides some insight into the actual solute valence which has been rather arbitrarily assigned in the

past. In effect one does not have to guess the solute ionization state but simply insert the number of known high energy electrons available for equilibration.

As the solution for Eq.32 requires an initial guess , it is quite appropriate to set **n** to **-Z** implying that all the available electrons are donated . Adding back fractional charge until ***n*=0** during each iteration explores the entire range of options from . Occasionally no solution is possible within the described limit. This suggests that some solutes either cannot equilibrate due to an insufficient number of valence electrons or that they must adopt a -ve valence. It is possible to expand the range of n to examine the actual numerical solutions, the significance of such solutions is not however obvious.

3.6 Determination of Equilibrium Radius for solute

Solving for ***n*** one can determine a value for the new radius ,

$$r = r_o\left(1 + \frac{n}{Z}\right)^{\frac{2}{9}}$$ **Equation [34]**

where r_o is the original radius. **Z** is the original valence.

Solutions for ***n*** , were found by implementing a computer program written for the task, **iter.cpp** (source code presented in the appendix) . The value of ***n*** , was found by iteration of the polynomial expression for values of ***n*** between -ve valence and +valence, in increments of .025, for the particular element being examined as an impurity within a particular solvent. Recall that alpha is the solvent ***Emax*** value. With this program any

number of elements could be evaluated as impurities within the particular solvent system and predictions on their possible ΔQ values determined based on the relative differences in ***Emax*** and radius of the impurity ion subsequent to equilibration. The impurity ion equilibrium radius was calculated based on the charge transfer ***n*** . Since in most instances n is a fractional quantity and it was assumed only integral numbers of electrons could be redistributed , the radius for the solute was also determined for transfer of the full integral charge value. In effect three values for the impurity radius were determined the base atomic radius based on the pure metal, the statistical equilibrium radius based on the value of the charge transfer quantity ***n*** required to make the energy of the solute equilibrate with the solvent and finally the radius for a whole number of electrons rounded up or down from the value of ***n*** based on whether it is positive or negative valued. The term ,

$$Z+n \quad ,$$

is regarded as the ionization state of the solute in solvent In this manner the question of the solute ionization state can be finally answered. Further investigation of this issue was not pursued beyond a simple calibration check to insure that in the case of allotropic elements that the reported ionic radii for specific ionization states coincided with the those predicted.

3.7 Prediction Parameters

The algorithm was designed to evaluate the respective energy values for the solvent and each of more than 70 solutes. The first major component of analysis is the determination of the differences in Emax energy and a prediction of possible ΔQ according to the

Modified Le Claire Model. Note the solution algorithm does not deal with the Relative Valence Model , that is accomplished within the spreadsheet since it is simply a difference between the bulk valences for solute and solvent.

The next stage of evaluation is a comparison of the atomic radius of the solute with that of the solvent. If the solute energy is lower than the solvent (more negative) then a potential well exists that attracts electrons. The exact value of that charge transfer is iteratively calculated and the new equilibrium radius of the solute is compared with that of the solvent.

There is some ambiguity regarding the radius of the solvent. Knowing the valence of a solvent it is possible to look up the Goldschmidt ionic radius , however X-ray diffraction data implies that the solvent still takes on a crystallographic spacing , the interatomic distances of twice the atomic distance with the high energy valence electrons in the sea of electrons. It appears that the sea is evenly dispersed nevertheless and the interatomic distance maintained inspite of the decrease in the ionic radius.

If the atomic radius of solute is less than solvent interatomic distance / 2 it is assumed the solute will have a $-\Delta\mathbf{Q}$ regardless of the charge transfer. The assumption was arbitrarily made and ignores the fact that relaxation of solvent atoms in the vicinity of a vacancy tends to decrease the volume of the vacancy by some variable percent of the solvent atomic volume (Shewmon, 1989). There was no simple means to predict a relaxation

volume for the vacancy and it was hoped that if a trend of correlation was evident this would not strongly affect the observed results. In the case of charge transfer to the solute another arbitrary assumption was made, that the atom could not dilate beyond its atomic diameter. Therefore a small solute gaining charge would remain small and still express a $-\Delta Q$, while a large charge accepting solute would inevitably remain too large and would express a $+ \Delta Q$ value. In logical terms the solution algorithm first determines the direction of charge transfer by comparing the Emax values of the solute and solvent,

if solute Emax is > solvent then U is negative and charge leaves the solute.

then If the solute atomic radius, or the solute equilibrium radius, or the solute next full charge radius is < solvent atomic radius **ΔQ** is negative for the solute. If all three conditions are false then **ΔQ** is positive. Essential the only time this model contradicts the Le Claire model is when all three conditions are false, yielding a reversal of the prediction. (*It later became clear that ion states larger than the solvent were capable of demonstrating* $-\Delta Q$ *values inspite of being somewhat larger. As there appeared to be increased kinetics associated with these charge donators, a problem of an upper limit to the cutoff became apparent. The assumption that the cutoff limits are identical to the atomic diameter of the solvent appear to be less than ideal . Unfortunately there did not appear to be a simple means of adapting these concepts at the time and only revealed themselves after the analysis*)

If the Emax is < solvent then U is positive and charge enters the solute,

then If the solute atomic radius is > solvent atomic radius **ΔQ** is positive

(note occasionally solutes of this class were bumped up, i.e. their radii were within .03A of the solvent and this was thought to be too close to qualify as smaller . This brings up the issue of a lower cutoff limit which must be considered as being in some way related to the relaxation phenomenon)

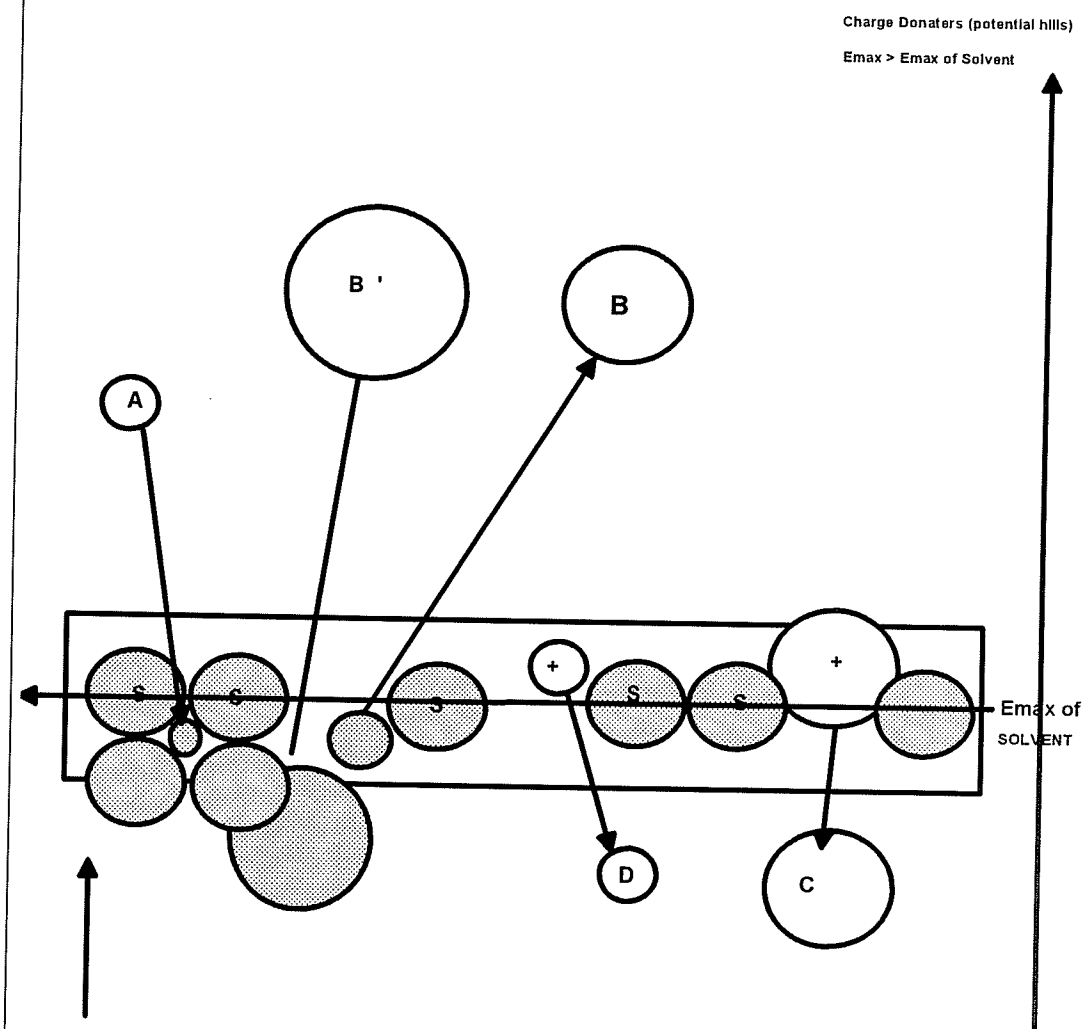
If the solute atomic radius is < solvent interatomic radius ΔQ is negative

(Reversing the LeClaire prediction)

It is possible for a very large impurity to lose charge during equilibration and still after contracting be larger than the solvent so a positive value of delta Q is still expected. In addition, if charge was transferred only in integral amounts , the next whole number of charge was examined as to its effects on the solute radius. If whole charge is the only physical quantity to be transferred then the solute would in effect never actually achieve a stable equilibrium but would be constantly either too high or too low with charge continuously tunnelling back and forth between solvent and solute. If one considers then that the solute exists in two states for different periods of time and statistically equilibrates then the radius of those states may be such that one is larger and the other smaller than the solvent average atomic radius. If in the larger state the impurity would be expected to have a positive delta Q then in the smaller state it might have a negative delta Q . As the diffusion data on solutes represents a statistical average of the events it is probable that an oscillator would appear to have a negative delta Q though not as dramatic as for a solute that existed in two states both of which were smaller than the solvent radius. Additionally it was considered a possibility that a charge donator could

adopt an ionic radius small enough to allow the solute to begin diffusion using the interstitial mechanism. The only way to verify this possibility was to examine manually, specific solutes and check their frequency factors. In this case the approximation of Shewmon(1989) where a ratio of 10:1 for A_0 and A_2 to be indicative of vacancy mechanism while much higher ratios would be taken as an indication of interstitial diffusion.

The value of delta Q for a solute would then appear to be a function of the differences compared with the solvent ,in energy , atomic radius, of the ground state and equilibrated state as well as the frequency with which the solute changed states. It is clearly beyond the scope of this paper to answer these later issues. It remains the goal to verify if in fact the addition of a radius compensating formula to the original model of Le Claire could become the basis of general model for making qualitative predictions on the differences in activation energy between solute in the solvent and self-diffusion for the solvent.



A- will always fit into a solvent vacancy therefore -ve dQ

B- will only fit into vacancy after losing charge and adopting an ionic radius less than that of the solvent. If this is possible it will be a -ve dQ

B'- even after losing charge still too large therefore +ve dQ

C -after accepting charge inevitably too large therefore +ve dQ

D-after accepting charge may still be small enough to fit into vacancy therefore -ve dQ

Note D and C cases , it seems unlikely that these impurities can actually get significantly larger than their basic atomic diameter

FIGURE 3

3.8 ANOMALOUS RESULTS AND TREATMENT

The nature of this project was rather complex in that not only were several models being compared as to their relative merits but also at issue was the actual diffusion mechanism. Subsequent to the early analysis of the data according to the previously listed procedures certain anomalous results with large solutes and very low activation energies (primarily the alkali metals) suggested further investigation. This included small tests as to the impact of varying the cut off points. Initially the assumption was to set the cutoff point identical with half the interatomic distance of the solvent. Later tests were conducted to evaluating points slightly greater and lower than half the crystal interatomic distance. This was simply a change to the manner in which the algorithm made a prediction. Later yet this concept was mathematically embodied into the energy equilibration program.

The principle used was, that large solutes could not possibly exist within a smaller solvent atom crystal without adopting a new dimension determined by the crystal spacing. Using as an upper limit half the interatomic distance x 1.05 as the solute's cut-off point , the Ef of the solute was recalculated using the solvent atomic radius and making the required modifications to the Emax value of the solute. As a consequence of "squeezing" these large solutes their Emax values tended to increase ,requiring a different solution to charge transfer than expected only on the basis of the solute's bulk properties. This procedure was hoped to provide a means of eventually incorporating relaxation factors, strain energy and their influence on solute energy levels. The results of this procedure employed in solvent systems; Gold, Copper and Aluminium are presented in the results section .

4.0 RESULTS

4.1 Solvent Systems

The diffusion data in the results section Tables (24-47) has been taken from the Impurity Diffusion Parameter Tables (3-22). References for the diffusion values are given in the latter in order to conserve space in the former.

4.1.1 Aluminum (31 samples),

(see Table 3 for impurity diffusion data, appendix Table 24 for equilibration data)

There was experimental diffusion data available for 31 solute elements. The energy difference models , predicted the correct sign for **ΔQ** in 19 of the cases while the Radius Compensating Model **(R.C.M.) predicted** the correct sign of **ΔQ** in 20 cases. The R.C.M. reversed the sign due to the size of the solute and predicted a **ΔQ** incorrectly in 4 cases.

Examination of the scatterplot **(Fig.5)** of Delta radius versus Delta Q reveals a large number of solutes with large atomic radii exhibiting **-ΔQ** values as well as some small solutes exhibiting **+ΔQ** values . These make up the error predictions. The scatter plots for the other solvent systems showed this problem to varying degrees. It was noticed that there was a relatively high incidence of predicting the large Alkali metals and the low melt point metals on the right of the noble metals incorrectly for many solvent systems. This relationship prompted the re-evaluation of the radius used to calculate solute energies. Cesium while not common as a solute in diffusion experiments was relatively consistent in having low activation energies in spite of its enormous size, in whatever

solvent . See Section **4.1.21** for the results of this alternative strategy for calculating solute energies and equilibrium radius.

(Note all solvent systems include the solvent as solute in order to check the ability of the models to zero energy differences and demonstrate a common reference. The use of the solvent as a solute was also used as a check for errors in the data base. Clearly the Relative Valence Model is incapable of dealing with homovalency and suffers seriously from this short coming.)

The original model of Le Claire (1962) , the Relative Valence Model proved to be able to correctly predict the sign of the experimental activation energies for solutes in 10 cases. If the Homovalent impurity model of Le Clair is used to fill in the missing values of the R.V.M. then the aggregate success is improved slightly to 45%.

In fact examination of Fig.5 shows a reasonable line could be drawn through the points with the exception of Be and Co, lending more credence to the R.C.M.. This trend is more obvious when large solutes are forced to accommodate the aluminium radius, Fig.25 and Table 44.

The **Relative Valence Model (R.V.M.)** success was 32.26%

The **Ground State Energy Difference Model (U)** success was 61.29%

The **M.L.M** success was 61.29%.

The **R.C.M** success was 64.52%

4.1.2 Beryllium (11 samples),

(see Table 4 for impurity diffusion data, appendix Table 25 for equilibration data)

There was experimental diffusion data for 11 solute elements in Beryllium . The energy difference models U and M.L.M., were able to predict the sign of ΔQ correctly in only 3 and 4 cases, respectively while the radius compensating model predicted the correct sign of ΔQ in all 10 cases. The Emax value of Be is very low at -8.173 eV and as such most of the solutes would be expected to donate electrons becoming $-\Delta Q$, according to the M.L.M. however due to the small atomic radius of Be the R.C.M. predicts few if any of these elements with the exception of Carbon actually shrink enough to occupy a Beryllium vacancy. As a consequence the R.C.M. predicted that these elements would all have $+\Delta Q$.

The R.V.M. managed to predict the correct sign of ΔQ in only two cases of the ten.

The value of the R.C.M. seems to be most evident when the solvent is radically different from the solute atoms in dimension.

The R.V.M. success was 45.5%

The **U** success was 27.3%

The M.LeC.M success was 36.4%.

The R.C.M success was 100%

4.1.3 Cobalt (9 samples)

(see Table 5 for impurity diffusion data, appendix Table 26 for equilibration data)

The M.L.M. predicted the correct sign of ΔQ in only 5 of the 9 cases for which ΔQ were available. The R.C.M. predicted the sign correctly in 6 of the 9 cases. The two errors of the R.C.M. were also common to the M.L.M. where potential wells appear to have much higher rates of diffusion than predicted . Only in the case of Ni and alpha Iron did the R.C.M. reverse the M.L.M. model predictions thereby predicting correctly the additional two cases. The U model was correct in all cases but for Carbon. This is the best performance for this model of any solvent system. The U model appears to be better in predicting the sign of the activation energy in heterovalent systems than the point charge model or the R.V.M. . In fact over all the systems investigated , see Table 26, the U model was better by over 10% however the results were highly variable.

The R.V.M. success was 33.33%.

The **U** success was 89 %

The M.L.M success was 55.55%.

The R.C.M success was 77.77%

4.1.4 Copper (32 samples)

(see Table 6 for impurity diffusion data, appendix Table 27 for equilibration data) The M.L.M and the R.C.M correctly predicted the sign of **ΔQ** in only 20 and 17 of the 32 elements, respectively for which **ΔQ** were available. In 8 cases the two models had the same error , predicting a solute to be a potential well expecting a +**ΔQ** when the data indicated -**ΔQ**.

(Note this system was re-evaluated using the solvent lattice dimension as the upper limit for radius of large solutes and the results presented in **4.1.22**)

The U model correctly predicted the correct sign of **ΔQ** in only 14 cases.

The Relative Valence model correctly predicted 17 of the 32 solutes. Of the four models tested this is a poor performance. Copper is one of the original solvent systems along with Silver and Gold, on which this very model was based. It is a bit surprising that the performance is so poor .

The R.V.M. success was 53.12%.

The **U** success was 43.75 %

The M.LeC.M success was 62..5%.

The R.C.M success was 53.12%

4.1.5 Gold (16 samples)

(see Table 7 for impurity diffusion data, appendix Table 28 for equilibration data)

The M.L.M. predicted the correct sign for ΔQ in 11 of the 16 cases for which ΔQ values were available. The R.C.M. predicted only 9 correct signs for ΔQ, which included all five of the same errors made by the M.L.M. and an additional 2 errors.
(Note this system was re-evaluated using the solvent lattice dimension as the upper limit for radius of large solutes and the results presented in **4.1.23**)

Of the 5 common errors, 4 were for potential hills with expectant $-\Delta Q$ that demonstrated $+\Delta Q$. Note that Gold has a very low Emax , at -9.877 eV and there is a general expectation for solutes to become donors with $-\Delta Q$. In addition the Gold Atomic radius at 1.44 Angstroms is quite large . Most solutes averaging closer to 1.25 A.

The Relative Valence Model was capable of correctly predicting the sign of ΔQ in 10 of the 16 systems examined. While the U model made only 8 correct predictions. In this system combining the U and R.V. models would result in 13 correct predictions clearly supporting the logic of Le Clair (1964) in proposing the Homovalent impurity modifications to correct the deficiencies of the R.V.model. However this was not generally the case when extended to systems not originally considered.

The R.V.M. success was 62.5%.

The U model success was 50%

The M.L.M success was 68.8%.

The R.C.M success was 56.3%

4.1.6 α-Iron(25 samples)

(see Table 8 for impurity diffusion data, appendix Table 29 for equilibration data)

Both the M.L.M and the R.C.M. predicted 19 of the 25 **ΔQ** correctly. The **ΔQ** values in brackets ,see Table 8, are those of Hirano (*****) and where possible these were used as the basis of comparison. It is clear that the wide variety of experimental values creates a difficulty in assessing the predictions. However in only three cases is the Hirano(*****) data at odds with the Smithell's values. In other cases it is the only data or it is corroborated by Smithell's. Only three of the incorrect predictions are common to both models. Where 4 of the incorrect predictions are for potential hills some of which are faster and some slower than would be predicted. Looking specifically at the solute Al with experimental **ΔQ** of -4.8 Kj/mole , one could see that this is extremely small value. The radius predicted for the Al ion at equilibrium is 1.377 A and at the full deficit of one electron would be 1.3 which is still larger than the alpha Iron atom at 1.26 A if only slightly. Intuitively one might guess that the actual activation energy would be close to that of iron. The equilibrium charge transfer n for Al is -.4665 less than one full electron. If Al then would be oscillating between 0 and +1 ionization states it would never exist as an ion smaller than iron. However it raises the issue of the impact of the oscillation rate, could this rate effect the **ΔQ** negatively or positively?

The R.V.M. success was 44 %

The U model success was 60%

The M.L.M success was 76%.

The R.C.M success was 76%

4.1.7 γ-Iron(20 samples)

(see Table 9 for impurity diffusion data, appendix Table 30 for equilibration data)

The R.V.M. correctly predicted only 8 of the 20 signs of the **ΔQ** for experimental solute data . The M.L.M. correctly predicted only 6 of the 20 signs. The R.C.M. was only slightly better at predicting 11 correct signs of **ΔQ**. The improvement due to the reversing of prediction based on Energy differences alone. The two models shared 9 incorrect predictions, where potential wells with expected +**ΔQ** were found experimentally to have much lower activation energies ,-**ΔQ**. The value of Emax calculated for the solvent may in fact be too high at -3.066 . If the actual Emax for the solute was more negative by a factor of 2, it would still not correct the errors. Some of these fast diffusers have extremely low Emax values and no simple explanation presents itself at this time. No model was capable of adequate performance when compared with the experimental data in this system. Combining the U and R.V.M. models would result in 10 correct predictions, for 50% success, This is a case where performance of either model is enhanced by union.

The R.V.M. success was 40%

The U model success was 40%

The M.L.M success was 30%.

The R.C.M success was 55%

4.1.8 Lead (16 samples)

(see Table 10 for impurity diffusion data, appendix Table 31 for equilibration data)

The M.L.M. predicted 9 of the 16 **ΔQ** signs correctly. The R.C.M. predicted the sign of **ΔQ** correctly in 14 of the 16 cases. The Emax of lead is -9.633 , which is quite low, implying that many of the solutes would become potential hills with - **ΔQ** values. Whenever the M.L.M. predicts a potential well the R.C.M. reverses all of those predictions because the size of the solute is still too small , even at the full atomic diameter, to show a retarded diffusion rate. The lead atom is one of the largest with a radius of 1.75 A. It appears that even large atoms like gold can still diffuse quite freely. The lead solvent system clearly demonstrates the ability of the R.C.M. to improve on predictions based solely on energy differences. The union of R.V.M. and U models results in a success rate of only 37.5%.

The R.V.M. success was 37.5%

The U model success was 31.25%

The M.LeC.M success was 56.25%

The R.C.M success was 87.5%

4.1.9 Lithium (12 samples)

(see Table 11 for impurity diffusion data, appendix Table 32 for equilibration data)

This is the first example of the total failure of the Relative Valence Model too get even a single correct prediction of **ΔQ**. The U model in fact is the best with 9 correct predictions but when combined with the R.V.M. the success is marginal 16.6%. The

predictions of the sign of solute activation energy are not good for any of the newer models. The M.L.M with 7 of 12 correct. The R.C.M. having also only 7 correct predictions. The R.C.M. incorrectly predicted that 3 of the potential wells would have $-\Delta Q$ since their atomic radii were less than that of Lithium ,1.52 A. These 3 were Zn 1.33A, Cd 1.5A, and Hg also 1.5A. The vacancy relaxation phenomenon may account for some of this error. A possible solution is to refine the cutoff limit at some percentage less than the solvent radius. In this case the lower limit would have to be the size of the Zn atom which is 15% smaller than the full atomic radius of Lithium. The values of ΔQ in the case of these three elements are also the three lowest $+\Delta Q$ of all adding some support to the trend for small differences with solutes similar to solvent in size.

The R.V.M. success was 0%

The U model success was 75%

The M.L.M success was 58.33%

The R.C.M success was 58.33%

4.1.10 Magnesium (10 samples)

(see Table 12 for impurity diffusion data, appendix Table 33 for equilibration data)

Identical results for both the M.L.M. and R.C.M. models , this clearly demonstrates the fact that the R.C.M. is not an independent model but rather an extension of the M.L.M. The U model with 6 correct predictions is significantly better at dealing with heterovalent solvent/solute systems than the R.V.M. by itself , which had only one correct prediction. Combining the two models of LeClaire improves the success to only 30 %. All

errors identical and suggestive of an inability to set cutoff limits based on the solvent atomic radii. Rather a compensation factor for relaxation should be included. If the relaxation factor was set at 15% less than the solvent radius , that would have brought the cutoff down to 1.36 A. correcting all three incorrect predictions. By changing the cutoff to 1.36A. we find the M.L.M. prediction success unchanged but the R.C.M. improved. Since there is no way to verify the validity of mixed sign experimental data , for the sake of these evaluations both are given a correct score under the assumption that over the entire test of 20 systems the distribution of undeserved correct predictions will not favour one model over another. It would be just as meaningless to count both models wrong. Since clearly one must always be correct if they are different answers.

The R.V.M. success was 10%.

The U model success was 60%

The M.L.M success was 70%

The R.C.M success was 70%

4.1.11 Molybdenum (13 samples)

(see Table 13 for impurity diffusion data, appendix Table 34 for equilibration data)

The M.L.M. predicted the sign of the solute ΔQ correctly in 9 of the 13 cases for which experimental data for solutes in Mo exists. The earlier U model based on ground energy differences was able to predict only 7 cases correctly, while the R.V.M. was correct in only 4 instances. The R.C.M. was correct in 11 of the 13 cases.

The Mo Emax is of concern since it appears to be positive valued and this does not appear to be justified in theory. The calculations for Emax appear to be at fault principally in the values attributed to the I_T , s-p transition energy and the free and mean interaction energies. Regardless of whether the value of E_f for Mo was calculated with the mass volume approach or atomic volume, it was quite high . Several other elements demonstrated the peculiar results as can be seen graphically in FIG(2). Acknowledging that the issue was the relative values of the energies, the analysis of Mo was run anyway. The result of the analysis is peculiar for another reason. This is the first time the computer program was unable to find solutions to the polynomial solution within the range allowed. Recall that it was again arbitrarily determined that only high energy electrons could engage in equilibration of the solute Emax. The number of high energy electrons corresponding to the Z value. In effect the computer program is implying that many solutes, to raise their Emax to that of Mo would require more electrons to be donated than the number of their Z electrons. Solutions to the polynomial are in fact possible, by allowing greater numbers of electrons to be donated than the value of Z, but the relevance of this procedure is in doubt. It appears that many solutes in Mo can in fact not reach equilibrium. The analysis is not compromised by this situation since a potential well is not actually allowed to dilate beyond the atomic radius , and the sign of $\Delta\mathbf{Q}$ is a function of the difference between the solute and solvent atomic radii. The incredibly low $-\Delta\mathbf{Q}$ of the Yttrium solute is remarkable when one considers the solute's size, 1.81 A and the fact that it is a deep potential well. Examination of Fig.15 shows a highly linear arrangement of points with the exception of Y .

The R.V.M. success was 30.76%

The U model success was 53.84%

The M.L.M success was 69.23%.

The R.C.M success was 84.61%

4.1.12 Nickel (23 samples)

(see Table 14 for impurity diffusion data, appendix Table 35 for equilibration data)

The R.V.M. and U models were capable of 15 correct predictions of the sign of the solute activation energy difference. Combining the two models, that is restricting R.V.M. to heterovalent systems and using the U model for homovalent , results in 17 correct predictions.

The M.L.M predicted the correct sign of ΔQ in 18 cases out of the 23 samples for which ΔQ were available. The R.C.M. was significantly poorer , with only 14 correct predictions. Only 2 errors were common to both models. The R.C.M. was unable to predict in 7 cases that large solute atoms could reduce radius sufficiently at equilibrium to actually become $-\Delta Q$, rather the R.C.M. predicted that these solutes would remain too large and have $+\Delta Q$. This situation was seen earlier in the Aluminum system and also the γ-Iron to a lesser degree . (.Note this system was re-evaluated using the solvent lattice dimension as the upper limit for radius of large solutes and the results presented in **4.1.24**)

The R.V.M. success was 65.23%

The U model success was 65.2%

The M.L.M success was 78.26%.

The R.C.M success was 60.86%

4.1.13 Niobium (18 samples)

(see Table 15 for impurity diffusion data, appendix Table 36 for equilibration data)

The R.V.M. was correct in predicting the sign of ΔQ in only 3 cases, while the U model was much more successful with 13 correct predictions. Combining the two models would only improve the R.V.M. by two for 27.7% success. Often the effect of combining the two models is to downgrade or dilute the success of the U model.

Both the M.L.M and R.C. models are correct in predicting the sign of , 15 of the 18 experimental values for ΔQ. Two of the errors are common to both . The accuracy is quite high probably due to the very low, -12.584 Emax value for the solvent and the large atomic diameter . Most elements would be expected to have smaller atomic radii initially and smaller yet as the consequence of charge donation. The role of the R.C.M. does not contribute significantly to improved accuracy in this system but neither does the R.C.M. evidence any loss of accuracy under these circumstances.

Fig. 17 shows a degree of linearity in the distribution of points, with the lines always passing through the solvent self diffusion 0 point.

The R.V.M. success was 16.66%

The U model success was 72.2%

The M.L.M success was 83.3%

The R.C.M success was 83.3%

4.1.14 Praseodymium (11 samples)

(see Table 16 for impurity diffusion data, appendix Table 37 for equilibration data)

The R.V.M. and the U model were very poor in predicting the sign of solute ΔQ , the rates of success were 0 and 2 respectively while combining the two would have yielded only a single correct prediction for the self diffusion case.

This system like that of Molybdenum has a very high Emax value , and the analysis was performed under the same assumptions, as previously discussed. The M.L.M. was unable to predict more than 2 of the 11 samples correctly however the R.C.M. correctly predicted the sign of ΔQ in 10 of the 11 cases. It appears that whenever the solvent system takes on extreme values of Emax or radius the R.C.M. provides better accuracy than the M.L.M . The plot of ΔQ versus ΔRadius shown in Fig. 18 shows a peculiar non-linear distribution of points .

The R.V.M. success was 0% .

The U model success was 18.2%

The M.L.M success was 18.2%.

The R.C.M success was 90.90%

4.1.15 Silver (20 samples)

(see Table 17 for impurity diffusion data, appendix Table 38 for equilibration data)
The very high success rate for the Relative Valence Model , 17 correct of the 20 solutes is at least a good argument for the development of the model in the first place .However of the original three solvents for which LeClaire(1962) proposed the R.V.M. it is the only one for which the data supports the effort. The U model however correctly predicted only 4 cases. Combining the two leads to a slight improvement over the success of the R.V.M., yielding 19 correct predictions.

The M.L.M. correctly predicted the sign of the experimental values of solute ΔQ in 13 cases of the 20 total. The R.C.M. correctly predicted the sign of ΔQ in 18 of the 20 cases. This is a remarkable improvement from the prediction rates for copper and gold . No errors were common to both models.

One of the two errors for the R.C.M. in this system is that of the solute Sn , predicted to be a potential hill, but also a very large atom. With a charge transfer at equilibrium of -1.012 it did not seem likely that tin would go to an ionization state of +2 with the radius of 1.35 A .in order to become smaller than Ag. The **ΔQ** value for Sn is very low at -100.3 kj/mole, in fact it is the lowest of all impurity diffusion rates recorded in Ag. A remarkable attainment for such a large atom especially when compared with Beryllium.
(Sn is one of the low melt point metals with large atomic radius that consistently is predicted to have a $+\Delta Q$ on the basis of size. This metal along with the Alkalis is however

quite amenable to correct predictions if the method of re-evaluation previously discussed is employed.)

The second R.C.M. error with Pt is due to the small difference in size between the two species.

The R.V.M. success was 85%

The U model success was 20%

The M.L.M success was 65%.

The R.C.M success was 90%

4.1.16 Tin (13 samples)

(see Table 18 for impurity diffusion data, appendix Table 39 for equilibration data)

The R.V.M. was correct in predicting the sign of solute ΔQ in only 4 of 13 cases while the U model was correct in 9 cases. Combining the two methods benefits the R.V.M. only in detecting the null condition for the self solute.

The M.L.M. was correct in 5 of the 13 cases. The R.C.M. was correct in predicting the sign of the experimental values of solute ΔQ in 11 of the 13 cases. Sn is a relatively large atom with a fairly typical Emax value of -4.327 eVolts. In the case of the solute, In the imposition of the lower cutoff limit would have predicted the sign correctly .

It is worth noting that when the solute Sn was placed in the solvent Sn the iteration routine will return very low values of n due in part to roundoff errors during the iteration process. If one refers to the top line of each of the solvent system tables , this round off error shows up occasionally . In general the value of charges as low as 0.005 seem insignificant, as would differences in radii of .01 A. The arbitrary choice of manipulating **In** seems of little consequence since the important issue is to evaluate the potential merit of these models and possible modifications to improve their application.

Fig.20 shows a very linear relationship between **ΔQ** and **ΔRadius** for solutes in the Tin system.

The R.V.M. success was 38.46%

The U model success was 69.23%

The M.L.M success was 38.46%.

The R.C.M success was 84.6%

4.1.17 β-Thorium (12 samples)

(see Table 19 for impurity diffusion data, appendix Table 40 for equilibration data)

The Thorium solvent is unusual in that it has one of the largest Atomic radius investigated similar to Pr and Pb. The Emax is typical at -%.138 eVolts. The M.LeC.M correctly predicted the sign of the experimental values of **ΔQ** in only 7 of the 12 samples. The

R.C.M. was correct in every case. The success of the R.C.M. again suggests that the fact that a solute accepts charge does not in and of itself guarantee a $+\Delta\mathbf{Q}$ value for the solute. It seems absolutely essential to check the solute radii against that of the solvent before making a prediction.

The R.V.M. and U models were capable of only 3 and 1 correct predictions of $\Delta\mathbf{Q}$. Combining the two models would improve the apparent success only by including a null value for solvent self diffusion.

Fig.21 for solutes in Thorium , shows a roughly linear distribution of points for $\Delta\mathbf{Q}$ versus **ΔRadius.**

The R.V.M. success was 27.27%

The U model success was .09%

The M.L.M success was 63.6%%

The R.C.M success was 100%

4.1.18 Tungsten (12 samples)

(see Table 20 for impurity diffusion data, appendix Table 41 for equilibration data)

The R.V.M. was correct in predicting the sign of solute $\Delta\mathbf{Q}$ in only 2 cases, while the U model was correct in 11 cases. The combination of the two models improves the R.V.M.

by five additional correct predictions. Overall it appears the success of the combined technique is less than the success rate employing the U model exclusively.

The M.L.M predicted the correct sign of impurity activation energy difference in 10 of the 12 cases for which experimental data was available. The R.C.M. made 3 errors, in the case of Osmium there is the recurring problem of negligible differences in radii . The situation with Yttrium is similar to other very large atoms with high diffusion rates, which shows some correction when the solute radius is forced to accommodate to the solvents lattice parameter. Two solute elements in Tungsten have mixed ΔQ values in the literature . Ir with an initial atomic radius of 1.35A is very similar to W @ 1.37A, and it was expected to become a donor of electrons due to having a higher Emax value than the solvent . The data itself may be at fault but more than likely this situation points to the difficulty the R.C.M. has with discriminating solutes and solvents that have small differences in charge and radius. Any error in calculating the Emax values could lead to mistaken sign of charge transfer.

In general upon reviewing the results of the two energy difference models there is a surprising degree of correspondence. In Table 23 the overall performance of the various models is tabulated and a slightly better performance for the Emax method is seen.

The R.V.M. success was 16.67%

The U model success was 91.67%

The M.L.M success was 91.67%

The R.C.M success was 75%

4.1.19 γ-Uranium (10 samples)

(see Table 21 for impurity diffusion data, appendix Table 42 for equilibration data)

Uranium, though not particularly large at 1.38 A, does however, have a very high Emax value of -1.759 eVolts. Note that since some of the ionization potentials for U were unavailable , the missing values were borrowed from Thorium , which otherwise were very similar.

The R.V.M. was correct in only 1 of the ten systems , while the U model was correct 5 times. The union of the two models produces only five correct predictions.

The M.L. M. correctly predicted only 4 of the 10 signs of the difference in activation energy. The R.C.M. however , was correct in **ΔQ** sign in all but one instance , that of Carbon as solute. The value of which , + 3.8 kj/mole , is rather odd when one regards its **ΔQ** in other systems, where it typically has a -**ΔQ**.

The scatterplot of **ΔQ** versus **ΔRadius** for solutes in Uranium (Table 23) demonstrates a high degree of linearity , with the exception of Carbon.

The R.V.M. success was 10%

The U model success was 50%

The M.L.M success was 40%.

The R.C.M success was 90%.

4.1.20 Zinc (11 samples)

(see Table 22 for impurity diffusion data, appendix Table 43 for equilibration data)

The R.V.M. made 6 correct predictions of the sign of solute **ΔQ**. Combining this with the U model improves the success to 10 correct predictions.

Clearly the M.L.M. and the U model were superior in predicting the sign of solute **ΔQ** values when compared with the R.C.M. with 7 and 8 correct predictions versus 5 for the later model. In 4 cases, very large atoms are diffusing at much faster rates than expected and have remarkably low activation energies. This system was examined subsequently under the imposition of lattice parameters on large solutes and the results presented in section **4.1.26** .

The R.V.M. success was 54.5 %

The U model success was 72.7%

The M.L.M success was 63.63%.

The R.C.M success was 45.45%.

4.1.21 Recalculation of Aluminium Solvent (Table 44 and Figure 25)

(forcing solutes 5% larger than aluminium to adopt radius of 1.43 A x 1.05 for the purposes of Emax determination)

Improves the success of the R.C.M. from 67.% to 77.4% . This turns out to be 3 additional correct predictions. There is a trend seen in Fig 25 for a shift of large solutes to the left , or toward smaller dimensions. The process leaves smaller solutes unmodified.

4.1.22 Recalculation of Copper Solvent (Table 45 and Figure 26)

Improves the success of the R.C.M. from 53.1% to 65.6%, or a gain of 4 additional correct predictions.

4.1.23 Recalculation of Gold Solvent (Table 46 and Figure 27)

Improves the success of the R.C.M. from 56.3% to 62.5 %, which is in fact a gain of only a single correct prediction.

4.1.24 Recalculation of Nickel Solvent (Table 47 and Figure 28)

Improves the success of the R.C.M. from 60.9% to 80%. This system benefited greatly from the recalculation of solute Fermi and Emax energies based on solvent dimensions. In Fig.28 evidence of linearity is quite distinct.

4.1.25 Recalculation of α-Iron Solvent (Table 48 and Figure 29)

Improves the success of the R.C.M. from 76.0% to 80 % which is actually only a gain of one additional correct prediction. However the linearity of the scatterplot as seen in Fig.29 is much improved.

4.1.26 Recalculation of Zinc Solvent (Table 49 and Figure 30)

The impact was marginal for recalculation of solute energies on the basis of solvent atomic dimensions. There was in fact only a gain of 1 additional correct prediction.

4.2 EVIDENCE OF INTERSTITIAL DIFFUSION

Wharburton and Turnbull (1975) give the diffusivities of a number of solutes in lead over a range of temperatures and concluded that the fast diffusion seen with Cu,Pd, Au, Ni, Zn, and Ag was due to interstitial diffusion while slow diffusers such as Tl, Sn, Na, Hg, and Cd were engaged in vacancy diffusion. When the R.C.M. analysis for lead (Table Inset Below) was reviewed it was found that the solutes listed by Wharburton and Turnbull (1975) had the following atomic and ionic radii subsequent to equilibration of Emax values. (Recall that of the listed solutes R.C.M. incorrectly predicted only the ΔQ of Na.)

Slow Diffusers

	Atomic Radius	Equilibrium Ionic Radius	Charge Transfer	
Na	1.86	1.6269	-n	$+\Delta Q$
Hg	1.5	+	+n	$-\Delta Q$
Cd	1.5	+	+n	$-\Delta Q$
Tl	1.71	1.6568	-n	$-\Delta Q$
Sn	1.58	1.4478	-n	$-\Delta Q$

Fast diffusers

	Atomic Radius	Equilibrium Ionic Radius	Charge Transfer	
Cu	1.28	.96	-n	$-\Delta Q$
Ag	1.44	1.13	-n	$--\Delta Q$
Au	1.44	+	**+n**	$--\Delta Q$
Zn	1.33	1.31	-n	$-\Delta Q$
Pd	1.37	+	+n	$--\Delta Q$
Ni	1.25	1.22	-n	$--\Delta Q$

Pb 1.75A (Atomic radius equivalent to half the interatomic distance)

Slow diffusers with equilibrium sizes from 1.75 A to 1.44 A approx. 1.0 to .83 of solvent size then vacancy diffusion likely mechanism.

If solute equilibrium radius of solute less than .82 x Solvent radius then interstitial mechanism appears possible , at least in the case of lead solvent.

Fast diffusers with equilibrium sizes from 1.44 A to .96 A

where + indicates full atomic radius. taken from Warburton and Turnbull (1975)

It is not clear if activation energy is relevant in this case but it appears that the slow diffusers have the largest atomic radii and even at the equilibrium radius appear to be the larger ions. It seems that the fast diffusers tend to be less than 1.44 A radius in the atomic state and none exceed that after equilibrium. The slow diffusers are all larger than 1.44 A as atoms and as ions still remain larger. Sn appears to have the potential as does Na of dropping the next full electron and dramatically reducing size . The fact that they are slow diffusers implies that they do not . The size ranges are uncomfortably close and even appear to overlap, but clearly the largest atoms are slow diffusers with Ao values in the range of $10^{-8}\_to\_10^{-9}$ cm2/sec while the fast diffusers range from $5\times10^{-7}\_to\_10^{-5}$ cm2/sec. The fastest diffusers were Cu and Ni, the slowest Tl and Sn. It appears based on these results that there is a potential to use the R.C.M. to corroborate such data that was deemed "anomalous diffusion" by Shewmon (1989). Reports of similar results of impurity diffusion in tin were not investigated. The fact that the R.C.M. shows promise in the clarification of frequency factors suggests strongly that the model is in fact general in application.

4.3 RADIUS CONVERGENCE RATES

The fact that the radius formula $r = r_o\left(1+\frac{n}{Z}\right)^{\frac{2}{9}}$ tended to converge to the reported Goldschmidt ionic radii of the various elements was reassuring. Being somewhat sceptical an analysis of the rate of convergence or the deviation from the ideal

Goldschmidt radius at a particular ionization state was performed. The results suggest that as charge transfer nears the full number of valence electrons a solution is no longer possible i.e. n =-Z where the power term becomes $(0)^{\frac{2}{9}}$. However by iterating toward the singularity a check on convergence was possible. In general convergence with the Goldschmidt ionic radius for most elements appears to occur at n= - Z+.15 where Z is between 1 and 6. However , this was by no means universal. In several groups of elements convergence occurred much sooner, in fact as early as -Z+.3. The premature convergence was not proportional to valence. It appeared that certain groups of elements simply have a different radius response rate to ionization than do other groups. While the radius formula tends to be generally very accurate it can be significantly off especially with Z=1 solutes. Presentation of this data was beyond the scope of this project , due to the large volume taken up by the iterative data. However the source code for the iterative solution algorithm is included in the appendix (**A5**) and is relatively straightforward to compile and run. It is not clear what if any noticeable affect premature convergence has on the outcome of the R.C.M. other than it may tend occasionally overestimate the amount of shrinking that a solute undergoes for a given charge loss. This is only potentially a problem with potential hills, solute Emax higher than solvent's, and would only affect the predictions relating to impurities initially larger than the solvent where the final equilibrium radius falls within some size range very close to that of the solvent. A possible method of correction is to re-examine the solution to the differential equations that generate the radius equation.

Recall that the assumption was made that

$$\left(\frac{dE_o}{dr}\right)_{r_o} \equiv -\left(\frac{dE_f(Z)}{dr}\right) r_o$$

where the ***Qm*** term was dropped since it was very small.

There is another problem with the radius formula that was only considered late in the analysis of the data. Taking as an example the solute Aluminum; if it were expected to donate some charge and donated the outer valence electron in the p shell that leaves two s shell electrons . The diameter of the s shell is considered to remain the same, or nearly so, whether their are one or two electrons contained therein. The radius formula is continuous in that it converges to the 3+ state but intermediate values are not necessarily captured adequately. Assuming that Aluminum does donate one electron then the new radius would be that of the underlying s shell. The radius formula would expect a radius for charge donation of 1 electron larger than for 2 electrons when in fact the radii would be identically that of the s shell. This could point to an entirely different approach to the calculation of radii based on a quantum mechanical approach. Conversely for 2+ atoms that give up a charge of 1 electron a radius less than that of the of the s shell is determined by the radius formula when in fact no change may actually occur until both are donated. This could explain why the predictions for Hg and Cadmium are rather inaccurate.

4.4 OSCILLATION

The solute ion oscillates in position according to the vibration frequency which is inversely proportional to its mass. The jump frequency is positively correlated with the diffusion rate. Lighter atoms vibrate at higher frequencies and are therefore expected to jump more frequently. The gain and loss of electrons tunnelling between solvent and

solute most play some role in the vibrational frequency of the ions. The relationship between diffusion rates and vibration frequency has been discussed regularly as part of the isotope effect theory. The work in lead has produced inconclusive results with fast diffusers, that on the basis of isotope effect would not appear to be able to do so. Shewmon's remarks regarding the fast diffuser, gold suggested that the mass of the saddle barrier in lead appears to be greater than expected. This due to a larger than expected fraction of the activation energy be required to cross the activated complex. A possibility exists that the unknown driving force behind fast diffusion was the state oscillation in addition to the position oscillation. For example if a Nickel atom donates a single electron , Ni +1, the atomic volume goes from 8.18 A^3 down to 1.98 A^3 This simply the change from the atomic radius of 1.25 A to the ionic of .78 A . The loss in volume is expected to occur simultaneously with the loss of the electron. In addition a disrupt change in the frequency of vibration must also be expected. The kinetic effect of the loss of the single electron coupled with the decreased volume might account for higher than expected rates of diffusion. In the previously mentioned study by Warburton and Turner (1975) , Nickel was identified as a fast diffuser in lead.

4.5 SUMMARY OF MODEL ACCURACY

Overall 20 solvent systems were evaluated and results tabulated (Table 23), totalling 324 solvent-solute systems. The Modified LeClaire Model (**M.L.M**.) predicted the correct sign of solute ΔQ in 197 of 324 systems for which experimental data existed, for a total accuracy of 60.8% correct. The Radius Compensating Model (**R.C.M**) , which is an

Summary of Model Results

TABLE 23

Solvent	# of Solute Elements	R.V.M. Correct Predictions		Homovalent Correct Predictions		M.L.C. Correct Predictions		R.C.M. Correct Predictions	
Aluminum	31	10	32.3%	20	64.5%	20	64.5%	21	67.7%
Berylium	11	5	45.5%	3	27.3%	4	36.4%	11	100.0%
Cobalt	9	3	33.3%	8	88.9%	5	55.6%	7	77.8%
Copper	32	17	53.1%	14	43.8%	20	62.5%	17	53.1%
Gold	16	10	62.5%	8	50.0%	11	68.8%	9	56.3%
a-Iron	25	11	44.0%	15	60.0%	19	76.0%	19	76.0%
g-Iron	20	8	40.0%	8	40.0%	6	30.0%	11	55.0%
Lead	16	6	37.5%	5	31.3%	9	56.3%	14	87.5%
Lithium	12	0	0.0%	9	75.0%	7	58.3%	7	58.3%
Magnesium	10	1	10.0%	6	60.0%	7	70.0%	7	70.0%
Molybdenum	13	4	30.8%	7	53.8%	9	69.2%	11	84.6%
Nickel	23	15	65.2%	15	65.2%	18	78.3%	14	60.9%
Niobium	18	3	16.7%	13	72.2%	15	83.3%	15	83.3%
Praseodymium	11	0	0.0%	2	18.2%	2	18.2%	10	90.9%
Silver	20	18	90.0%	4	20.0%	13	65.0%	18	90.0%
Tin	13	4	30.8%	9	69.2%	5	38.5%	11	84.6%
b-Thorium	11	3	27.3%	1	9.1%	7	63.6%	11	100.0%
Tungsten	12	1	8.3%	9	75.0%	9	75.0%	9	75.0%
g-Uranium	10	1	10.0%	5	50.0%	4	40.0%	9	90.0%
Zinc	11	6	54.5%	8	72.7%	7	63.6%	5	45.5%
Totals	324	126	38.9%	169	52.2%	197	60.8%	236	72.8%
Without Self-Solute	304	126	41.4%	147	48.4%	177	58.2%	217	71.4%

R.C.M modified to Squeeze Solute to fit Solvent lattice parameters		
24	77.4%	31
		11
		9
21	65.6%	32
10	62.5%	16
20	80.0%	25
		20
		16
		12
		10
		13
20	87.0%	23
		18
		11
		20
		13
		11
		12
		10
6	54.5%	11

Improvement or Loss/ total # samples

3	31
4	32
1	16
1	25
6	23
1	11
16	138

11.6% Improvement rate for samples tested

extension of the previous model that bases its predictions on Energy differences as well as differences in equilibrium radii , was correct in determining the sign of solute ΔQ in 236 of the 324 cases. The R.C.M. had an overall success of 72.8% correct. The M.L.M. appears to have little better than a random success at predicting the correct sign of ΔQ for a solute when extended to a wide variety of systems. The use of the M.L.M. is restricted to a few systems where the significance of relative size effects are cancelled out, such as solvents with large radii and low Emax values. The R.C.M. success overall seems to be unlikely due to a random process. In only 1 of the systems did the R.C.M. prove less than 50% accurate. In 13 systems the accuracy was in excess of 70% with 7 systems having near perfect scores (0 to 1 wrong). The R.C.M. appears capable of modelling the principals determining the sign of the solute activation energy and further is capable of incorporating successfully concepts related to relaxation factors effecting the activation volume of the solvent.

The impact of imposing limits based on solvent lattice parameters on the solute atomic volume are also shown for 6 systems in TABLE 23. The impact of this procedure is to improve the prediction success rate for the systems tested (Al, Au, a-FE, Cu, Ni, and Zn), totalling 138 sample solvent-solute systems, by 11.6%. The benefit of the "squeezing " procedure is selective for only solutes much larger than the solvent. It appears to simply enhance the R.C.M. without compromising the previous successes for various systems. If applied generally to all models the improvement could be expected to be in the order of 5% , raising the potential success rate to about 77%.

The poor success of the Relative Valence model ,which predicts that solutes with a higher valence than the solvent exhibit $-\Delta Q$ is extraordinary. A large but variable proportion of the errors incurred by the R.V.M. are due to its inability to cope with homovalent solutes. So serious is this limitation that the R.V.M. can not even predict a NULL value for a solvent in itself. Recall all other models the U, M.LeC.M . and the R.C.M. are however capable of detecting such a situation. Both of these newer models are open to modifications with respect to the Ef and radius values assumed for the solute.

The Relative Valence Model has no potential for improvement as long as it neglects radius effects. Combining the original point charge model or R.V.M. for use in heterovalent systems with the U method for homovalent systems does not in effect result in any benefit overall. The U model by itself is better than the R.V.M. in predicting the sign of ΔQ in heterovalent systems than is the R.V.M. . The concept of using the difference in energies of solvent and solute is vastly more meaningful than the comparison of valence.

The issue of success rate is actually of no meaning to the merit of energy methods when they are viewed as part of an analysis system. The true value of the energy methods lies in their ability to indicate the direction of transfer of charge . Further the energy methods are sensitive to the changes in atomic volumes of solutes induced by solvent lattice parameters.

5.0 DISCUSSION

It appears that the R.C.M. is relatively robust and with a few exceptions can predict the correct sign of the impurity activation energy difference in about 70 % of the cases. If one accepts the possibility that some of the diffusion data is less than perfect , the success may be as much as 10% better. The R.C.M. clearly is a significant improvement over the energy difference models, and the relative valence models. The use of atomic size differences between solute and solvent is not new by any means. The literature includes several examples of experimental data rationalised by the difference in atomic radii. It is just that the previous procedures for determining the activation energy of the solute have sought solutions independent of radius. The R.C.M. appears to be capable of becoming a general model for diffusion in metals.

The Relative Valence Model of Le Claire (1962) seems totally inadequate when compared with either the Modified Le Claire model based on Emax values or the Radius Compensating model based on energy equilibration and charge transfer. The overall success rate was seldom better than 50% correct and averaged overall only 38.9% correct in predicting the sign of solute activation energy differences, $\Delta \mathbf{Q}$. Furthermore the point charge concept as proposed by Corless and March(1961) and Le Claire(1962) appears to have no justification, principally due to its failure to include radius effects. These results put into serious question the entire structure of Le Claire's 1962 work on the calculations for predicting quantitatively values for solute activation energy.

Considering the work of Hahn and Averback (1986, 1987, 1988) with the solvents a-Ti, a-Zr and the alloy a-Ni-Zr , there are three additional examples of radius and diffusion correlated solvent systems.

Recall that in the past all modelling attempts have sought a solution based on a single equation relating only one atomic variable , either valence or energy difference. The R.C.M. is an algorithmic approach based on initial energy differences with subsequent conditional rules to finally determine the actual sign of the impurity activation energy difference. This approach is somewhat more complicated than a single solution and may well be more realistic. The R.C.M. is capable of incorporating within the algorithm any number of new conditionals based on specific physical phenomena. For example the initial model,as presented, made no effort to deal with the relaxation factors affecting the activation volume. However it is a simple matter to modify the cutoff limit to approximate such a condition. If in fact oscillation between ionization states imparts kinetic energy to a solute , then a modification of the upper cutoff limit can easily be employed. The setting of such an upper limit could be a function of the charge transfer, i.e. upper limits for a solvent system may be individually set for each solute based on differences in thermal coefficients and Young's moduli. No investigation of the scale of n was undertaken in this study but it appears that the size of the charge transfer may be significant. If the transfer is only a very small amount required to reach equilibrium oscillation may not be that frequent. If on the other hand the charge transfer is close to a full electron the ionization state might well be quite stable , that is the ion would rather remain constantly

in that state than dropping back to the atomic state. Intermediate charge transfers would be relatively unstable in either state and as such oscillation might be expected to be more frequent.

The value of a statistical average equilibrium charge transfer becomes more suspect as one examines Qm and Qf since neither can be solved on the basis of fractional charges. The meaning of electron pair interaction energy is lost when one considers fractions. Promotion energies again are meaningless for fractional charges. It may seem inappropriate to confess to such misgivings at such a late state of this project. Unfortunately it only became apparent as a consequence of the success of the simplistic model. It appears then that quantitative predictions of ΔQ and D are not amenable to simple solutions. Rather these values appear to be averages of chaotic like phenomena.

The work of Petry ,et al(1991) proposed a "pumping mechanism", the result of dynamic interactions between solvent and solute attributed to thermal oscillations, which was capable of dramatic and periodic, lowering of the activation energy required by a migrating atom greatly enhancing diffusion in B.C.C. metals. The existence of such a mechanism in other crystal structures was not considered . Limoge (1992) suggested that many of the unresolved issues regarding diffusion might lend themselves to illumination if research were refocused toward specific systems. Concentration being directed to producing good measurements in a given family of alloys. By good, Limoge

was clearly implying reproducible and systematic measurements and conversely that much data was not trustworthy. Using such an approach would clear up a number of issues. The wide range in reported solute diffusion parameters makes the testing of any theoretical model more difficult.

The radius formula adapted from Varley(1954) is not as precisely correlated with the known Goldshcmidt Ionic radii as might be desired. Further improvements to the accuracy might be obtained by including the electron free and mean interactions into this model. It is possible that quantum dynamics model might be more appropriate when charge transfer means that one electron remains in the s shell.

The methods used to determine the Eo values for the various elements were a compromise. Not all the elements have had their ionization potentials determined and it was necessary to approximate these where missing based on the values of neighbouring elements. The **s-p** transition energies were approximated based on values used by Varley(1954) and much improvement could be evidenced with regard to this issue. The screening factor q_o is also a term with which great liberty was taken. At the time these terms seemed so small that it was not considered significant with respect to the overall relative values calculated for Emax .

Undoubtedly even after correction for these terms the relative Emax values will not be altered appreciably. However there may be small alterations that could effect specific solvents and yield improvements to the precision of the model.

Several important consequences of this technique include the ability to determine the possible ionization states for a solute, and the possible mechanism for diffusion i.e. either interstitial or substitutional . Of particular importance is the fact that apparently anomalous diffusion data has a rational and consistent explanation. There are issues that impinge on this model that at first glance appear to be peripheral but may ultimately provide the basis for a clearer picture of diffusion processes. For instance the work of Varley(1954) was not concerned with diffusion in the least but rather with alloy heats of formation. Further that work concerned itself with the issue of strain energy due to mismatch in the sizes of the solvent and solute. It was suggested that the strain energy was one source of the energy required for equilibration. Charge transfer being proposed as a method by which strain energy could be reduced. This then suggests that charge transfer calculations would have to be altered to take into account the strain energy contributions.

Differential rates of oscillation due to differences in thermal expansion coefficients raises another issue on the dynamics of diffusion with regards to its effects on strain energy. The role of strain energy in vacancy diffusion rates may ultimately be a productive area of investigation. The most salient feature of this model is the ease with which it can be

adapted to integrate with a number of diffusion and metallurgical issues. Rather than being a model requiring a new set of tools and procedures , it is in simplest terms , a procedure to integrate a large body of existing principles and procedures. If in fact the model or some later refined version has a potential for exploring in greater detail issues such as solute ion kinetics and solvent relaxation processes, the impact on materials engineering may be quite significant.

If this model is valid, as we suspect , it begs an obvious question , is it applicable then to multiple solute systems. First impressions suggest that in multiple solutes the pertinent issue is the availability of charge. If a solute with a very low Emax value is attracting a large electron cloud about itself, it seems then that a second ion in the vicinity would be in competition with the well . If that second solute was a donor a different local equilibrium might be the consequence. If donors tend to oscillate between ionization states it is possible that a well might tend to dampen the rate of oscillation , with subsequent alterations to diffusion rates. If the assumption of a self-consistant field is valid a third solute equilibrium Emax may well be that of some average of the solvent and the primary solute. Obviously these thoughts are highly speculative and based on the premise that the R.C.M. is in fact valid and extendible. Perhaps in view of past models being so readily accepted on such marginal evidence and by comparison with the huge data base used for the R.C.M. , these are overly cautious sentiments.

The R.C.M. is not necessarily a model of what governs the mechanics of diffusion. Rather it simulates a process that approximates closely the empirical data. Whereas earlier models sought to define the model as being the basis for the actual process.

It is after much thought about reconciling the data observed in this thesis with the R.C.M. that some possible mechanisms present themselves.

If one accepts the concept of an Emax value for any atomic species, then we can in a sense plot Emax (y-axis) vs Atomic radius(x-axis) for all elements. Picking an arbitrary solvent from within the scatter plot as the new 0, 0-point,we see that larger atoms lie to the right along the x-axis and elements with higher Emax (y-axis) above the zero point for the solvent and lower Emax elements to the bottom. Strain energy would increase with increasing distance to the right, falling to zero to the left . Let's assume a solute is arbitrarily chosen from the right side of the solvent x intercept. Adding strain energy to these elements would increase their Energy levels.

Now this is not as unwarranted as it may sound , since Ef values were calculated on the basis of atomic radius. Lets now assume Cesium with atomic radius of 2.65 Ang. is trying to fit within the crystal structure of Aluminium with an inter atomic spacing of 1.4Angstroms.This is only one eighth or so of the former atomic volume. If Cesium were to be somehow compressed to this size then the Ef would increase dramatically from that of the atomic state. Recall that atomic radius squared was used in the denominator of **Equation 23** to determine **Ef**. This increase might be expected to push electrons to such

high energy levels that they could easily find lower energy bands around neighbouring Aluminium ions. In this manner a potential well was transformed into a potential hill contradicting what one would expect from bulk data alone. And conversely Cobalt with atomic radius based on crystal lattice parameters of 1.25 Angstroms might rattle around on a crystal lattice site even dilating to accommodate the space available thereby dropping its energy level and becoming a potential well .The free Co atom is reported to have a radius of 1.67 Ang. If Cobalt then were to expand it could easily fill the available site. For the purposes of this thesis the dilation of solutes beyond the atomic radius was ignored since no appropriate means was available to determine accurately values. In this manner a loose solute with an initially higher Emax could drop its energy and equilibrate without the need for charge transfer. In fact if it dilates enough it could actually become a potential well drawing in electrons from the solvent. If high energy electrons from the conduction band of a solute can find lower unoccupied energy bands within the solvent , charge transfer seems probable in order to reduce the overall energy of the crystal. However if the solute electron is of lower energy than the available sites in the solvent then the likelihood of transfer is decreased. It is curious to note that the early work of Le Claire(1962) which focused on the noble metals may have been influenced by this situation. All the solutes were adjacent to the solvent and would have had similar energy bands even overlapping enhancing the prospect of charge transfer.

It was clearly beyond the scope of the resources available to continue the project in any more detail. If time had permitted it would have been desirable to evaluate the potential of calculating the solute Ef using solvent crystal dimensions.

A minor example of this concept was applied to solutes in the Aluminium, Gold, Copper alpha Iron, Nickel and Zinc solvent systems. The fermi energies for any solute larger than the solvent atomic radius plus 5% were recalculated under the assumption that they would be forced to adopt radii based on the solvent interatomic distances. For example Cesium could not exist at 2.65 A in the Aluminum lattice of 1.43 A . So rather than calculate the solutes fermi energy on the basis of its bulk atomic radius , the solvent dimension was used. The consequence was the elevation of the Ef and thus Cesium becomes a potential hill. In order to equilibrate Emax it donates charge and shrinks to 1.25 A. The net result is a prediction of $-\Delta\mathbf{Q}$ as a solute in Aluminum which is in fact the value obtained experimentally. The effect of this technique was to improve R.C.M results by approximately 5%. An extension of this principle to other systems could account for significant improvements in the R.C.M primarily with average sized crystal structures.

Solute radius and the solute activation energy are highly likely to be correlated but not necessarily directly. Overall the linearity of scatterplots of ΔQ versus ΔRadius was disappointing. The remaining issues are what manner of mechanisms are at work effecting radius adaptations. It seems clear that the relative size of the solvent as with the high atomic number elements swamps all other effects and only radius is visible. At the other end with small atomic radius elements radius dominates again. The difficulties seem to arise for solvents between 1.2 and 1.5 Angstroms. Within these solvents strain energy and unoccupied energy bands take on greater significance.

Finally , the issue of making quantitative estimates of the ΔQ for impurity diffusion begs to be asked. It is our considered opinion that due to the lack of definite linearity the actual value of ΔQ is not directly related to radius. Unfortunately it may be that the diffusion rate and the activation energy are functions of mass and kinetics as well as the ionic volume of the solute species. The process of diffusion may be a function of electron density in as far as it appears to affect the ability of the solute to donate electrons. Diffusion rates might be expected to increase when the density of donors is lower it is easier for the solute to ionize and take on a smaller effective atomic volume .

6.0 CONCLUSIONS

a) The Relative Valence Model is incapable of determining the correct sign of solute DQ in more than half the 324 samples tested.

b) The U or Ground State Energy difference model had only slightly better overall performance.

c) Energy difference models based on the sum of Ground State and Fermi energies are only slightly better than random chance in predicting the sign of solute DQ.

d) None of the above models can be used to predict the quantitative value of solute DQ if they cannot predict the qualitative value.

e) The Radius Compensating Model can correctly predict the sign of solute DQ in more than 70% of the samples tested. It can in fact approach near perfect scores in many systems. This model is based on the assumption that subsequent to transfer of equilibrating charge the solute takes on a new ionic radius and that the relative

difference between the equilibrated solute ion radius and that of the solvent determines whether or not a solute has a lower ,-DQ ,or higher ,+DQ ,value for activation energy than that of the solvent.

f) The R.C.M. can be used to determine the solute ionization state and its atomic volume. The technique permits the discrimination between vacancy and interstitial solute diffusion for various solutes in different solvents.

g) The diffusion parameters of a solute are determined by the solvent lattice parameters and energy states and the ability of the solute to equilibrate to these conditions. The R.C.M. provides a method of predicting solute DQ even in transition metals where radii and energy levels are very similar.

h) Anomalous fast diffusion by alkali metals has been shown to be easily explained by the imposition of solvent lattice parameters on the solute which tends to increase their tendency to become charge donators as solutes with consequent small ionic radii.

i) The R.C.M. appears to have settled conclusively the issue of what determines the activation energy of a solute. The R.C.M. is proposed as a method to determine diffusion parameters in ternary systems.

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APPENDIX A1

Table 2 -Atomic table of elements and intrinsic properties sorted by valence

Figure 2 -Atomic Table of Elements ; sorted by valence and Emax

Atomic Table of Element Bulk Parameters

TABLE 2

	element	Self Qo Kjoules	val	at rad	ion rad	Heat of vapor. Evolts Kjoules/mole	Ef	Eo=-1/Z(Hv+Slp+ZEf-Qf+Qm) Eo	Emax	Qf lt=8		Qm	q0/r0	Sum of Z Ionization Potentials	element	Ionization potentials in Evolts First	second	third	fourth	fifth	sixth
55	Cs		1	2.650	1.650	65.900	0.683	1.200	-5.777	-3.777	Cs			3.894	Cs	3.894	25.1				
37	Rb	39.3	1	2.510	1.490	69.200	0.717	1.338	-6.232	-4.002	Rb			4.177	Rb	4.177	27.28	40	52.6	71	84.4
19	K	39.2	1	2.310	1.330	77.530	0.804	1.580	-6.724	-4.091	K			4.341	K	4.341	31.625	45.72	60.91	82.66	100
11	Na	42.2	1	1.860	0.980	89.040	0.923	2.437	-8.498	-4.438	Na	0		5.139	Na	5.139	47.286	71.64	98.91	138.39	172.15
3	Li	53.8	1	1.520	0.780	134.680	1.396	3.648	-10.436	-4.356	Li	0		5.392	Li	5.392	75.638	122.45			
47	Ag	181.7	1	1.440	1.130	255.060	2.644	4.065	-14.285	-7.510	Ag		0.9	7.576	Ag	7.576	21.49	34.83			
29	Cu	211	1	1.280	0.960	304.600	3.157	5.145	-16.028	-7.453	Cu		1.200	7.726	Cu	7.726	20.292	36.83	55.2	79.9	103
79	Au	172.3	1	1.440	1.370	324.430	3.363	4.065	-16.653	-9.878	Au		0.900	9.225	Au	9.225	20.5				
1	H		1	0.460	1.540	0.900	0.009	39.836	-53.444	12.950	H			13.598	H	13.598					
28	Ni	275.7	2	1.250	0.780	371.830	3.854	8.564	-22.326	-8.053	2.533 Ni	0.4	0.6	25.803	Ni	7.635	18.168	35.17	54.9	75.5	108
26	Fe	250.6	2	1.240	0.870	351.040	3.638	8.702	-22.592	-8.088	0.310 Fe	0.4	0.6	24.050	Fe	7.87	16.18	30.651	54.8	75	99
4	Be	161	2	1.140	0.540	292.400	3.031	10.296	-25.333	-8.173	0.889 Be	0.4	0.6	27.533	Be	9.322	18.211	153.89	217.71		
56	Ba		2	2.170	1.430	150.920	1.564	2.842	-13.036	-8.300	-3.208 Ba	0.4	0.6	15.216	Ba	5.212	10.004				
38	Sr		2	2.150	1.270	138.910	1.440	2.895	-13.510	-8.685	-2.665 Sr	0.4	0.6	16.725	Sr	5.695	11.03	43.6	57	71.6	90.8
20	Ca	161.1	2	1.970	1.060	149.950	1.554	3.448	-14.538	-8.792	-2.242 Ca	0.4	0.6	17.984	Ca	6.113	11.871	50.908	67.1	84.41	108.78
21	Sc		2	1.600	0.830	304.800	3.159	5.227	-17.546	-8.835	-1.740 Sc	0.4	0.6	19.340	Sc	6.54	12.8	24.76	73.47	91.66	111.1
30	Zn	93.9	2	1.330	0.830	115.310	1.195	7.564	-21.556	-8.949	0.570 Zn	0	1	27.358	Zn	9.394	17.964	39.722	59.4	82.6	108
12	Mg	133.9	2	1.600	0.780	128.660	1.334	5.227	-17.740	-9.028	-0.611 Mg	0.4	0.6	22.681	Mg	7.646	15.035	80.143	109.24	141.26	186.5
82	Pb	109	2	1.750	1.320	179.410	1.860	4.369	-16.915	-9.633	-0.384 Pb	0.4	0.6	22.448	Pb	7.416	15.032	31.937	42.32	68.8	
48	Cd	80	2	1.500	1.030	99.870	1.035	5.947	-19.658	-9.746	-0.085 Cd	0.4	0.6	25.901	Cd	8.993	16.908	37.48			
46	Pd	266.3	2	1.370	0.500	393.300	4.076	7.129	-21.707	-9.825	3.000 Pd	0.4	0.6	27.680	Pd	8.34	19.34	32.93			
80	Hg		2	1.500	1.120	59.150	0.613	5.947	-20.891	-10.979	0.319 Hg	0.4	0.6	29.193	Hg	10.437	18.756	34.2			
78	Pt	276.4	2	1.380	0.520	510.450	5.291	7.026	-22.872	-11.161	1.563 Pt	0.4	0.6	27.563	Pt	9	18.563				
22.1	Ti_a	122.7	2	1.470	0.760	428.860	4.445	6.192	-46.826	-36.505	-28.731 Ti_a	0.2	0.800	47.891	Ti	6.82	13.58	27.491	43.266	99.22	119.36
24	Cr	308.6	3	1.250	0.640	348.780	3.615	11.222	-21.017	-2.315	30.654 Cr	2.2	0.800	54.226	Cr	6.766	16.5	30.96	49.1	69.3	90.56
5	B		3	0.970	0.200	538.900	5.586	18.635	-33.555	-2.497	34.408 B	2.2	0.800	71.382	B	8.298	25.154	37.93	259.37	340.22	
26	Fe	291.3	3	1.260	0.670	351.040	3.638	11.044	-21.473	-3.066	29.252 Fe	2.2	0.800	54.701	Fe	7.87	16.18	30.651	54.8	75	99
22.2	Ti_b	251	3	1.470	0.690	428.860	4.445	8.114	-17.432	-3.909	26.582 Ti_b	2.2	0.800	47.891	Ti	6.82	13.58	27.491	43.266	99.22	119.36
69	Tm		3	1.740	1.040	191.000	1.980	5.791	-14.101	-4.449	21.190 Tm	2.2	0.800	41.940	Tm	6.18	12.05	23.71			
59.1	Pr		3	1.930	1.000	332.530	3.445	5.236	-13.225	-4.499	19.270 Pr	2.2	0.800	37.590	Pr	5.42	10.55	21.62	38.95	57.45	
70	Yb	146.7	3	1.930	1.000	128.900	1.336	4.707	-12.435	-4.590	23.976 Yb	2.2	0.800	43.624	Yb	6.254	12.17	25.2			
58	Ce_g	153.1	3	1.920	1.180	313.800	3.252	5.293	-13.924	-5.102	16.080 Ce_g	2.2	0.800	36.520	Ce	5.47	10.85	20.2	36.72		
62	Sm		3	1.810	1.130	191.630	1.986	5.352	-14.156	-5.236	13.650 Sm	2.2	0.800	35.875	Sm	5.63	11.07	19.175			
60	Nd		3	1.820	1.150	283.680	2.940	5.293	-14.088	-5.266	14.140 Nd	2.2	0.800	35.385	Nd	5.49	10.72	19.175			
45	Rh		3	1.340	0.680	495.390	5.135	9.765	-21.550	-5.275	28.580 Rh	2.2	0.800	56.600	Rh	7.46	18.08	31.06			
31	Ga	293	3	1.350	0.620	256.060	2.654	9.621	-21.341	-5.307	26.911 Ga	2.2	0.800	57.219	Ga	5.999	20.51	30.71	64		
33	As		3	1.250	0.690	34.760	0.360	11.222	-24.253	-5.551	20.259 As	2.2	0.800	56.794	As	9.81	18.633	28.351	50.13	62.63	127.6
13	Al	142	3	1.430	0.570	293.720	3.044	8.574	-20.049	-5.759	24.080 Al	2.2	0.800	53.261	Al	5.986	18.828	28.447	119.99	153.71	190.47
66	Dy		3	1.770	1.070	230.900	2.393	5.597	-15.136	-5.808	12.750 Dy	2.2	0.800	36.775	Dy	5.93	11.67	19.175			
67	ho		3	1.760	1.050	251.040	2.602	5.660	-15.416	-5.982	12.530 ho	2.2	0.800	36.995	ho	6.02	11.8	19.175			
63	Eu	143.9	3	2.040	1.130	175.730	1.821	4.213	-13.109	-6.087	13.430 Eu	2.2	0.800	36.095	Eu	5.67	11.25	19.175			
57	La_g	125.1	3	1.870	1.220	399.570	4.141	5.014	-14.494	-6.137	13.713 La_g	2.2	0.800	35.812	La	5.577	11.06	19.175	guess value for all the yellow cells		

Atomic Table of Element Bulk Parameters

TABLE 2- continued

	element	Self Qo	val	at rad	ion rad	KJoules/mole Hvapor	Ev	EvCahoc Eo=-1/Z(Hv+Slp+ZEf-Qf+Qm) Ef	Varle	VEo	vEmax	Qf lt=8		Qm	q0/r0	Sum of Z ion	lement	Ionization potentials in Ev First	second	third	fourth	fifth	sixth
68	Er	301.9	3	1.75	1.04	292.88	3.036	5.725		-15.765	-6.223	12.320	Er	2.2	0.800	37.205	Er	6.1	11.93	19.175			
49	In	78.2	3	1.57	0.92	226.35	2.346	7.113		-18.389	-6.533	23.405	In	2.2	0.800	52.685	In	5.786	18.869	28.03	54		
64	Gd	136.8	3	1.80	1.11	311.71	3.231	5.412		-15.657	-6.638	12.110	Gd	2.2	0.800	37.415	Gd	6.14	12.1	19.175			
39	Y	128.9	3	1.81	1.06	393.3	4.076	5.352		-15.684	-6.764	14.420	Y	2.2	0.800	39.140	Y	6.38	12.24	20.52	61.8	77	93
71	Lu		3	1.73	0.99	355.9	3.689	5.858		-16.980	-7.216	11.024	Lu	2.2	0.800	38.501	Lu	5.426	13.9	19.175			
27	Co	287.6	3	1.25	0.65	382.42	3.964	11.222		-26.164	-7.462	5.430	Co	2.2	0.800	44.095	Co	7.86	17.06	19.175			
51	Sb	165.3	3	1.61	0.90	67.91	0.704	6.764		-18.746	-7.472	17.429	Sb	2.2	0.800	50.471	Sb	8.641	16.53	25.3	44.2	56	108
83	Bi		3	1.82	1.20	104.8	1.086	5.293		-16.521	-7.699	19.141	Bi	2.2	0.800	49.539	Bi	7.289	16.69	25.56	45.3	56	88.3
81	Tl	95.2	3	1.71	1.06	162.09	1.680	5.996		-17.704	-7.710	25.124	Tl	2.2	0.800	56.366	Tl	6.108	20.428	29.83			
61	Pm		3		1.06							13.900	Pm	2.2	0.800	35.625	Pm	5.55	10.9	19.175			
6	C	682	4	0.77	0.20	355.8	3.688	35.825		-49.566	10.142	101.946	C	5.2	0.800	148.022	C	11.26	24.383	47.887	64.492	392.08	489.98
25	Mn		4	1.37	0.52	219.74	2.278	11.317		-17.957	0.904	88.858	Mn	5.2	0.800	107.942	Mn	7.435	15.64	33.667	51.2	72.4	95
42	Mo	405.7	4	1.36	0.68	594.13	6.158	11.484		-18.328	0.812	80.791	Mo	5.2	0.800	96.809	Mo	7.099	16.15	27.16	46.4	61.2	68
59.2	Pr	123.1	4	1.83	1.00	332.63	3.448	6.343		-9.824	0.746	71.260	Pr	5.2	0.800	76.540	Pr	5.42	10.55	21.62	38.95	57.45	
58	Ce_d	90	4	1.82	1.02	313.8	3.252	6.412		-10.426	0.262	65.640	Ce_d	5.2	0.800	73.240	Ce	5.47	10.85	20.2	36.72		
65	Tb		4	1.77	0.89	330.9	3.430	6.780		-11.362	-0.063	64.590	Tb	5.2	0.800	74.290	Tb	5.85	11.52	20.2	36.72		
44	Ru		4	1.34	0.65	567.77	5.885	11.829		-20.045	-0.330	76.530	Ru	5.2	0.800	98.310	Ru	7.37	16.76	28.47	45.71		
14	Si	424	4	1.17	0.39	384.22	3.982	15.516		-26.236	-0.375	69.435	Si	5.2	0.800	103.129	Si	8.151	16.345	33.492	45.141	166.77	205.05
32	Ge	297.4	4	1.22	0.44	334.3	3.465	14.271		-24.608	-0.824	71.077	Ge	5.2	0.800	103.763	Ge	7.899	15.934	34.22	45.71	93.5	
41	Nb	401.9	4	1.43	0.74	696.64	7.221	10.387		-19.462	-2.150	60.660	Nb	5.2	0.800	84.540	Nb	6.88	14.32	25.04	38.3	50.55	102.6
40.1	Zr_a	190.5	4	1.58	0.87	581.58	6.028	8.508		-17.625	-3.445	52.060	Zr_a	5.2	0.800	77.300	Zr	6.84	13.13	22.99	34.34	81.5	
40.2	Zr_b	272.8	4	1.58	0.87	581.58	6.028	8.508		-17.625	-3.445	52.060	Zr_b	5.2	0.800	77.300	Zr	6.84	13.13	22.99	34.34	81.5	
75	Re		4	1.38	0.72	707.1	7.329	11.153		-22.448	-3.859	71.096	Re	5.2	0.800	103.744	Re	7.88	16.934	34.22	45.71		
74	W	504.5	4	1.37	0.68	799.14	8.283	11.317		-22.899	-4.038	70.996	W	5.2	0.800	103.844	W	7.98	15.934	34.22	45.71		
50	Sn	106.1	4	1.58	0.74	290.37	3.010	8.508		-18.508	-4.327	61.724	Sn	5.5	0.500	93.212	Sn	7.344	14.632	30.502	40.734	72.28	
72.2	Hf_b	161.9	4	1.59	0.84	661.07	6.852	8.402		-19.365	-5.362	46.700	Hf	5.2	0.800	78.500	Hf	7	14.9	23.3	33.3		
52	Te	195.4	4	1.43	0.89	50.63	0.525	10.387		-22.898	-5.586	48.661	Te	5.2	0.800	92.979	Te	9.009	18.6	27.96	37.41	58.75	70.7
77	Ir	438.3	4	1.35	0.66	563.58	5.841	11.655		-25.498	-6.074	59.722	Ir	5.2	0.800	104.054	Ir	9.1	18.6	27.96	37.41		
76	Os		4	1.35	0.67	627.6	6.505	11.655		-25.506	-6.082	48.970	Os	5.2	0.800	92.670	Os	8.7	18.6	27.96	37.41		
90	Th	418.4	4	1.80	1.10	543.86	5.637	6.556		-15.655	-4.729	40.820	Th	5.2	0.800	66.380	Th	6.08	11.5	20	28.8		
92	U	119.2	4	1.38	1.05	422.57	4.380	11.153		-19.993	-1.404	40.710	U	5.2	0.800	66.490	U	6.19	11.6	20	28.8		
15	P	115.5	5	1.09	0.35	12.129	0.126	20.745		-43.554	-8.979	72.066	P	9.2	0.800	176.784	P	10.486	19.725	30.18	51.37	65.023	230.43
23	V	309.4	5	1.32	0.40	458.57	4.753	14.146		-36.944	-13.368	62.898	V	9.5	0.500	162.637	V	6.74	14.65	29.31	46.707	65.23	128.12
53	I		5	1.36	0.94	41.71	0.432	13.326		-43.419	-21.209	39.858	I	9.2	0.800	180.692	I	10.451	19.131	33	45.71	72.4	
73	Ta	460.2	5	1.47	0.68	753.12	7.806	11.406		-41.159	-22.149	44.396	Ta	9.2	0.800	176.154	Ta	7.89	15.934	34.22	45.71	72.4	
7	N		5		0.15	5.59	0.058					112.417	N	9.2	0.800	266.943	N	14.534	29.601	47.448	77.472	97.888	552.06
41	Nb	401.9	5	1.43	0.74	696.64	7.221	12.053		-32.673	-12.585	48.410	Nb	9.2	0.800	135.090	Nb	6.88	14.32	25.04	38.3	50.55	102.6
8	O		6	0.60	1.32	6.82	0.071	77.313		-101.938	26.917	161.496	O	14.2	0.800	294.976	O	13.618	35.116	54.934	77.412	113.9	138.12
16	S	215.1	6	1.06	0.34	9.62	0.100	24.771		-19.794	21.491	159.980	S	14.2	0.800	115.820	S	10.36	23.33	34.83	47.3	72.68	88.049
34	Se	125	6	1.16	0.35	26.32	0.273	20.684		-39.154	-4.681	76.658	Se	14.2	0.800	173.006	Se	9.752	21.19	30.82	42.944	68.3	81.7

All energies in Electron Volts , Radii in Angstroms. Activation Energy , Q, in Kilo Joules /mole

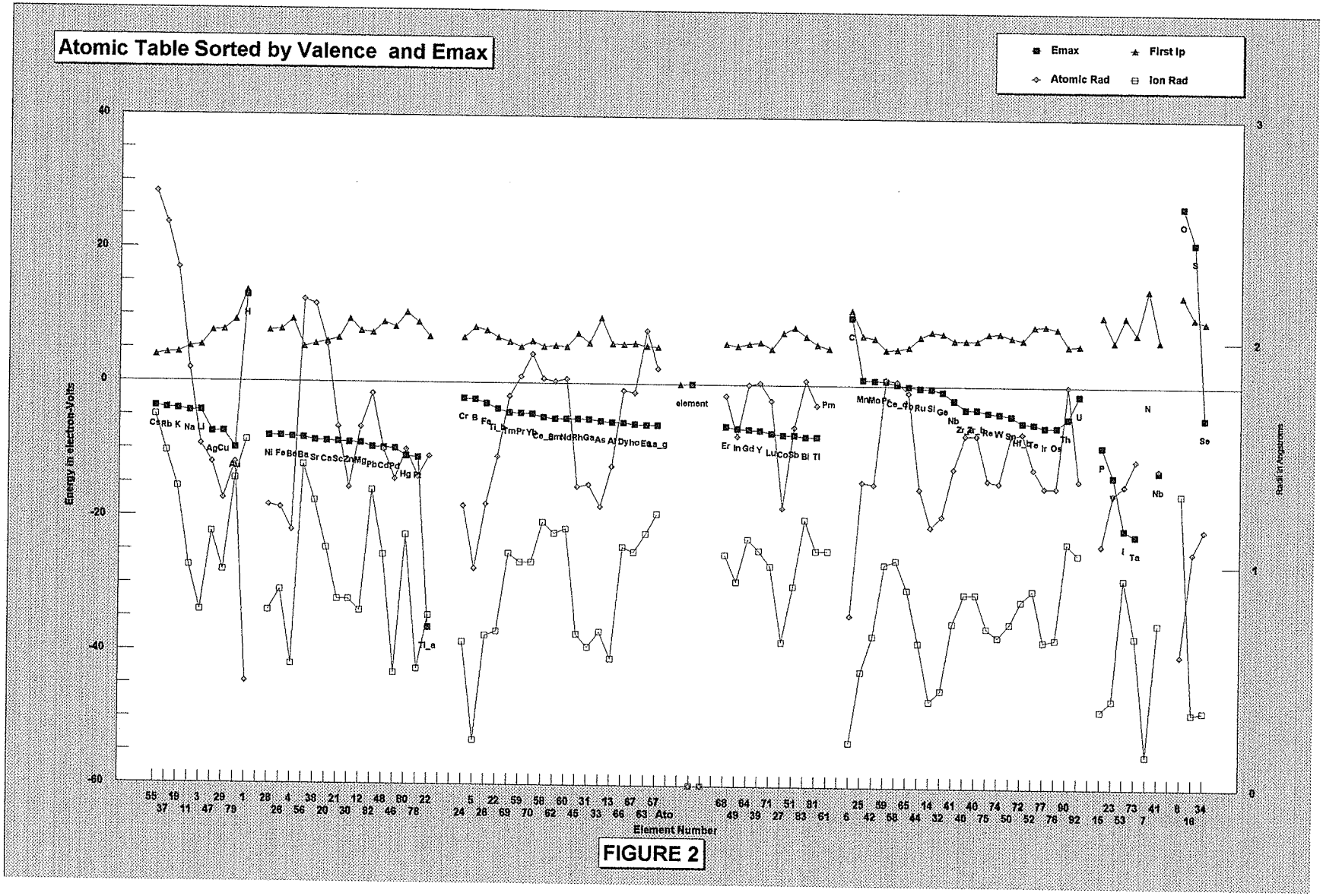
Atomic Table Sorted by Valence and Emax
Emax
First Ip
Atomic Rad
Ion Rad
Energy in electron-Volts
Radii in Angstroms
Element Number
element
40
20
0
-20
-40
-60
3
2
1
0

FIGURE 2

APPENDIX A2

Tables 3-22 Tables of Impurity diffusion Parameters for 20 Solvent Systems

Impurity Diffusion Parameters **TABLE 3** **SOLUTES IN ALUMINUM**

Solvent	Element	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Valence
Aluminum	Al	13	K	1.71E+00	142				Cahoon&Sherby,1992	Al			
				cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules			2.699	26.98	3
					/mole		/mole	/mole					

Solute Elements

	He	2				3.00E+00	154.88	12.88	Mroewec,1980	He			
	Pu	94				7.20E+09	318.14	176.14	Mroewec,1980	Pu			
	U	92	798-898			1.00E-01	117.20	-24.8	Smithells,1967	U			
	U	92				1.00E-01	117.21	-24.79	Mroewec,1980	U			
	Ag	47	450-632	2.78E-01	181.70	8.00E-02	116.80	-25.2	Mroewec,1980	Ag	10.49	107.88	1
	Ag	47	360-640	2.78E-01	181.70	3.2E-02	108.84	-33.16	Fricke,1972	Ag	10.49	107.88	1
	Ag	47	615-883	2.78E-01	181.70	1.3E-01	117.20	-24.8	Smithells,1967	Ag	10.49	107.88	1
	Ag	47	644-928	2.78E-01	181.70	1.2E-01	116.50	-25.5	Smithells,1967	Ag	10.49	107.88	1
	Au	79		5.60E-02	172.30	2.20E+00	133.95	-8.05	Fricke,1972	Au	19.32	197	1
	Au	79	290-650	5.60E-02	172.30	2.20E+00	134.00	-8	Mroewec,1980	Au	19.32	197	1
	Au	79	642-928	5.60E-02	172.30	1.31E-01	116.40	-25.6	Smithells,1967	Au	19.32	197	1
	Au	79	696-882	5.60E-02	172.30	7.70E-02	113.00	-29	Smithells,1967	Au	19.32	197	1
	Cs	55	453-573			1.04E-02	99.20	-42.8	Smithells,1967	Cs	1.9	132.91	1
	Cs	55				2.70E-08	33.07	-108.9	Mroewec,1980	Cs	1.9	132.91	1
	Cu	29	350-630	7.80E-01	211.00	1.50E-01	126.40	-15.6	Mroewec,1980	Cu	8.96	63.54	1
	Cu	29	375-619	7.80E-01	211.00	1.30E+00	138.20	-3.8	Fricke,1972	Cu	8.96	63.54	1
	Cu	29	300-500	7.80E-01	211.00	3.30E+00	146.51	4.51	Mroewec,1980	Cu	8.96	63.54	1
	Cu	29	594-928	7.80E-01	211.00	6.54E-01	136.00	-6	Smithells,1967	Cu	8.96	63.54	1
	H	1				2.10E-01	46.04	-95.96	Fricke,1972	H	9E-05	1.01	1
	Li	3		1.40E-01	53.80	4.50E+00	138.14	-3.86	Fricke,1972	Li	0.534	6.94	1
	Li	3	803-923	1.40E-01	53.80	3.50E-01	126.00	-16	Smithells,1967	Li	0.534	6.94	1
	Na	11	719-863	1.45E-01	42.20	6.70E-04	97.10	-44.9	Smithells,1967	Na	0.971	22.99	1
	Na	11		1.45E-01	42.20	8.10E-07	7.11	-134.9	Fricke,1972	Na	0.971	22.99	1
	Na_high	11		1.45E-01	42.20	1.10E+00	133.95	-8.05	Fricke,1972	Na_high	0.971	22.99	1
	Be	4		5.70E-05	161.00	5.2E+01	167.44	25.44	Fricke,1972	Be	1.85	9.01	2
	Cd	48	714-907	1.4E-01	80.00	1.04E+00	124.30	-17.7	Smithells,1967	Cd	8.65	112.41	2
	Cd	48	360-640	1.4E-01	80.00	3.20E-04	62.79	-79.21	Fricke,1972	Cd	8.65	112.41	2
	Cd	48	400-630	1.4E-01	80.00	7.94E-08	90.90	-51.1	Mroewec,1980	Cd	8.65	112.41	2
	Co	27		1.66E+00	287.60	4.60E+02	175.81	33.81	Mroewec,1980	Co	8.85	58.94	2
	Co	27	724-930	1.66E+00	287.60	5.1E+02	175.70	33.7	Smithells,1967	Co	8.85	58.94	2
	Co	27	673-913	1.66E+00	287.60	2.5E+02	174.60	32.6	Smithells,1967	Co	8.85	58.94	2
	Co	27	400-640	1.66E+00	287.60	2.5E+02	173.30	31.3	Mroewec,1980	Co	8.85	58.94	2
	Fe	26	793-930	2.76	250.60	5.30E+01	183.40	41.4	Smithells,1967	Fe	7.87	55.85	2
	Fe	26	360-630	2.76	250.60	4.10E-09	58.20	-83.8	Fricke,1972	Fe	7.87	55.85	2
	Fe	26	20-642	2.76	250.60	1.20E-01	134.80	-7.2	Mroewec,1980	Fe	7.87	55.85	2
	Fe	26		2.76	250.60	1.10E+05	259.53	117.53	Fricke,1972	Fe	7.87	55.85	2
	Fe	26	823-913	2.76	250.60	1.35E+02	192.60	50.6	Smithells,1967	Fe	7.87	55.85	2
	Hg	80	718-862			1.53E+01	141.80	-0.2	Smithells,1967	Hg	13.55	200.61	2
	Mg	12	667-928	1.00E+00	133.90	1.24E+00	130.40	-11.6	Smithells,1967	Mg	1.74	24.32	2
	Mg	12	394-655	1.00E+00	133.90	1.24E+00	130.42	-11.58	Fricke,1972	Mg	1.74	24.32	2
	Mg	12	300-500	1.00E+00	133.90	6.30E-02	113.20	-28.8	Mroewec,1980	Mg	1.74	24.32	2
	Mg	12	598-923	1.00E+00	133.90	6.23E-02	115.00	-27	Smithells,1967	Mg	1.74	24.32	2
	Ni	28	742-924	1.39E+00	275.70	4.40E+00	145.80	3.8	Smithells,1967	Ni	8.9	58.71	2
	Ni	28		1.39E+00	275.70	1.10E-06	83.72	-58.28	Mroewec,1980	Ni	8.9	58.71	2
	Ni	28	360-630	1.39E+00	275.70	2.90E-08	65.70	-76.3	Mroewec,1980	Ni	8.9	58.71	2
	Pb	82	777-876	1.37E+00	109	5.00E+01	145.60	3.6	Smithells,1967	Pb	11.36	207.21	2
	Pd	46	400-630	2.10E-01	266.30	1.92E-07	84.60	-57.4	Fricke,1972	Pd	12.02	106.4	2
	Pd	46		2.10E-01	266.30	1.90E-07	83.72	-58.28	Fricke,1972	Pd	12.02	106.4	2
	Zn	30	688-928	1.60E-01	93.90	3.25E-01	117.90	-24.1	Smithells,1967	Zn	7.13	65.38	2
	Zn	30	614-920	1.60E-01	93.90	2.45E-01	119.60	-22.4	Smithells,1967	Zn	7.13	65.38	2
	Zn	30	300-500	1.60E-01	93.90	4.00E-03	100.46	-41.54	Mroewec,1980	Zn	7.13	65.38	2
	Zn	30	340-640	1.60E-01	93.90	2.00E-01	120.60	-21.4	Mroewec,1980	Zn	7.13	65.38	2
	Zn	30	700-900	1.60E-01	93.90	3.00E-01	121.40	-20.6	Mroewec,1980	Zn	7.13	65.38	2

Impurity Diffusion Parameters **TABLE 3- continued** **SOLUTES IN ALUMINUM**

Solvent	Element	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Valence
Aluminum	Al	13	K	1.71E+00	142				Cahoon&Sherby,1992	Al			
				cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules			2.699	26.98	3
					/mole		/mole	/mole					

Solute Elements

	Al	13	130-200	1.71E+00	142.00	1.9E-01	124.00	-18	Mroewec,1980	Al	2.699	26.98	3
	Al	13		1.71E+00	142.00	2.00E-02	100.46	-41.54	Fricke,1972	Al	2.699	26.98	3
	Al*26	13	400-610	1.71E+00	142.00		144.40	2.4	Mroewec,1980	Al*26	2.699	26.98	3
	Ce	58				1.9E-06	113.02	-28.98	Fricke,1972	Ce	6.77	140.13	3
	Ce_D	58		1.2E-02	90.00				Smithells,1967	Ce_D	6.77	140.13	3
	Ce_G	58		5.5E-01	153.10				Fricke,1972	Ce_G	6.77	140.13	3
	Cr	24	859-923	2.00E-01	308.60	1.85E+03	253.00	111	Smithells,1967	Cr	7.19	52.01	3
	Cr	24	360-630	2.00E-01	308.60	1.10E-06	83.30	-58.7	Fricke,1972	Cr	7.19	52.01	3
	Cr	24	500-645	2.00E-01	308.60	8.00E+05	255.34	113.34	Fricke,1972	Cr	7.19	52.01	3
	Ga	31	350-640			3.10E-02	100.46	-41.54	Fricke,1972	Ga	5.907	69.72	3
	Ga	31	680-926			4.90E-01	123.10	-18.9	Smithells,1967	Ga	5.907	69.72	3
	In	49	715-929	3.20E+00	78.20	1.16E+00	122.70	-19.3	Smithells,1967	In	7.286	114.82	3
	In	49	673-873	3.20E+00	78.20	1.23E-01	115.60	-26.4	Smithells,1967	In	7.286	114.82	3
	In	49	400-630	3.20E+00	78.20	1.42E-08	92.90	-49.1	Smithells,1967	In	7.286	114.82	3
	In	49		3.20E+00	78.20	1.20E-01	117.21	-24.79	Mroewec,1980	In	7.286	114.82	3
	La	57				1.40E-06	113.02	-28.98	Fricke,1972	La	6.146	138.9	3
	La_B	57		1.5E+00	188.70				Fricke,1972	La_B	6.146	138.9	3
	La_G	57		1.1E-01	125.10				Smithells,1967	La_G	6.146	138.9	3
	Nd	60				4.80E-07	104.65	-37.35	Fricke,1972	Nd	7.008	144.24	3
	Sb	51	721-893	1.05E+00	165.30	9.00E-02	121.70	-20.3	Smithells,1967	Sb	6.697	121.75	3
	Sb	51	448-620	1.05E+00	165.30	9.00E-02	121.80	-20.2	Mroewec,1980	Sb	6.697	121.75	3
	Sm	62				3.50E-07	96.28	-45.72	Mroewec,1980	Sm	7.52	150.4	3
	Tl	81	737-862			1.16E+00	152.70	10.7	Smithells,1967	Tl	11.87	204.37	3
	V	23		2.88E-01	309.40	6.10E-08	83.72	-58.28	Fricke,1972	V	6.1	50.95	3
	Ge	32	674-926	1.30E+01	297.40	4.81E-01	121.30	-20.7	Smithells,1967	Ge	5.32	72.59	4
	Ge	32	350-640	1.30E+01	297.40	3.20E-03	83.72	-58.28	Fricke,1972	Ge	5.32	72.59	4
	Mn	25	460-660			1.04E+02	20.90	-121.1	Mroewec,1980	Mn	7.43	54.94	4
	Mn	25	450-650			2.20E-01	120.60	-21.4	Mroewec,1980	Mn	7.43	54.94	4
	Mn	25	500-650			1.28E+03	229.00	87	Mroewec,1980	Mn	7.43	54.94	4
	Mn	25	500-645			3.80E+02	221.86	79.86	Mroewec,1980	Mn	7.43	54.94	4
	Mn	25	730-933			1.04E+02	211.40	69.4	Smithells,1967	Mn	7.43	54.94	4
	Mo	42	898-928	5.00E-01	405.70	1.40E+01	250.00	108	Smithells,1967	Mo	10.22	95.95	4
	Mo	42	400-630	5.00E-01	405.70	1.04E-09	54.80	-87.2	Fricke,1972	Mo	10.22	95.95	4
	Mo	42				1.00E-09	54.41	-87.59	Fricke,1972	Mo	10.22	95.95	4
	Nb	41		1.10E+00	401.90	1.70E-07	83.72	-58.28	Fricke,1972	Nb	8.57	92.91	4
	Pr	59		8.70E-02	123.00	3.60E-07	100.46	-41.54	Fricke,1972	Pr	6.773	140.9	4
	Si	14	344-631	2.00E+01	424.00	3.46E-01	123.90	-18.1	Fricke,1972	Si	2.33	28.09	4
	Si	14	350-550	2.00E+01	424.00	1.80E-01	150.69	8.69	Fricke,1972	Si	2.33	28.09	4
	Si	14	753-893			2.48E+00	137.00	-5	Smithells,1967	Si	2.33	28.09	4
	Sn	50	673-873	9.20E+00	106.10	2.45E-01	119.30	-22.7	Smithells,1967	Sn	7.3	118.7	4
	Sn	50	400-630	9.20E+00	106.10	3.05E-07	84.60	-57.4	Fricke,1972	Sn	7.3	118.7	4
	Sn	50		9.20E+00	106.10	2.50E-01	121.39	-20.61	Fricke,1972	Sn	7.3	118.7	4
	V	23	400-630	2.88E-01	309.40	6.05E-08	82.10	-59.9	Fricke,1972	V	6.1	50.95	4
	Zr	40				3.43E+02	218.10	76.1	Mroewec,1980	Zr	6.49	91.22	4
	Zr	40				7.28E+02	241.60	99.6	Mroewec,1980	Zr	6.49	91.22	4
	Zr	40				5.48E+05	289.30	147.3	Mroewec,1980	Zr	6.49	91.22	4
	Zr	40	804-913			7.28E+02	242.00	100	Smithells,1967	Zr	6.49	91.22	4
	I	53	442-656			1.16E+00	122.30	-19.7	Fricke,1972	I	4.94	126.91	5

Impurity Diffusion Parameters TABLE 4 SOLUTES IN BERYLLIUM

Solvent	Element	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Berylium	Be	4		5.70E-06	161				Smithells	Beryli	1.85	9.01	2
				cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole					

Solute Elements

	Ag	47	923-1183		181.7	6.20E+00	193	32	Smithells	Ag			1
	Ag	47	929-1170		181.7	4.30E-01	164.5	3.5	Smithells	Ag			1
	Ag	47	929-1170		181.7	1.76E+00	180.9	19.9	Smithells	Ag			1
	Co	27	1253-1493		287.6	2.70E+01	287.2	126.2	Smithells	Co			2
	Fe	26	973-1349		250.6	5.30E-01	216.9	55.9	Smithells	Fe			2
	Fe	26	1073-1373		250.6	1.00E+00	221.9	60.9	Smithells	Fe			2
	Ni	28	1073-1523		275.7	2.00E-01	243	82	Smithells	Ni			2
	Al	13	1068-1356		142	1.00E+00	168.3	7.3	Smithells	Al			3
	Ce	58	1223-1513		153.1	3.10E+02	303.5	142.5	Smithells	Ce			3
	V	23	1173-1423		309.4	2.90E+01	243	82	Smithells	V			3
	C	6			682	3.20E-05	158.6	-2.4	Smithells	C			4
	Nb	41	1318-1513		401.9	2.00E+04	359.6	198.6	Smithells	Nb			4
	Te	52	693-1273		181.9	4.20E-01	193.3	32.3	Smithells	Te	6.237	127.6	4
	Te	52	733-1273		181.9	3.80E-01	198.6	45.5	Smithells	Te	6.237	127.6	4

Impurity Diffusion Parameters TABLE 5 SOLUTES IN COBALT

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Smithells		At.Wt.	Density	Val
Cobalt_A				1.66E+00	287.6					Co_A	8.85	58.94	2
				cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole					
	Cu		1158,1273		211	1.20E-01	275	-12.6	Smithells	Cu			1
	Fe		Tc-1573		250.6	1.60E-01	248.7	-38.9	Smithells	Fe			2
	Fe		1081-Tc		250.6	3.40E-01	259.6	-28	Smithells	Fe			2
	Fe		1223-1643		250.6	1.10E-01	253.3	-34.3	Smithells	Fe			2
	Mn		1133-1378			3.15E-02	232.4	-55.2	Smithells	Mn			2
	Mn		1424-1519			1.10E-02	217.7	-69.9	Smithells	Mn			2
	Ni		1409-1643		275.7	4.00E-01	282.2	-5.4	Smithells	Ni			2
	Ni		1045-1321		275.7	3.40E-01	269.2	-18.4	Smithells	Ni			2
	Ni		1465-1570		275.7	1.00E-01	252	-35.6	Smithells	Ni			2
	Pt		1354-1481		276.4	6.50E-01	279.3	-8.3	Smithells	Pt			2
	Zn		1081-Tc		93.9	1.20E-01	266.7	-20.9	Smithells	Zn			2
	Zn		Tc-1573		93.9	8.00E-02	254.5	-33.1	Smithells	Zn			2
	C		1073-1673		682	3.10E-01	153.7	-133.9	Smithells	C			4
	C		723-1073		682	8.72E-02	149.3	-138.3	Smithells	C			4
	S		1423-1523		215.1	1.30E+00	226.1	-61.5	Smithells	S			4

Impurity Diffusion Parameters **TABLE 6** **SOLUTES IN COPPER**

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		At.Wt.	Density	Val
Copper				7.80E-01	211				Cahoon	Cu	8.96	63.54	1
				cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole					
	Ag		873-1273		181.7	6.10E-01	194.7	-16.3	Smithells	Ag			1
	Au		633-1350		172.3	2.43E-01	197.8	-13.2	Smithells	Au			1
	Be		973-1348		161	6.60E-01	195.9	-15.1	Smithells	Be			2
	Cd		1032-1346		80	1.27E+00	194.6	-16.4	Smithells	Cd			2
	Cd		983-1309		80	1.20E+00	194	-17	Smithells	Cd			2
	Co		640-1351		287.6	7.36E+02	312.8	101.8	Smithells	Co			2
	Co		640-1351		287.6	7.40E-01	217.2	6.2	Smithells	Co			2
	Fe		1103-1347		250.6	1.40E+00	216.9	5.9	Smithells	Fe			2
	Fe		989-1329		250.6	1.01E+00	213.3	2.3	Smithells	Fe			2
	Hg		1053-1353			3.50E-01	184.2	-26.8	Smithells	Hg			2
	Mn		973-1348			7.40E-01	195.5	-15.5	Smithells	Mn			2
	Mn		773-976			1.42E+00	204.3	-6.7	Smithells	Mn			2
	Ni		613-1349		275.7	7.00E-01	225	14	Smithells	Ni			2
	Ni		613-1349		275.7	2.50E+02	299.3	88.3	Smithells	Ni			2
	Pb		1008-1225		109	8.62E-01	182.4	-28.6	Smithells	Pb			2
	Pd		1080-1329		266.3	1.71E+00	227.6	16.6	Smithells	Pd			2
	Pt		1149-1352		276.4	5.60E-01	233	22	Smithells	Pt			2
	Ti		973-1283		122.7	6.93E-01	196	-15	Smithells	Ti			2
	Zn		878-1322		93.9	3.40E-01	190.9	-20.1	Smithells	Zn			2
	Zn		1073-1313		93.9	2.40E-01	188.9	-22.1	Smithells	Zn			2
	As		1086-1348			2.02E-01	176.4	-34.6	Smithells	As			3
	Bi		1074-1348			7.66E-01	178.1	-32.9	Smithells	Bi			3
	Cr		999-1338		308.6	3.37E-01	195	-16	Smithells	Cr			3
	Cr		1073-1343		308.6	1.02E+00	224	13	Smithells	Cr			3
	Ga		1153-1352		298	5.23E-01	192.7	-18.3	Smithells	Ga			3
	In		602-1354		78.2	2.90E-01	179.6	-31.4	Smithells	In			3
	In		602-1354		78.2	3.11E+03	295.4	84.4	Smithells	In			3
	Rh		1023-1348			3.30E+00	242.8	31.8	Smithells	Rh			3
	Sb		1049-1349		165.3	4.80E-01	179.5	-31.5	Smithells	Sb			3
	Sb		873-1275		165.3	3.40E-01	175.8	-35.2	Smithells	Sb			3
	Tl		1058-1269		95.2	7.10E-01	181.3	-29.7	Smithells	Tl_B			3
	V		995-1342		309.4	2.48E+00	215	4	Smithells	V			3
	Ge		1110-1326		297.4	3.15E-01	185.5	-25.5	Smithells	Ge			4
	Ge		975-1289		297.4	3.97E-01	187.4	-23.6	Smithells	Ge			4
	Ir		1183-1303			1.06E+01	276.4	65.4	Smithells	Ir			4
	Nb		1080-1179		401.9	2.04E+00	251.5	40.5	Smithells	Nb			4
	Ru		1221-1335			8.50E+00	257.5	46.5	Smithells	Ru			4
	S		1073-1273		215.1	2.30E+01	206.6	-4.4	Smithells	S			4
	Si		973-1323		424	7.00E-02	171.7	-39.3	Smithells	Si			4
	Sn		1018-1355		106.1	6.70E-01	184.4	-26.6	Smithells	Sn			4
	Sn		1010-1321		106.1	8.42E-01	188.2	-22.8	Smithells	Sn			4
	Te		822-1214		181.9	9.70E-01	180.5	-30.5	Smithells	Te			4
	W		1163-1306		504.5	1.69E+00	225.7	14.7	Smithells	W			4
	P		847-1319		115.5	3.05E-03	136.1	-74.9	Smithells	P			5
	Se		878-1150		125.1	1.00E+01	180.5	-30.5	Smithells	Se			6

Impurity Diffusion Parameters TABLE 7 SOLUTES IN GOLD

Solvent	Au	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Gold	Au	79		5.60E-02	172.3				Cahoon				
			k	cm.sq/sec	kJoules	cm.sq/sec	kJoules	kJoules					
					/mole		/mole	/mole					
Solute Elements													
	Ag	47	1004-1323	2.78E-05	181.70	0.086	169.3	-3	Smithells	Ag	10.49	107.88	1
	Ag	47	972-1281	2.78E-05	181.70	0.072	168.3	-4	Smithells	Ag	10.49	107.88	1
	Cu	29	973-1179	7.80E-01	211.00	0.105	170.2	-2.1	Smithells	Cu	8.96	63.54	1
	Co	27	1030-1325	1.66E+00	287.60	0.25	185.2	12.9	Smithells	Co	8.85	58.94	2
	Co	27	973-1323	1.66E+00	287.60	0.22	183.4	11.1	Smithells	Co	8.85	58.94	2
	Fe	26	1027-1221	2.76	250.6	0.082	174.2	1.9	Smithells	Fe	7.87	55.85	2
	Fe	26	973-1323	2.76	250.6	0.19	172.5	0.2	Smithells	Fe	7.87	55.85	2
	Hg	80	877-1300			0.116	156.5	-15.8	Smithells	Hg	13.53	200.59	2
	Ni	28	973-1323	1.39E+00	275.70	0.25	188.4	16.1	Smithells	Ni	8.9	58.71	2
	Ni	28	1153-1210	1.39E+00	275.70	0.3	192.6	20.3	Smithells	Ni	8.9	58.71	2
	Pd	46	973-1273	2.10E-01	266.30	0.076	195.1	22.8	Smithells	Pd	12.02	106.4	2
	Pt	78	1173-1329	5.7E-01	276.4	7.6	255	82.7	Smithells	Pt	21.4	195.09	2
	Pt	78	973-1273	5.7E-01	276.4	0.095	201.4	29.1	Smithells	Pt	21.4	195.09	2
	Zn	30	969-1287	1.60E-05	93.9	0.082	158.1	-14.2	Smithells	Zn	7.13	65.38	2
	Al	13	773-1223	1.71E+00	142	0.052	143.6	-28.7	Smithells	Al	2.699	26.98	3
	In	49	973-1273	3.20E+00	78.20	0.075	153.7	-18.6	Smithells	In	7.286	114.82	3
	Sb	51	1003-1278	2E-01	115.5	0.0114	129.4	-42.9	Smithells	Sb	6.697	121.75	3
	Ge	32	1010-1287	1.30E+01	297.40	0.073	144.5	-27.8	Smithells	Ge	5.32	72.59	4
	Sn	50	970-1268	9.2E-04	106.1	0.0412	143.3	-29	Smithells	Sn	7.3	118.7	4
	Te	52	909-1145	1.96E+04	181.9	0.063	141.1	-31.2	Smithells	Te	6.24	127.6	4

Impurity Diffusion Parameters **TABLE 8** **SOLUTES IN A-IRON**

Solvent	Element	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Valence
Iron_A				2.76E+00	250.6				Cahoon	Fe_A	7.87	55.85	2
				cm.sq./sec	kJoules	cm.sq./sec	kJoules						
					/mole		/mole						

a	Ag		1021-1161		181.7	1.95E+03	288.9	38.3	Smithells	Ag			1
a	Ag		1053-1173		181.7	3.80E+01	259.2	8.6	Smithells	Ag			1
a	Ag		973-1033		181.7	2.30E+02	278	27.4	Smithells	Ag			1
a	Au		1055-1174		172.3	3.10E+01	261.2	10.6	Smithells	Au			1
a	Cu		1045-1173		211	3.00E+02	283.9	33.3	Smithells	Cu			1
a	*Ag				181.7	2.50E+00	233	-17.6	Hirano ?	*Ag			1
a	*Au				172.3	2.16E+01	257	6.4	Hirano ?	*Au			1
a	*Cu				211	4.20E+00	244	-6.6	Hirano ?	*Cu			1

a,b	Be		1073-1773		161	5.34E+00	218.1	-32.5	Smithells	Be			2
a	Co		1044-1177		287.6	1.18E+02	285.9	35.3	Smithells	Co			2
a	Co		956-1000		287.6	7.19E+00	260.4	9.8	Smithells	Co			2
a	Co		1081-1157		287.6	6.38E+00	257.1	6.5	Smithells	Co			2
a	Mn		1073-1173			3.50E-01	219.8	-30.8	Smithells	Mn			2
a	Mn		973-1033			1.49E+00	233.6	-17	Smithells	Mn			2
	Ni		1203-1323		275.7	7.70E-01	280.5	29.9	Smithells	Ni			2
a	Ni		873-953		275.7	1.40E+00	245.8	-4.8	Smithells	Ni			2
a	Ni		1054-1173		275.7	9.90E+00	259.2	8.6	Smithells	Ni			2
a	Ni		1083-1173		275.7	1.30E+00	234.5	-16.1	Smithells	Ni			2
d	Ni		1748-1767		275.7	9.70E+00	267.5	16.9	Smithells	Ni			2
	U		1223-1348			7.00E-05	133.2	-117.4	Smithells	U			2
a	Zn		1072-1169		93.9	6.00E+01	262.6	12	Smithells	Zn			2
a	*Be				161	1.71E+01	228	-22.6	Hirano ?	*Be			2
a	*Co				287.6	6.91E+00	258	7.4	Hirano ?	*Co			2
a	*Mn					7.60E-01	224.5	-26.1	Hirano ?	*Mn			2
a	*Ni				275.7	2.41E+00	242.2	-8.4	Hirano ?	*Ni			2
a	*Ti (Alpha)				122.7	6.80E+01	261.1	10.5	Hirano ?	*Ti			2
a	*Zn				93.9	2.03E+00	231.4	-19.2	Hirano ?	*Zn			2

a	*As					5.44E+00	223	-27.6	Hirano ?	As			3
a	As		1223-1653			4.30E+00	219.8	-30.8	Smithells	As			3
a	Cr		1043-1150		308.6	9.00E+01	271	20.4	Smithells	Cr			3
a	Cr		1070-1150		308.6	8.52E+00	250.8	0.2	Smithells	Cr			3
a	Sb		773-873		165.3	8.00E+01	269.9	19.3	Smithells	Sb			3
a	Sb		1040-1173		165.3	4.40E+02	270	19.4	Smithells	Sb			3
a	V		1058-1172		309.4	1.24E+02	274	23.4	Smithells	V			3
a	*Al				142	5.15E+00	245.8	-4.8	Hirano ?	*Al			3
a	*Cr				308.6	2.33E+00	238.8	-11.8	Hirano ?	*Cr			3
a	*Sb				165.3	1.41E+02	259.4	8.8	Hirano ?	*Sb			3
a	*V				309.4	3.05E+00	239.3	-11.3	Hirano ?	*V			3

a	Nb		1059-1162		401.9	5.02E+01	252	1.4	Smithells	Nb			4
a	S		973-1173		215.1	3.46E+01	231.5	-19.1	Smithells	S			4
a-g	Sn		1197-1653		106.1	8.45E-01	261.7	11.1	Smithells	Sn			4
a	Sn		900-1023		106.1	6.10E+04	316.4	65.8	Smithells	Sn			4
a	Sn		1073-1183		106.1	2.40E+00	221.9	-28.7	Smithells	Sn			4
a	Sn		973-1033		106.1	5.40E+00	232.4	-18.2	Smithells	Sn			4
a	*Hf				161.9	1.31E+00	290	39.4	Hirano ?	*Hf			4
a	*Mo				405.7	6.60E-01	224.2	-26.4	Hirano ?	*Mo			4
a	*S				215.1	1.56E+00	202.8	-47.8	Hirano ?	*S			4
a	*Si				424	7.40E-01	219.8	-30.8	Hirano ?	*Si			4
a	*Sn				106.1	2.24E+00	222.2	-28.4	Hirano ?	*Sn			4
a	*W				504.5	2.00E+00	246.2	-4.4	Hirano ?	*W			4

a	P		1078-1153		115.5	2.87E+02	271	20.4	Smithells	P			5
a	P		932-1057		115.5	1.38E+05	332	81.4	Smithells	P			5
a	*P				115.5	1.65E+00	221.5	-29.1	Hirano ?	*P			5

Impurity Diffusion Parameters TABLE 9 SOLUTES IN G-IRON

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Valence
Iron_G				8.90E-01	291.3				Cahoon				
				cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules		Fe_G	7.87	55.85	3
					/mole		/mole	/mole					
g	Be		1373-1723		161	1.00E-01	241.2	-50.1	Smithells	Be			1
g	Cu		1558-1641		211	2.86E+00	306.7	15.4	Smithells	Cu			1
g	Cu		1198-1323		211	1.90E-01	272.6	-18.7	Smithells	Cu			1
g	Cu		1378-1483		211	4.16E+00	305	13.7	Smithells	Cu			1
	*Be				161	3.30E-01	256	-35.3	Hirano ?	*Be			1
	*Cu				211	4.34E-01	280.1	-11.2	Hirano ?	*Cu			1
g	Co		1702-1794		287.6	6.38E+00	257.1	-34.2	Smithells	Co			2
g	Co		1409-1633		287.6	1.00E+00	301.9	10.6	Smithells	Co			2
g	Co		1233-1493		287.6	2.90E-02	247.4	-43.9	Smithells	Co			2
g	Mn		1193-1553			1.60E-01	261.7	-29.6	Smithells	Mn			2
g	Ni		1409-1673		275.7	3.00E+00	314	22.7	Smithells	Ni			2
g	Pd		1373-1573		266.3	4.10E-01	280.9	-10.4	Smithells	Pd			2
g	Pt		1233-1533		276.4	2.70E+00	296	4.7	Smithells	Pt			2
	*Co				287.6	2.86E-01	284	-7.3	Hirano ?	*Co			2
	*Ni				275.7	1.08E-01	273	-18.3	Hirano ?	*Ni			2
	*Pd				266.3	4.00E-01	278.6	-12.7	Hirano ?	*Pd			2
	*Pt				276.4	1.00E+00	283	-8.3	Hirano ?	*Pt			2
	*Ti alpha				122.7	6.80E+01	261.1	-30.2	Hirano ?	*Ti			2
	*Zn				93.9	6.20E-01	274.1	-17.2	Hirano ?	*Zn			2
g	As		1323-1573			5.80E-01	246.6	-44.7	Smithells	As			3
g	Cr		1233-1669		308.6	1.08E+01	291.8	0.5	Smithells	Cr			3
g	V		1210-1607		309.4	6.20E-01	273.5	-17.8	Smithells	V			3
g	V		1393-1653		309.4	7.50E-01	264.2	-27.1	Smithells	V			3
	*As					5.60E-01	245	-46.3	Hirano ?	*As			3
	*Cr				308.6	1.69E-01	263.9	-27.4	Hirano ?	*Cr			3
	*Mn					1.78E-01	264	-27.3	Hirano ?	*Mn			3
	*V				309.4	2.80E-01	264	-27.3	Hirano ?	*V			3
g	Hf		1438-1593		161.9	9.00E+04	473.1	181.8	Smithells	Hf			4
g	Hf		1371-1626		161.9	3.60E+03	407.4	116.1	Smithells	Hf			4
g	Nb		1210-1604		401.9	8.30E-01	266.5	-24.8	Smithells	Nb			4
g	S		1223-1523		215.1	1.70E+00	221.9	-69.4	Smithells	S			4
	*Hf				161.9	3.60E+03	407	115.7	Hirano ?	*Hf			4
	*Mo				405.7	3.60E-02	239.8	-51.5	Hirano ?	*Mo			4
	*Nb				401.9	5.60E+00	286	-5.3	Hirano ?	*Nb			4
	*S				215.1	7.52E+00	236.4	-54.9	Hirano ?	*S			4
	*Sn				106.1	4.00E-03	191	-100.3	Hirano ?	*Sn			4
	*W				504.5	5.10E-01	272	-19.3	Hirano ?	*W			4
g	P		1223-1573		115.5	6.30E-02	193.4	-97.9	Smithells	P			5
	*P				115.5	8.70E+00	273	-18.3	Hirano ?	*P			5

Impurity Diffusion Parameters TABLE 10 SOLUTES IN LEAD

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Lead	Pb	82		1.37E+00	109				Cahoon	Pb	11.4	207.2	2
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole	Cahoon				

Solute Elements

	Ag	47	398-598	2.78E-01	181.70	4.6E-02	60.5	-48.5	Smithells	Ag	10.49	107.88	1
	Ag	47	470-750	2.78E-01	181.70	4.8E-02	60.8	-48.2	Smithells	Ag	10.49	107.88	1
	Au	79	367-598	5.60E-02	172.30	4.1E-03	39.1	-69.9	Smithells	Au	19.32	197	1
	Au	79	334-563	5.60E-02	172.30	5.2E-03	38.6	-70.4	Smithells	Au	19.32	197	1
	Au	79	441-693	5.60E-02	172.30	5.8E-03	40.2	-68.8	Smithells	Au	19.32	197	1
	Cu	29	498-598	7.80E-01	211.00	7.9E-03	33.6	-75.4	Smithells	Cu	8.96	63.54	1
	Cu	29	491-803	7.80E-01	211.00	8.6E-03	34.2	-74.8	Smithells	Cu	8.96	63.54	1
	Na	11	522-586	1.45E-01	42.20	6.3	118.5	9.5	Smithells	Na	0.971	22.99	1
	Cd	48	423-593	1.4E-01	80.00	0.409	88.9	-20.1	Smithells	Cd	8.65	112.41	2
	Cd	48	523-823	1.4E-01	80.00	0.92	92.8	-16.2	Smithells	Cd	8.65	112.41	2
	Co	27	383-573	1.66E+00	287.60	9.0E-03	46.4	-62.6	Smithells	Co	8.85	58.94	2
	Hg	80	523-823			1.5	86.7	-22.3	Smithells	Hg	13.55	200.61	2
	Hg	80	466-573			1.05	95	-14	Smithells	Hg	13.55	200.61	2
	Ni	28	481-593	1.39E+00	275.70	9.4E-03	44.5	-64.5	Smithells	Ni	8.9	58.71	2
	Ni	28	432-523	1.39E+00	275.70	1.1E-02	45.4	-63.6	Smithells	Ni	8.9	58.71	2
	Pd	46	470-590	2.10E-01	266.30	3.4E-03	35.4	-73.6	Smithells	Pd	12.02	106.4	2
	Pt	78	490-593			1.1E-02	42.3	-66.7	Smithells	Pt	21.4	195.09	2
	Zn	30	453-773	1.60E-01	93.90	1.65E-02	47.8	-61.2	Smithells	Zn	7.13	65.38	2
	In	49	437-493	3.20E+00	78.20	33	112.2	3.2	Smithells	In	7.286	114.82	3
	Sb	51	461-588	1.05E+00	165.30	0.29	92.9	-16.1	Smithells	Sb	6.697	121.75	3
	Tl	81	480-596			0.511	101.9	-7.1	Smithells	Tl	11.87	204.37	3
	Sn	50	523-723	9.20E+00	106.10	0.41	94.4	-14.6	Smithells	Sn	7.3	118.7	4
	Sn	50	468-595	9.20E+00	106.10	0.29	99.4	-9.6	Smithells	Sn	7.3	118.7	4

Impurity Diffusion Parameters TABLE 11 SOLUTES IN LITHIUM

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Li				1.40E-01	53.8				Cahoon	Li	0.53	6.94	1
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole					

Solute Elements

	Ag	47	340-434	2.78E-01	181.7	3.70E-01	53.72	-0.08	Smithells	Ag	10.49	107.88	1
	Ag	47	323-423	2.78E-01	181.7	5.40E-01	53.72	-0.08	Smithells	Ag	10.49	107.88	1
	Au	79	319-426	5.60E-02	172.3	2.10E-01	46.01	-7.79	Smithells	Au	19.32	197	1
	Cu	29	323-394	7.80E-01	211.00	4.70E-02	38.6	-15.2	Smithells	Cu	8.96	63.54	1
	Cu	29	363-420	7.80E-01	211.00	3.00E-01	41.87	-11.93	Smithells	Cu	8.96	63.54	1
	Na	11	325-449	1.45E-01	42.20	4.10E-01	52.8	-1	Smithells	Na	0.971	22.99	1
	Cd	48	355-449	1.4E-01	80.00	6.20E-01	62.8	9	Smithells	Cd	8.65	112.41	2
	Hg	80	331-447			1.04E+00	59.37	5.57	Smithells	Hg	13.55	200.61	2
	Pb	82	401-443	1.37E+00	109	1.60E+04	105.5	51.7	Smithells	Pb	11.36	207.21	2
	Zn	30	330-446	1.60E-01	93.90	5.70E-01	54.34	0.54	Smithells	Zn	7.13	65.38	2
	Bi	83	413-450			5.30E+14	198	144.2	Smithells	Bi	9.8	208.98	3
	Ga	31	389-447		298	2.10E-01	54.05	0.25	Smithells	Ga	5.907	69.72	3
	In	49	348-443	3.20E+00	78.20	3.90E-01	66.44	12.64	Smithells	In	7.286	114.82	3
	Sb	51	413-449	1.05E+00	165.30	1.60E+12	173.8	120	Smithells	Sb	6.697	121.75	3
	Sn	50	380-447	9.20E+00	106.10	6.20E-01	66.32	12.52	Smithells	Sn	7.3	118.7	4

Impurity Diffusion Parameters — TABLE 12 — SOLUTES IN MAGNESIUM

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Mg		12		1.00E-04	133.9				Cahoon	Mg	1.74	24.32	2
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole					
Solute Elements													
Mg	U	92	773-893		167.4	1.60E-05	95.9	-38	Smithells	U			
	Ag	47	752-913	2.78E-01	181.70	1.79E+01	148.2	14.3	Smithells	Ag	10.49	107.88	1
	Ag	47	752-913	2.78E-01	181.70	3.62E+00	133.1	-0.8	Smithells	Ag	10.49	107.88	1
	Cd	48	733-898	1.4E-01	80.00	1.29E+00	140.7	6.8	Smithells	Cd	8.65	112.41	2
	Cd	48	733-898	1.4E-01	80.00	4.60E-01	132.7	-1.2	Smithells	Cd	8.65	112.41	2
	Fe	26	673-873	2.76	250.60	4.00E-06	88.8	-45.1	Smithells	Fe	7.87	55.85	2
	Ni	28	673-873	1.39E+00	275.70	1.20E-05	95.9	-38	Smithells	Ni	8.9	58.71	2
	Zn	30	740-893	1.60E-01	93.90	4.10E-01	119.7	-14.2	Smithells	Zn	7.13	65.38	2
	In	49	747-906	3.20E+00	78.20	1.88E+00	142.4	8.5	Smithells	In	7.286	114.82	3
	In	49	747-906	3.20E+00	78.20	1.76E+00	143.4	9.5	Smithells	In	7.286	114.82	3
	Sb	51	781-896	1.05E+00	165.30	2.57E+00	137.3	3.4	Smithells	Sb	6.697	121.75	3
	Sb	51	781-896	1.05E+00	165.30	3.27E+00	138.2	4.3	Smithells	Sb	6.697	121.75	3
	C	6	773-873		682	2.10E-07	52.3	-81.6	Smithells	C	2.62	12.011	4
	Sn	50	748-903	9.20E+00	106.10	4.27E+00	149.9	16	Smithells	Sn	7.3	118.7	4

Impurity Diffusion Parameters — TABLE 13 — SOLUTES IN MOLYBDENUM

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Mo		42		5.00E-05	405.7				Cahoon	Mo	10.22	95.95	4
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole					
Solute Elements													
	Re	75	1973-2373			9.70E-02	396.5	-9.2	Smithells	Re	21	186.2	2
	Li	3	1843-2243	1.40E-01	53.80	1.00E-02	470.6	64.9	Smithells	Li	0.53	6.94	1
	Co	27	1273-1773	1.66E+00	287.60	6.00E+00	324.5	-81.2	Smithells	Co	8.85	58.94	2
	Co	27	2123-2623	1.66E+00	287.60	1.80E+01	446.7	41	Smithells	Co	8.85	58.94	2
	Fe	26	1273-1623	2.76	250.60	1.50E-01	346.2	-59.5	Smithells	Fe	7.87	55.85	2
	Fe	26	1200-1478	2.76	250.60	3.70E-03	291.8	-113.9	Smithells	Fe	7.87	55.85	2
	Ni	28	1623	1.39E+00	275.70	2.80E-12			Smithells	Ni	8.9	58.71	2
	W	74	1973-2533	5.4E-01	504.5	1.70E+00	460.5	54.8	Smithells	W	19.3	183.85	2
	W	74	2093-2453	5.4E-01	504.5	1.40E+02	569.4	163.7	Smithells	W	19.3	183.85	2
	W	74	1973-2423	5.4E-01	504.5	4.50E-04	324.5	-81.2	Smithells	W	19.3	183.85	2
	Cr	24	1273-1773	2.00E-01	308.60	2.50E-04	226.1	-179.6	Smithells	Cr	7.19	52.01	3
	Cr	24	1273-1423	2.00E-01	308.60	1.88E+00	342.5	-63.2	Smithells	Cr	7.19	52.01	3
	V	23	1803-1998	2.88E-01	309.40	2.90E+00	473.1	67.4	Smithells	V	6.1	50.95	3
	Y	39	1473-1873	5.5E-06	128.9	1.80E-04	214.8	-190.9	Smithells	Y	4.5	88.9	3
	C	6	493-543		682	2.00E-03	115.85	-289.9	Smithells	C	2.62	12.011	4
	C	6	1533-2283		682	1.04E-02	139	-266.7	Smithells	C	2.62	12.011	4
	Nb	41	1998-2453	1.1	401.9	2.90E+00	569.4	163.7	Smithells	Nb	8.57	92.91	4
	Nb	41	2123-2623	1.1	401.9	1.40E+01	452.6	46.9	Smithells	Nb	8.57	92.91	4
	Nb	41	1973-2373	1.1	401.9	1.70E-02	379.3	-26.4	Smithells	Nb	8.57	92.91	4
	U	92	1773-2273		167.4	7.60E-03	319.9	-85.8	Smithells	U	18.9	238.02	4
Mo	U	92	2073-2373		167.4	1.30E-06	316.5	-89.2	Smithells	U	18.9	238.02	4
	P	15	2273-2493	3.6E+09	115	1.90E-01	337	-68.7	Smithells	P	1.82	30.97	5
	Ta	73	1193-1423	2	460.2	3.50E-04	347.5	-58.2	Smithells	Ta	16.6	180.94	5
	Ta	73	2098-2449	2	460.2	1.90E+00	473.1	67.4	Smithells	Ta	16.6	180.94	5
	S	16	1238-1443	2.0E+17	215.1	3.40E-02	297.3	-108.4	Smithells	S	2.07	32.06	6
	S	16	2493-2743	2.0E+17	215.1	3.20E+01	422.9	17.2	Smithells	S	2.07	32.06	6

Impurity Diffusion Parameters TABLE 14 SOLUTES IN NICKEL

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Nickle	Ni	28		1.39E+00	275.7					Ni	8.9	58.71	2
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole	Cahoon				

Solute Elements

	Ag	47	1297-1693	2.78E-01	181.70	8.94	279.4	3.7	Smithells	Ag	10.49	107.88	1
	Ag	47	1123-1323	2.78E-01	181.70	8.25	282.2	6.5	Smithells	Ag	10.49	107.88	1
	Au	79	1173-1373	5.60E-02	172.30	2	272.1	-3.6	Smithells	Au	19.32	197	1
	Cu	29	1080-1613	7.80E-01	211.00	0.61	255	-20.7	Smithells	Cu	8.96	63.54	1
	Cu	29	1327-1632	7.80E-01	211.00	0.57	258.3	-17.4	Smithells	Cu	8.96	63.54	1
	Cu	29	1048-1323	7.80E-01	211.00	0.27	255.5	-20.2	Smithells	Cu	8.96	63.54	1
	Be	4	1293-1673	5.70E-05	161.00	0.019	193.4	-82.3	Smithells	Be	1.85	9.01	2
	Co	27	1335-1696	1.66E+00	287.60	2.77	285.1	9.4	Smithells	Co	8.85	58.94	2
	Co	27	1123-1643	1.66E+00	287.60	0.59	269.6	-6.1	Smithells	Co	8.85	58.94	2
	Fe	26	1223-1643	2.76	250.60	0.22	252.9	-22.8	Smithells	Fe	7.87	55.85	2
	Fe	26	1478-1669	2.76	250.60	1	269.4	-6.3	Smithells	Fe	7.87	55.85	2
	Pt	78	1354-1481	5.7E-01	276.4	2.5	286.8	11.1	Smithells	Pt	21.4	195.09	2
	U	92	1248-1348			1	236.1	-39.6	Smithells	U	18.9	238.03	2
	W	78	1373-1568	5.4E-01	504.5	2	299.4	23.7	Smithells	W	19.3	183.85	2
	W	78	1346-1668	5.4E-01	504.5	2.87	308.1	32.4	Smithells	W	19.3	183.85	2
	Al	13	914-1212	1.71E+00	142.00	1	260	-15.7	Smithells	Al	2.699	26.98	3
	As	33	1239-1634			1.39	251.8	-23.9	Smithells	As	5.72	74.92	3
	Ce	58	973-1370			0.66	254.6	-21.1	Smithells	Ce	6.77	140.13	3
	Cr	24	1373-1541	2.00E-01	308.60	1.1	272.6	-3.1	Smithells	Cr	7.19	52.01	3
	Nd	60	973-1373			0.44	250.5	-25.2	Smithells	Nd	7.008	144.24	3
	Sb	51	1203-1674	1.05E+00	165.30	3.85	264	-11.7	Smithells	Sb	6.697	121.75	3
	C	6	873-1673			0.12	137.3	-138.4	Smithells	C	2.62	12	4
	Ge	32	939-1675	1.30E+01	297.40	2.1	264	-11.7	Smithells	Ge	5.32	72.59	4
	Hf	72	1023-1423	1.2E-03	161.9	1.8	251	-24.7	Smithells	Hf	13.1	178.49	4
	Sn	50	1242-1642	9.20E+00	106.10	4.56	267.2	-8.5	Smithells	Sn	7.3	118.7	4
	Te	52	1135-1553	1.96E+04	181.9	2.6	254	-21.7	Smithells	Te	6.24	127.6	4
	V	23	1073-1573	2.88E-01	309.40	0.87	278.4	2.7	Smithells	V	6.1	50.95	5
	S	16	1078-1495	2.0E+17	215.1	1.4	219	-56.7	Smithells	S	2.07	32.06	6

Impurity Diffusion Parameters TABLE 15 SOLUTES IN NIOBIUM

Solvent	Element	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Niobium	Nb	41	1151-2668	1.10E+00	401.9				Cahoon	Nb	8.55	92.9	4
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole					
Solute Elements													
	U	92	1773-2273		167.4	8.90E-06	321.5	-80.4		U	18.90	238.02	2
	Cu	29	1909	7.80E-01	211.00	1.02E-09				Cu	8.96	63.54	1
	Co	27	1834-2325	1.66E+00	287.60	7.40E-01	295.2	-106.7	Smithells	Co	8.85	58.94	2
	Co	27	1580-1920	1.66E+00	287.60	1.10E-01	274.7	-127.2	Smithells	Co	8.85	58.94	2
	Co	27	1347-2173	1.66E+00	287.60	4.18E-02	257.2	-144.7	Smithells	Co	8.85	58.94	2
	Fe	26	1663-2168	2.76	250.60	1.40E-01	294.3	-107.6	Smithells	Fe	7.87	55.85	2
	Fe	26	1663-2373	2.76	250.60	1.50E+00	325.3	-76.6	Smithells	Fe	7.87	55.85	2
	Ni	28	1261-1519	1.39E+00	275.70	9.30E+00	336.6	-65.3	Smithells	Ni	8.9	58.71	2
	Ni	28	1433-2168	1.39E+00	275.70	7.70E-02	264.2	-137.7	Smithells	Ni	8.9	58.71	2
	Tl	22	1898-2348			4.00E-01	370.5	-31.4	Smithells	Tl	4.5	47.9	2
	Tl	22	1267-1765			9.90E-02	364	-37.9	Smithells	Tl	4.5	47.9	2
	W	78	2175-2473		504.5	7.00E+04	653	251.1	Smithells	W	19.3	183.85	2
	W	78	2073-2473		504.5	5.00E-04	383.9	-18	Smithells	W	19.3	183.85	2
	Al	13	1700-2000	1.71E+00	142.00	4.50E+02	430.1	28.2	Smithells	Al	2.699	26.98	3
	Cr	24	1220-1766	2.00E-01	308.60	1.30E-01	337.5	-64.4	Smithells	Cr	7.19	52.01	3
	Cr	24	1226-1708	2.00E-01	308.60	3.00E-01	349.6	-52.3	Smithells	Cr	7.19	52.01	3
	V	23	1898-2348	2.88E-01	309.40	4.70E-01	377	-24.9	Smithells	V	6.1	50.95	3
	V	23	1273-1673	2.88E-01	309.40	2.21E+00	355.9	-46	Smithells	V	6.1	50.95	3
	Y	39	1473-1873	5.5E-06	128.9	1.50E-03	232.8	-169.1	Smithells	Y	4.5	88.9	3
	C	6	403-2613		682	1.00E-03	141.92	-260	Smithells	C	2.62	12	4
	Mo	42	1998-2455	5.00E-01	405.70	9.20E+01	511	109.1	Smithells	Mo	10.22	95.95	4
	Mo	42	1973-2298	5.00E-01	405.70	1.30E-02	350.4	-51.5	Smithells	Mo	10.22	95.95	4
	Ru	44	2026-2342			2.93E+01	460.1	58.2	Smithells	Ru	12.2	101.07	4
	Sn	50	2123-2663	9.20E+00	106.10	1.40E-01	330.3	-71.6	Smithells	Sn	7.3	118.7	4
	Zr	40	1923-2523		190.5	0.85	379.4	-22.5	Smithells	Zr	6.49	91.22	4
	Zr	40	1855-2357		190.5	4.70E-01	364	-37.9	Smithells	Zr	6.49	91.22	4
	P	15	1573-2073	3.6E+09	115	5.10E-03	215.6	-186.3	Smithells	P	1.82	30.97	5
Nb	Ta	73	1376-2346	2	460.2	1.00E+00	415.7	13.8	Smithells	Ta	16.6	180.94	5
	S	16	1370-1770	2.0E+17	215.1	2.60E+03	306	-95.9	Smithells	S	2.07	32.06	6

Impurity Diffusion Parameters TABLE 16 SOLUTES IN PRASEODYMIUM

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Praseodymium		59		8.70E-02	123				Cahoon	Pr	6.77	140.9	4
			K	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole					
Solute Elements													
	Ag	47	886-1040	2.78E-01	181.70	1.4E-01	106.3	-16.7	Smithells	Ag	10.49	107.88	1
	Ag	47	1085-1195	2.78E-01	181.70	3.2E-02	90	-33	Smithells	Ag	10.49	107.88	1
	Au	79	870-1015	5.60E-02	172.30	4.3E-02	82.5	-40.5	Smithells	Au	19.32	197	1
	Au	79	1075-1185	5.60E-02	172.30	3.3E-02	84.2	-38.8	Smithells	Au	19.32	197	1
	Cu	29	926-1059	7.80E-01	211.00	8.4E-02	75.8	-47.2	Smithells	Cu	8.96	63.54	1
	Cu	29	-101	7.80E-01	211.00	5.7E-02	74.5	-48.5	Smithells	Cu	8.96	63.54	1
	Co	27	885-1036	1.66E+00	287.60	4.7E-02	68.7	-54.3	Smithells	Co	8.85	58.94	2
	Fe	26	885-1060	2.76	250.60	2.1E-03	39.4	-83.6	Smithells	Fe	7.87	55.85	2
	Fe	26	1075-1180	2.76	250.60	4.0E-03	43.5	-79.5	Smithells	Fe	7.87	55.85	2
	Zn	30	1095-1194	1.60E-01	93.90	6.3E-01	113	-10	Smithells	Zn	7.13	65.38	2
	Zn	30	876-1040	1.60E-01	93.90	1.8E-01	103.8	-19.2	Smithells	Zn	7.13	65.38	2
	Ho	67	1085-1180			9.5E-03	110.1	-12.9	Smithells	Ho	8.8	164.93	3
	In	49	1075-1200	3.20E+00	78.20	9.6E-02	121	-2	Smithells	In	7.286	114.82	3
	La	57	1080-1190	3.20E+00	78.20	1.8E-02	107.6	-15.4	Smithells	La	6.146	138.9	3

Impurity Diffusion Parameters TABLE 17 SOLUTES IN SILVER

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Valence
Silver	Ag	47	973-1223	2.78E-01	181.7				Cahoon	Ag	10.5	107.86	1
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole					
Solute Elements													
	Au	79	991-1198	5.60E-02	172.30	0.85	202.1	20.4	Smithells	Au	10.49	107.88	1
	Cu	29	990-1218	7.80E-01	211.00	1.23	193	11.3	Smithells	Cu	8.96	63.54	1
	Cu	29	699-897	7.80E-01	211.00	0.029	164.1	-17.6	Smithells	Cu	8.96	63.54	1
	Cd	48	866-1210	1.4E-01	80.00	0.44	174.6	-7.1	Smithells	Cd	8.65	112.41	2
	Co	27	973-1214	1.4E-01	80.00	1.9	204.1	22.4	Smithells	Co	8.85	58.94	2
	Fe	26	1073-1205	2.76	250.60	2.6	205.2	23.5	Smithells	Fe	7.87	55.85	2
	Hg	80	926-1122			0.079	159.5	-22.2	Smithells	Hg	13.55	200.61	2
	Ni	28	903-1200	1.39E+00	275.70	15	217.3	35.6	Smithells	Ni	8.9	58.71	2
	Ni	28	1022-1223	1.39E+00	275.70	21.9	229.3	47.6	Smithells	Ni	8.9	58.71	2
	Pb	82	973-1098	1.37E+00	109	0.22	159.5	-22.2	Smithells	Pb	11.36	207.21	2
	Pd	26	1008-1212	2.10E-01	266.30	9.57	237.6	55.9	Smithells	Pd	12.02	106.4	2
	Pt	78	923-1223	5.7E-01	276.4	6	238.2	56.5	Smithells	Pt	21.4	195.09	2
	Pt	78	1094-1232	5.7E-01	276.4	1.9	235.7	54	Smithells	Pt	21.4	195.09	2
	Zn	30	916-1197	1.60E-01	93.90	0.54	174.6	-7.1	Smithells	Zn	7.13	65.38	2
	Zn	30	970-1225	1.60E-01	93.90	0.532	174.6	-7.1	Smithells	Zn	7.13	65.38	2
	Al	13	873-1223	1.71E+00	142.00	0.13	159.5	-22.2	Smithells	Al	2.699	26.98	3
	As	33	915-1213			0.42	149.6	-32.1	Smithells	As	5.72	74.92	3
	Cr	24	1023-1215	2E-01	308.6	3.29	210	28.3	Smithells	Cr	7.19	52.01	3
	Cr	24	976-1231	2E-01	308.6	1.07	192.6	10.9	Smithells	Cr	7.19	52.01	3
	Ga	31	873-1213			0.42	162.9	-18.8	Smithells	Ga	5.907	69.72	3
	In	49	886-1209	3.20E+00	78.20	0.41	170.1	-11.6	Smithells	In	7.286	114.82	3
	In	49	553-838	3.20E+00	78.20	0.36	169	-12.7	Smithells	In	7.286	114.82	3
	Sb	51	743-1215	1.05E+00	165.30	0.169	160.4	-21.3	Smithells	Sb	6.697	121.75	3
	Tl	22	1051-1220			1.33	198	16.3	Smithells	Tl	4.5	47.9	3
	Tl	81	918-1073			0.15	158.7	-23	Smithells	Tl	11.87	204.37	3
	Ge	32	943-1123	1.3E+01	297.4	0.084	152.8	-28.9	Smithells	Ge	5.32	72.59	4
	Mn	25	883-1212			4.29	196	14.3	Smithells	Mn	7.43	54.94	4
	Ru	44	1066-1219			180	275.5	93.8	Smithells	Ru	12.2	101.07	4
	Sn	50	865-1210	9.20E+00	106.10	0.25	165	-16.7	Smithells	Sn	7.3	118.7	4
	Te	52	650-1169			0.21	154.7	-27	Smithells	Te	6.24	127.6	4
	V	23	1012-1218	2.88E-01	309.40	2.72	209	27.3	Smithells	V	5.8	50.94	5
	S	16	873-1173	2.0E+17	215.1	1.65	167.5	-14.2	Smithells	S	2.07	32.06	6
	Se	34	759-1109	5.0E+01	125.1	0.285	157.4	-24.3	Smithells	Se	4.8	78.96	6

Impurity Diffusion Parameters TABLE 18 SOLUTES IN TIN

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Tin	Sn	50		9.20E+00	106.10				Cahoon	Sn	7.3	118.69	4
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole					
Solute Elements													
par	Ag	47	408-498	2.78E-01	181.70	7.1E-03	51.5	-54.6	Smithells	Ag	10.49	107.88	1
perp	Ag	47	408-498	2.78E-01	181.70	0.18	77	-29.1	Smithells	Ag	10.49	107.88	1
par	Au	79	408-498	5.60E-02	172.30	5.8E-03	46.1	-60	Smithells	Au	19.32	197	1
perp	Au	79	408-498	5.60E-02	172.30	0.16	74.1	-32	Smithells	Au	19.32	197	1
par	Cu	29	298	7.80E-01	211.00	2E-06			Smithells	Cu	8.96	63.54	1
perp	Cu	29	413-503	7.80E-01	211.00	2.4E-03	33.1	-73	Smithells	Cu	8.96	63.54	1
par	Cd	48	463-498	1.4E-01	80.00	220	118.1	12	Smithells	Cd	8.65	112.41	2
perp	Cd	48	463-498	1.4E-01	80.00	0.18	77	-29.1	Smithells	Cd	8.65	112.41	2
	Co	27	413-490	1.66E+00	287.60	5.5	92.1	-14	Smithells	Co	8.85	58.94	2
	Fe	26	387-462	2.76	250.60	4.8E-04	51.1	-55	Smithells	Fe	7.87	55.85	2
par	Hg	80	447-499			7.5	105.9	-0.2	Smithells	Hg	13.55	200.61	2
perp	Hg	80	447-499			30	112.2	6.1	Smithells	Hg	13.55	200.61	2
par	Ni	28	298-373	1.39E+00	275.70	1.92E-02	18.1	-88	Smithells	Ni	8.9	58.71	2
perp	Ni	28	393-473	1.39E+00	275.70	1.87E-02	54.2	-51.9	Smithells	Ni	8.9	58.71	2
perp	Zn	30	408-496	1.60E-01	93.90	8.4	89.2	-16.9	Smithells	Zn	7.13	65.38	2
par	Zn	30	408-496	1.60E-01	93.90	1.1E-02	50.2	-55.9	Smithells	Zn	7.13	65.38	2
par	In	49	453-494	3.20E+00	78.20	12.2	107.2	1.1	Smithells	In	7.286	114.82	3
perp	In	49	453-494	3.20E+00	78.20	34.1	108	1.9	Smithells	In	7.286	114.82	3
par	Sb	51	466-499	1.05E+00	165.30	7	121.8	15.7	Smithells	Sb	6.697	121.75	3
perp	Sb	51	466-499	1.05E+00	165.30	73	123.1	17	Smithells	Sb	6.697	121.75	3
	Tl	81	410-489			1.3E-03	61.5	-44.6	Smithells	Tl	11.87	204.37	3

Impurity Diffusion Parameters TABLE 19 SOLUTES IN B-THORIUM

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
B-Thorium	Th	90			418.4								4
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole	Cahoon				
Solute Elements													
	Co	27	1613-1898	1.66E+00	287.60	4E-03	65.3	-353.1	Smithells	Co	8.9	58.93	2
	Fe	26	1613-1898	2.76	250.60	4E-03	71.6	-346.8	Smithells	Fe	7.86	55.84	2
	Ni	28	1613-1898	1.39E+00	275.70	4E-04	38.1	-380.3	Smithells	Ni	8.9	58.7	2
	W	74	1683-1818	5.4E-01	504.5	0.103	160	-258.4	Smithells	W	19.3	183.85	2
	C	6	713-1193		682	2.2E-02	113	-305.4	Smithells	C	2.62	12.011	4
	Mo	42	1698-1873	5.00E-01	405.70	15.1	216	-202.4	Smithells	Mo	10.22	95.95	4
	Nb	41	1643-1933	1.10E+00	401.90	0.5	201.8	-216.6	Smithells	Nb	8.57	92.91	4
	Re	75	1663-1943			4.04E-03	84	-334.4	Smithells	Re	21	186.2	4
	Zr	40	1773-1873			1.73E+04	384	-34.4	Smithells	Zr	6.49	91.22	4
	Ta	73	1648-1933	2	460.2	0.57	210.6	-207.8	Smithells	Ta	16.6	180.94	5
	V	23	1643-1933	2.88E-01	309.40	1.9E-02	129.8	-288.6	Smithells	V	5.8	50.94	5

Impurity Diffusion Parameters TABLE 20 SOLUTES IN TUNGSTEN

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Tungsten	W	74		5.40E-01	504.5					W	19.3	183.85	2
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole	Cahoon				
Solute Elements													
	Fe	26	1213-1513	2.76	250.60	0.014	276.3	-228.2	Smithells	Fe	7.87	55.85	2
	Y	39	1473-1873	5.5E-06	128.9	6.7E-03	285.1	-219.4	Smithells	Y	4.5	88.9	3
	C	6	2073-3073		682	9.22E-03	169.1	-335.4	Smithells	C	2.62	12.011	4
	C	6	373-673		682	3.15E-03	172	-332.5	Smithells	C	2.62	12.011	4
	Ir	77	2007-2960			0.32	506.2	1.7	Smithells	Ir	22.5	192.22	4
	Mo	42	1909-2658	5.00E-01	405.70	1.4	567.3	62.8	Smithells	Mo	10.22	95.95	4
	Mo	42	1973-2373	5.00E-01	405.70	0.3	423	-81.5	Smithells	Mo	10.22	95.95	4
	Mo	42	2273-2673	5.00E-01	405.70	0.05	506.6	2.1	Smithells	Mo	10.22	95.95	4
	Nb	41	1578-2640	1.10E+00	401.90	3.01	576.1	71.6	Smithells	Nb	8.57	92.91	4
	Os	76	2105-2928			0.64	538.4	33.9	Smithells	Os	22.4	190.2	4
	Re	75	2939-3501			275	681.6	177.1	Smithells	Re	21	186.2	4
	Re	75	2110-2900			4	597	92.5	Smithells	Re	21	186.2	4
	U	92	1973-2473	2.3E-03	119.2	2E-03	433.3	-71.2	Smithells	U	18.9	238.03	4
	U	92	2245-300	2.3E-03	119.2	1.8E-02	389.4	-115.1	Smithells	U	18.9	238.03	4
	P	15	2153-2453	3.6E+09	115.5	26.8	510	5.5	Smithells	P	1.82	30.97	5
	Ta	73	1578-2648	2	460.2	3.05	585.7	81.2	Smithells	Ta	16.6	180.94	5
	S	16	2153-2453	2E+17	215.1	2.17E-05	292.2	-212.3	Smithells	S	2.07	32.06	6

Impurity Diffusion Parameters TABLE 21 SOLUTES IN G-URANIUM

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
g-Uranium	U	92		2.30E-03	119.2								
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					
					/mole		/mole	/mole	Cahoon				
Solute Elements													
	Au	79	1057-1280	5.60E-02	172.30	4.86E-03	127.3	8.1	Smithells	Au	19.32	197	1
	Cu	29	1059-1312	7.80E-01	211.00	1.96E-03	100.7	-18.5	Smithells	Cu	8.96	63.54	1
	Co	27	1056-1263	1.66E+00	287.60	3.51E-04	52.6	-66.6	Smithells	Co	8.85	58.94	2
	Fe	26	1059-1263	2.76	250.60	2.69E-04	50.3	-68.9	Smithells	Fe	7.87	55.85	2
	Ni	28	1059-1313	1.39E+00	275.70	5.36E-04	65.57	-53.63	Smithells	Ni	8.9	58.71	2
	Cr	24	1070-1311	2.00E-01	308.60	5.47E-03	102.4	-16.8	Smithells	Cr	7.19	52.01	3
	C	6	1130-1270		682	0.218	123	3.8	Smithells	C	2.62	12.011	4
	Mn	25	1060-1212			1.81E-04	58.1	-61.1	Smithells	Mn	7.43	54.94	4
	Nb	41	1063-1376	1.10E+00	401.90	4.87E-02	166	46.8	Smithells	Nb	8.57	92.91	4

Impurity Diffusion Parameters TABLE 22 SOLUTES IN ZINC

Solvent	Solute	At.Num.	Temp.range	Self Do	Self Qo	Imp Do	Imp Qo	Delta Q	Reference		Density	At.Wt.	Val
Zn (average)		30		1.60E-05	93.9				Cahoon				
			k	cm.sq./sec	kJoules	cm.sq./sec	kJoules	kJoules					2
					/mole		/mole	/mole					

Solute Elements

p	Ag	47	544-686	2.78E-01	181.70	3.20E-01	108.9	15	Smithells	Ag	10.49	107.88	1
o	Ag	47	544-686	2.78E-01	181.70	4.50E-01	115.6	21.7	Smithells	Ag	10.49	107.88	1
p	Au	79	588-688	5.60E-02	172.30	9.70E-01	124.3	30.4	Smithells	Au	19.32	197	1
o	Au	79	588-688	5.60E-02	172.30	2.90E-01	124.3	30.4	Smithells	Au	19.32	197	1
o	Cu T	29	611-688	7.80E-01	211.00	2.00E+00	125.3	31.4	Smithells	Cu T	8.96	63.54	1
p	Cu =	29	611-688	7.80E-01	211.00	2.22E+00	123.6	29.7	Smithells	Cu =	8.96	63.54	1
p	Cd	48	498-689	1.4E-01	80.00	1.14E-01	86	-7.9	Smithells	Cd	8.65	112.41	2
o	Cd	48	498-689	1.4E-01	80.00	1.17E-01	85.5	-8.4	Smithells	Cd	8.65	112.41	2
o	Hg	80	533-686			7.30E-02	84.5	-9.4	Smithells	Hg	13.55	200.61	2
p	Hg	80	533-686			5.60E-02	82.5	-11.4	Smithells	Hg	13.55	200.61	2
p	Ni	28	564-664	1.39E+00	275.70	8.10E+00	136.6	42.7	Smithells	Ni	8.9	58.71	2
o	Ni	28	564-664	1.39E+00	275.70	4.30E-01	121.5	27.6	Smithells	Ni	8.9	58.71	2
p *smithel	Ga	31	513-676	5.3E-13	293	1.60E-02	77	-16.9	Smithells	Ga	5.907	69.72	3
o	Ga	31	513-676	5.3E-13	293	1.80E-02	76	-17.9	Smithells	Ga	5.907	69.72	3
p	In	49	444-689	3.20E+00	78.20	6.20E-02	80	-13.9	Smithells	In	7.286	114.82	3
o	In	49	444-689	3.20E+00	78.20	1.40E-01	82.1	-11.8	Smithells	In	7.286	114.82	3
	C	6	439-656		682	1.00E-05	50.2	-43.7	Smithells	C	2.62	12.011	4
p	Sn	50	571-673	9.2E-04	106.1	1.50E-01	81.2	-12.7	Smithells	Sn	7.3	118.7	4
o	Sn	50	571-673	9.2E-04	106.1	1.30E-01	77	-16.9	Smithells	Sn	7.3	118.7	4

APPENDIX A3

Figure 4	**Legend and Guide to the interpretation of Tables 24-43**
Tables 24-43	**Tables of Model Results for 20 Solvent systems**
Figures 5-24	**Plots of ΔQ versus Δ Radius for 20 Solvent Systems**

The Relative Valence Model predicts that if the difference in relative valences betwqeen solute and solvent is negative then the activation energy of the solute will be less than that of the solvent self activation energy. This column gives a 0 value for a prediction of -ve Delta Q if the difference in valences is negative. It will conversely give a value of 1 if the valence difference is positive , predicting a positive value of solute Delta Q.Incorrect guesses are shaded, note R.V.M. also fails for homovalent solutes where no prediction is possible.

Atomic radius of element , based on half the interatomic spacing .

Data taken from Flinn and Trojan(1990)

U is the difference between solvent Eo and Solute Eo .. The difference in ground state energies is the basis of the Le Clair Homovalent Impurity model . Wher solutes with Eo values lower than the solvent are expected to be slow diffusers.

The difference in Emax values . Similar to Le Claire U which is the difference in Eo values,and does not consider the contribution due to Ef energy. The Modified Le Claire model predicts that if U is negative the solute is a potential well having a positive valued activation energy difference. If U is negative then the solute is a potential hill and will have a negative value for delta Q.

Delta radius is the difference between the atomic radius of the solvent and the equilibrium radius of the solute. Note the equilibrium radius listed is the the smallest possible ie the next full integer of charge transfer , loss of all valence electrons or the maximum or atomic size of a charge acceptor type solute.

Ionic radius of element for the ionization state indicated by the full valence.
These are the Goldscmidt Ionic Radii Taken from Flinn and Trojan(1990)

Experimental value of Solute Delta Q taken from literature. For references refer to the Impurity Diffusion Parameter Tables for the respective solvent system Tables 3-22

Solutes for which experimental data exists are listed along the side

Difference in valence , Solvent valence -solute valence

Calculated Values of the Fermi Energy , values generated by C++ program , iter.cpp

Prediction of the sign of solute Delta Q based on the energy difference , U. 1 predicts a -neg value for Delta Q while 0 predicts a +pos. value for solute Delta Q

Guesses highlighted are incorrect

Predictions of solute Delta Q , according to the Modified Le Claire Model .
0 predicts that the solute is a potential hill with a -ve value of Delta Q and 1 the opposite incorrect predictions are shaded.

Solvent basic atomic data presented in top row

Ground State Energy values for elements, calculated by C++

Equilibrium radius of solute upon transfer of energy equilibrating charge.

A_IRON solvent system

		val			at rad	Ion rad	Ef	Eo	U		Emax	Alpha															
26	Fe_a	2			1.24	0.87	8.702	-22.592	0.000		-8.087	-8.087	0	0	0	1.24											
SOLUTES			Relative Valence Model Predictions							Le Clair U Model Predictions Difference in Eo Values			Delta E	Mod. LeClaire Model Predictions		Charge transfer from iter.cpp	Equil.Ro at atomic diameter	acceptors fixed	Delta Radius	next full charge as continuous	Rad. Comp. calculated by ItsModel Predictions		Element	Experimental delta Q
16	S	6	-4	0	1.06	0.34	10.296	-25.333	2.742	1	21.492	-8.087	-29.579	0	N.S.		0.34	0.34	-0.900		0	16	S	-47.8
14	Si	4	-2	0	1.17	0.39	8.574	-20.049	-2.542	0	-0.374	-8.087	-7.713	0	-1.532	1.0509	1.0509	-0.789	1	0	0	14	Si	-30.8
15	P	5	-3	0	1.09	0.35	15.516	-26.236	3.644	1	-8.977	-8.087	0.89	1	0.175	1.09	1.09	-0.150			0	15	P	-29.1
50	Sn	4	-2	0	1.58	0.74	20.745	-43.554	20.962	1	-4.327	-8.087	3.76	0	-1.015	1.4805	1.35	0.110	1.35	1	0	50	Sn	-28.4
42	Mo	4	-2	0	1.36	0.68	6.192	-46.826	24.234	1	-5.55	-8.087	-2.537	0	-0.442	1.2064	1.2064	-0.034	1.14	0	0	33	As	-27.6
25	Mn	4	-2	0	1.37	0.52	14.146	-36.944	14.352	1	0.813	-8.087	8.9	0	-2.117	1.1503	0.99	0.250	0.99	0	0	42	Mo	-26.4
4	Beryllium	2	0	0	1.14	0.54	11.222	-21.017	-1.574	0	0.905	-8.087	8.992	0	-2.162	1.1525	1.1525	-0.087	1.01	0	0	25	Mn	-26.1
30	Zn	2	0		1.33	0.83	11.317	-17.957	4.634	0	-8.173	-8.087	0.006	1	0.01	1.14	1.14	-0.100			0	4	Be	-22.6
47	Ag	1	1	1	1.44	1.13	8.508	-18.508	-4.084	0	-8.948	-8.087	0.861	1	0.122	1.33	1.33	0.090		1	0	30	Zn	-19
29	Cu	1	1	1	1.28	0.96	6.764	-18.746	-3.845	0	-7.506	-8.087	0.578	0	-0.048	1.1245	1.13	-0.110	1.13	0	0	47	Ag	-17.6
26	Fe_a	2			1.24	0.87	8.402	-19.365	-3.227	0	-8.087	-8.087	0.634	0	-0.048	1.2662	0.96	-0.280	0.96	1	1	29	Cu	-6.6
41	Nb	5	-3	0	1.43	0.74	8.508	-18.508	-4.084	0	-12.584	-8.087	4.497	null				0			0		Fe_A	0
79	Au	1	1	1	1.44	1.37	6.764	-18.746	-3.845	0	-9.877	-8.087	1.79	1	1.24	1.43	1.43	0.190			1	41	Nb	1.4
27	Co	3	-1	0	1.25	0.65	8.402	-19.365	-3.227	0	-7.461	-8.087	0.626	1	0.155	1.44	1.44	0.200			1	79	Au	6.4
51	Sb	3	-1	0	1.61	0.9	11.317	-22.899	0.308	1	-7.472	-8.087	0.615	2	-0.105	1.2401	1.14	-0.100	1.14	0	0	27	Co	7.4
22	Ti_a	2	0		1.47	0.76	7.026	-22.872	0.280	1	-36.505	-8.087	28.436	2	-0.135	1.5936	1.47	0.230	1.47	1	1	51	Sb	8.8
46	Pd	2	0		1.37	0.5	4.065	-18.653	-5.939	0	-9.825	-8.087	1.738	1	N.S.		1.47	0.250			1	22	Ti_a	10.5
														1	0.25	1.37	1.37	0.130			1	46	Pd	30.3

SUCCESS RATE 44.00% — U Model 60.00% — 76.00% — 76.00%

Predictions 1 positive Delta Q
0 negative Delta Q * or null in case of self-diffusion Empty cell no prediction possible

total 25

Bottom rows summarize the results of the three models as to percent correct and total number of sample solutes for the solvent system

Charge transfer required for the solute to equilibrate with the solvent Emax value. Determined by the program ITER.cpp

N.S. implies the solute does not have enough valence electrons available to equilibrate or it must accept more electrons than the number of its valence electrons. In effect a solution is out of range of the solution algorithm ITER.cpp . A prediction can still be made under certain circumstances. If the solute must give up more than its Z electrons then it is assumed it gives up these and obtains a minimum radius of its Goldschmidt ralus. If it is expected to accept a large number of electrons then it is expected to reach a maimum radius equivalent to its atomic radius. In either case energy equilibration appears to be impossible if the solute alone is assumed to be the only adapting entity.

For charge donators the next full radius of the solute is presented. The R.C.M. prediction algorithm will use this as a minimum value for donators . The algorithm will assume all acceptors assume their atomic diameter.

The Radius Compensating Model prediction compares the atomic , equilibrium and next full radius of a solute with that of the the solvent . If any of the three states is smaller than the solvent then a -Delta Q value for solute diffusion is predicted, a 0 value.
If the solute is a charge acceptor it is assumed then that it remains at its full atomic radius. The R.C.M. checks this radius against that of the solvent ,should it be smaller then the solute is predicted to have a -Delta Q for diffusion if it is larger than a positive Delta Q , a 1 , is pr4edicted.

Note the solvent as solute is left as a 0 prediction or as NULL

Incorrect predictions are shaded.

Emax value for each element based on bulk atomic properties . Calculated by the program ITER.cpp . Where Emax = Eo+5/3 Ef.
The values are in electron Volts

Since the equilibrium radius is often a fractional quantity the next full integral value of charge is examined and a radius at that value of charge transfer calculated by the program ITER.cpp. The radius formula is taken from the work of Varley(1954)

Alpha is the Emax of the solvent, (top row) to which the solute is expected to equilibrate.
Units in eVolts

FIGURE 4

ALUMINUM solvent system

TABLE 24

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha										
13	Al	3			1.43	0.57	8.574	-20.049	-0.000		-5.758	-5.758	0	0	0	1.43						
SOLUTES			Delta Valence	Relative Valence Model Predictions					Le Clair U Model Predictions Difference In Eo Values				Delta Emax	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
1	Hydrogen	1	2	1	0.46	1.54	39.836	-53.444	33.394	1	12.952	-5.758	-18.71	0	-0.52	0.3908		-1.039		0	1	H	-95.96
3	Lithium	1	2	1	1.52	0.78	3.648	-10.436	-9.613	0	-4.355	-5.758	-1.403	0	-0.16	1.4622		-0.650	0.78	0	3	Li	-16
4	Beryllium	2	1	1	1.14	0.54	10.296	-25.333	5.284	1	-8.173	-5.758	2.415	1	0.34	1.14	1.14	-0.290		0	4	Be	25.44
11	Na	1	2	1	1.86	0.98	2.437	-8.498	-11.551	0	-4.437	-5.758	-1.321	0	-0.168	1.7856		-0.450	0.98	0	11	Na	-44.9
12	Mg	2	1	1	1.6	0.78	5.227	-17.740	-2.310	0	-9.028	-5.758	3.27	1	0.647	1.6	1.6	0.170		1	12	Mg	-27
13	Al	3	0		1.43	0.57	8.574	-20.049	-0.000	0	-5.758	-5.758	0	0	0	1.43		0		0	13	Al	0
14	Si	4	-1	0	1.17	0.39	15.516	-26.236	6.186	1	-0.374	-5.758	-5.384	0	-1.195	1.0813		-0.349	1.003	0	14	Si	-18.1
23	V	5	-2	0	1.32	0.4	14.146	-36.944	16.895	1	-13.367	-5.758	7.609	1	2.14	1.32	1.32	-0.110		0	23	V	-59
24	Cr	3	0		1.25	0.64	11.222	-21.017	0.968	1	-2.314	-5.758	-3.444	0	-0.705	1.1777		-0.252	1.142	0	24	Cr	-58.7
25	Mn	4	-1	0	1.37	0.52	11.317	-17.957	-2.092	0	0.905	-5.758	-6.663	0	-1.847	1.1937		-0.236	1.174	0	25	Mn	-21.4
27	Co	3	0		1.25	0.65	11.222	-26.164	6.115	1	-7.461	-5.758	1.703	1	0.338	1.25	1.25	-0.180		0	27	Co	32
28	Ni	2	1	1	1.25	0.78	8.564	-22.326	2.276	1	-8.052	-5.758	2.294	1	0.362	1.25	1.25	-0.180		0	28	Ni	-58.28
29	Cu	1	2	1	1.28	0.96	5.145	-16.028	-4.021	0	-7.453	-5.758	1.695	1	0.17	1.28	1.28	-0.150	0.000	0	29	Cu	-15
30	Zn	2	1	1	1.33	0.83	7.564	-21.556	1.507	1	-8.948	-5.758	3.19	1	0.535	1.33	1.33	-0.100		0	30	Zn	-23
31	Ga	3	0		1.35	0.62	9.621	-21.341	1.292	1	-5.306	-5.758	-0.452	0	-0.097	1.3401		-0.090	1.234	0	31	Ga	-18.9
32	Ge	4	-1	0	1.22	0.44	14.271	-24.658	4.609	1	-0.873	-5.758	-4.885	0	-1.15	1.1315		-0.298	1.046	0	32	Ge	-58.28
41	Nb	5	-2	0	1.43	0.74	10.387	-19.462	-0.587	0	-12.584	-5.758	6.826	1	2.14	1.43	1.43	0.000		0	41	Nb	-58.28
42	Mo	4	-1	0	1.36	0.68	11.484	-18.328	-1.722	0	0.813	-5.758	-6.571	0	-1.802	1.1905		-0.240	1.166	0	42	Mo	-87
46	Pd	2	1	1	1.37	0.5	7.129	-21.707	1.658	1	-9.825	-5.758	4.067	1	0.692	1.37	1.37	-0.060		0	46	Pd	-58
47	Ag	1	2	1	1.44	1.13	4.065	-14.285	-5.765	0	-7.509	-5.758	1.751	1	0.2	1.44	1.44	0.010		1	47	Ag	-25
48	Cd	2	1	1	1.5	1.03	5.947	-19.658	-0.392	0	-9.746	-5.758	3.988	1	0.745	1.5	1.5	0.070		1	48	Cd	-17
49	In	3	0		1.57	0.92	7.113	-18.389	-1.661	0	-6.533	-5.758	0.775	1	0.203	1.57	1.57	0.140		1	49	In	-26
50	Sn	4	-1	0	1.58	0.74	8.508	-18.508	-1.542	0	-4.327	-5.758	-1.431	0	-0.445	1.5391		0.052	1.482	1	50	Sn	-22
51	Sb	3	0		1.61	0.9	6.764	-18.746	-1.303	0	-7.472	-5.758	1.714	1	0.458	1.61	1.61	0.180		1	51	Sb	-20.3
53	I	5	-2	0	1.36	0.94	13.326	-43.419	23.370	1	-21.209	-5.758	15.451	1	4.42	1.36	1.36	-0.070		0	53	I	-19.7
55	Cs	1	2	1	2.65	1.65	1.200	-5.777	-14.272	0	-3.777	-5.758	-1.981	0	-0.295	2.4517		0.220	1.65	1	55	Cs	-42.8
59	Pr	4	-1	0	1.83	1	6.343	-9.824	-10.225	0	0.747	-5.758	-6.505	0	-2.477	1.4764		-0.085	1.345	0	59	Pr	-41.54
79	Au	1	2	1	1.44	1.37	4.065	-16.653	-3.397	0	-9.877	-5.758	4.119	1	0.447	1.44	1.44	0.010		1	79	Au	-25
80	Hg	2	1	1	1.5	1.12	5.947	-20.891	0.841	1	-10.979	-5.758	5.221	1	0.962	1.5	1.5	0.070		1	80	Hg	-0.02
81	Tl	3	0		1.71	1.06	5.996	-17.704	-2.346	0	-7.709	-5.758	1.951	1	0.548	1.71	1.71	0.280		1	81	Tl	10.7
82	Pb	2	1	1	1.75	1.32	4.369	-16.915	-3.134	0	-9.633	-5.758	3.875	1	0.827	1.75	1.75	0.320		1	82	Pb	3.6
# correct				10	14					19				19						20			
SUCCESS RATE				32.26%	45.16%					61.29%				61.29%						64.52%			
TOTAL 31																							

This cell shows the success rate that results from using the RVM for only heterovalent systems and the U model of Le Clair for the Homovalent Systems

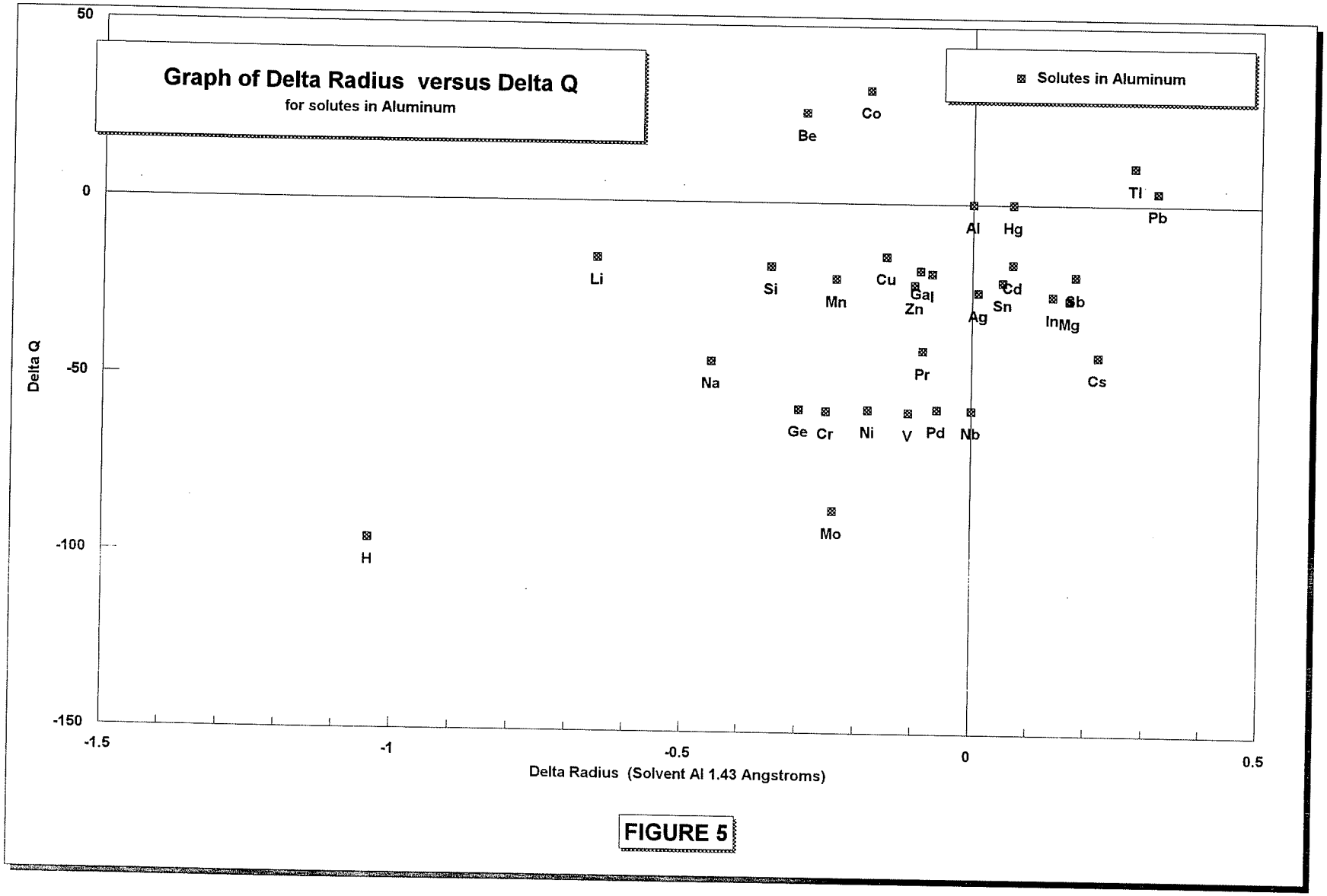
Graph of Delta Radius versus Delta Q
for solutes in Aluminum
Solutes in Aluminum
Delta Q
50
0
-50
-100
-150
-1.5
-1
-0.5
0
0.5
Delta Radius (Solvent Al 1.43 Angstroms)
Co
Be
Tl
Pb
Al
Hg
Li
Si
Mn
Cu
Ga
Zn
Cd
Sn
Ag
Sb
In
Mg
Na
Pr
Cs
Ge
Cr
Ni
V
Pd
Nb
Mo
H

FIGURE 5

BERYLLIUM solvent system

TABLE 25

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha										
4	Beryllium	2			1.14	0.54	10.296	-25.333	-0.000	0	-8.173	-8.173		0	1.14							
SOLUTES			Delta Valence	Relative Valence Model Predictions					Le Clair U Model Predictions Difference	in Eo Values			Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
6	Carbon	4	-2		0.77	0.2	35.825	-49.566	24.232	1	10.144	-8.173	-18.317	0	-2.065	0.6552		-0.4848	0.566	0	6	Carbon	-2.4
4	Beryllium	2	0		1.14	0.54	10.296	-25.333	-0.000	0	-8.173	-8.173	0	0	0.002	1.14	1.14	0		0	4	Beryllium	0
27	Co	3	-1	0	1.25	0.65	11.222	-26.164	0.831	1	-7.461	-8.173	-0.712	0	-0.12	1.2387		0.0987	1.142	1	27	Co	126.2
26	Fe_a	2	0		1.24	0.87	8.702	-22.592	-2.742	0	-8.087	-8.173	-0.086	0	-0.005	1.2393		0.0993	1.063	1	26	Fe_a	55.9
28	Ni	2	0		1.25	0.78	8.564	-22.326	-3.008	0	-8.052	-8.173	-0.121	0	-0.02	1.2472		0.1072	1.072	1	28	Ni	82
13	Al	3	-1		1.43	0.57	8.574	-20.049	-5.284	0	-5.758	-8.173	-2.415	0	-0.48	1.3756		0.2356	1.307	1	13	Al	7.3
52	Te	4	-2	0	1.43	0.89	10.387	-22.898	-2.436	0	-5.585	-8.173	-2.588	0	-0.625	1.377		0.237	1.341	1	52	Te	32.3
23	V	5	-3	0	1.32	0.4	14.146	-36.944	11.611	1	-13.367	-8.173	5.194	1	1.3	1.32	1.32	0.18		1	23	V	82
47	Ag	1	1	1	1.44	1.13	4.065	-14.285	-11.049	0	-7.509	-8.173	-0.664	0	-0.055	1.4219		0.2819	1.13	1	47	Ag	19.9
41	Nb	4	-2	0	1.43	0.74	10.387	-19.462	-5.871	0	-12.584	-8.173	4.411	1	1.218	1.43	1.43	0.29		1	41	Nb	198.6
58	Ce_g	3	-1	0	1.82	1.18	5.293	-13.924	-11.409	0	-5.102	-8.173	-3.071	0	-0.742	1.7085		0.5685	1.663	1	58	Ce_g	142.5
SUCCESS RATE				45.45%						27.27%				36.36%						100.00%			
TOTAL 11																							

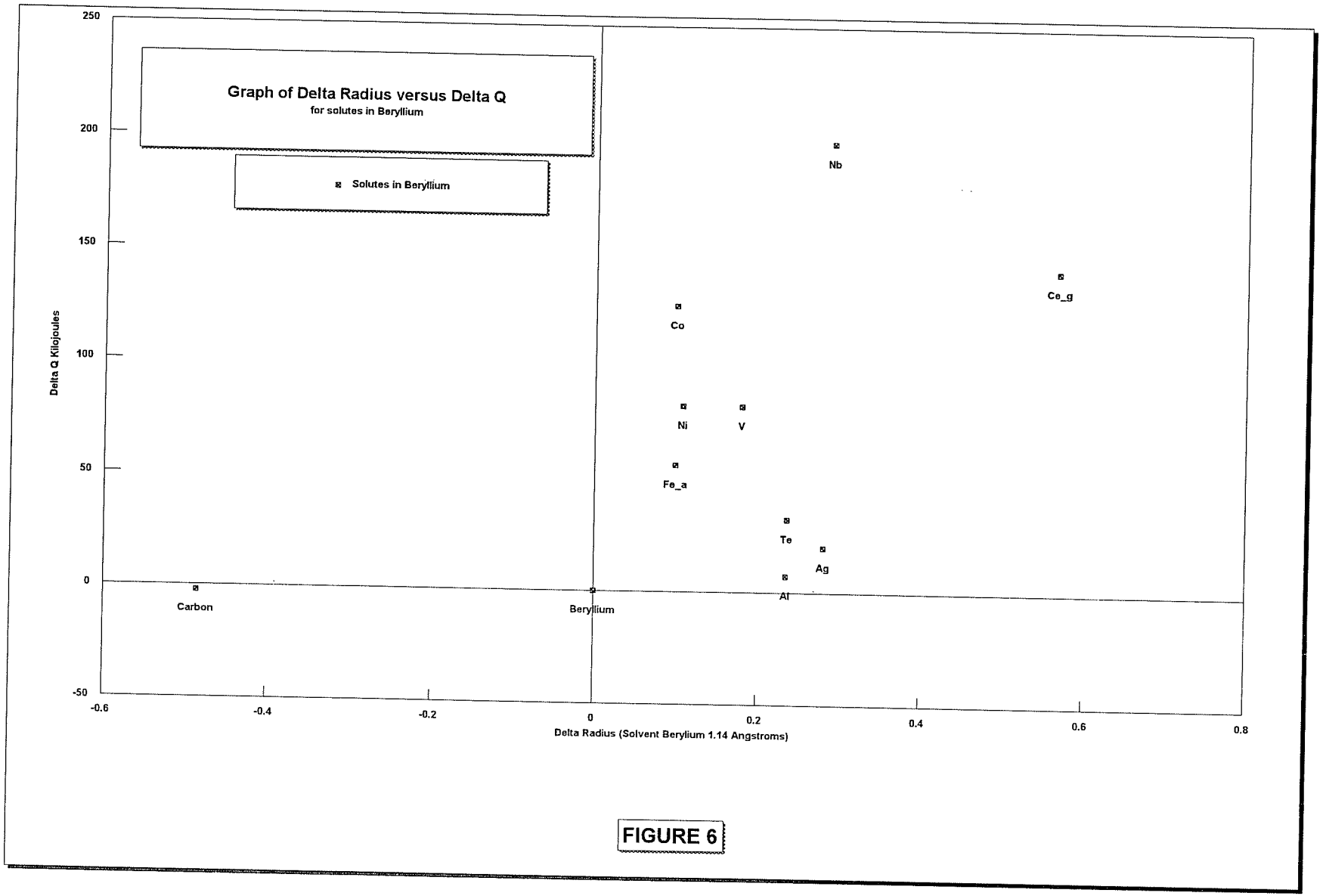
Graph of Delta Radius versus Delta Q
for solutes in Beryllium
Solutes in Beryllium
Delta Q Kilojoules
250
200
150
100
50
0
-50
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
Delta Radius (Solvent Beryllium 1.14 Angstroms)
Nb
Ce_g
Co
Ni
V
Fe_a
Te
Ag
Al
Carbon
Beryllium

FIGURE 6

COBALT solvent system

TABLE 26

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha										
27	Co	3			1.25	0.65	11.222	-26.1644	0.0000	1	-7.461	-7.461	0	0		1.25						
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference in Eo Values			Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
29	Cu	1	2	1	1.28	0.96	5.145	-16.028	-10.136	0	-7.453	-7.461	-0.008	0	-0.003	1.2793		-0.290	0.96	0	29	Cu	-12.6
28	Ni	2	1	1	1.25	0.78	8.564	-22.326	-3.839	0	-8.052	-7.461	0.591	1	0.085	1.25	1.25	0.000		0	28	Ni	-18.4
26	Fe_a	2	1	1	1.24	0.87	8.702	-22.592	-3.573	0	-8.087	-7.461	0.626	1	0.085	1.24	1.24	-0.010		0	26	Fe_a	-34.3
30	Zn	2	1	1	1.33	0.83	7.564	-21.556	-4.608	0	-8.948	-7.461	1.487	1	0.22	1.33	1.33	0.080		1	30	Zn	-20.9
78	Pt	2	1	1	1.38	0.52	7.026	-22.872	-3.293	0	-11.161	-7.461	3.7	1	0.557	1.38	1.38	0.130		1	78	Pt	-8.3
27	Co	3	0		1.25	0.65	11.222	-26.164	0.000	null	-7.461	-7.461	0	0	0	1.25		0.000	null	0	27	Co	0
6	Carbon	4	-1	0	0.77	0.2	35.825	-49.566	23.401	1	10.144	-7.461	-17.605	0	-2.027	0.658		-0.592	0.566	0	6	C	-138.3
25	Mn	4	-1	0	1.37	0.52	11.317	-17.957	-8.207	0	0.905	-7.461	-8.366	0	-2.08	1.1638		-0.086	1.007	0	25	Mn	-55.2
16	S	6	-3	0	1.06	0.34	24.771	-19.794	-6.370	0	21.492	-7.461	-28.953	0		0.34		-0.910	0.909	0	16	S	-61.5
SUCCESS RATE				33.33%						88.89%				55.56%						77.78%			
TOTAL 9																							

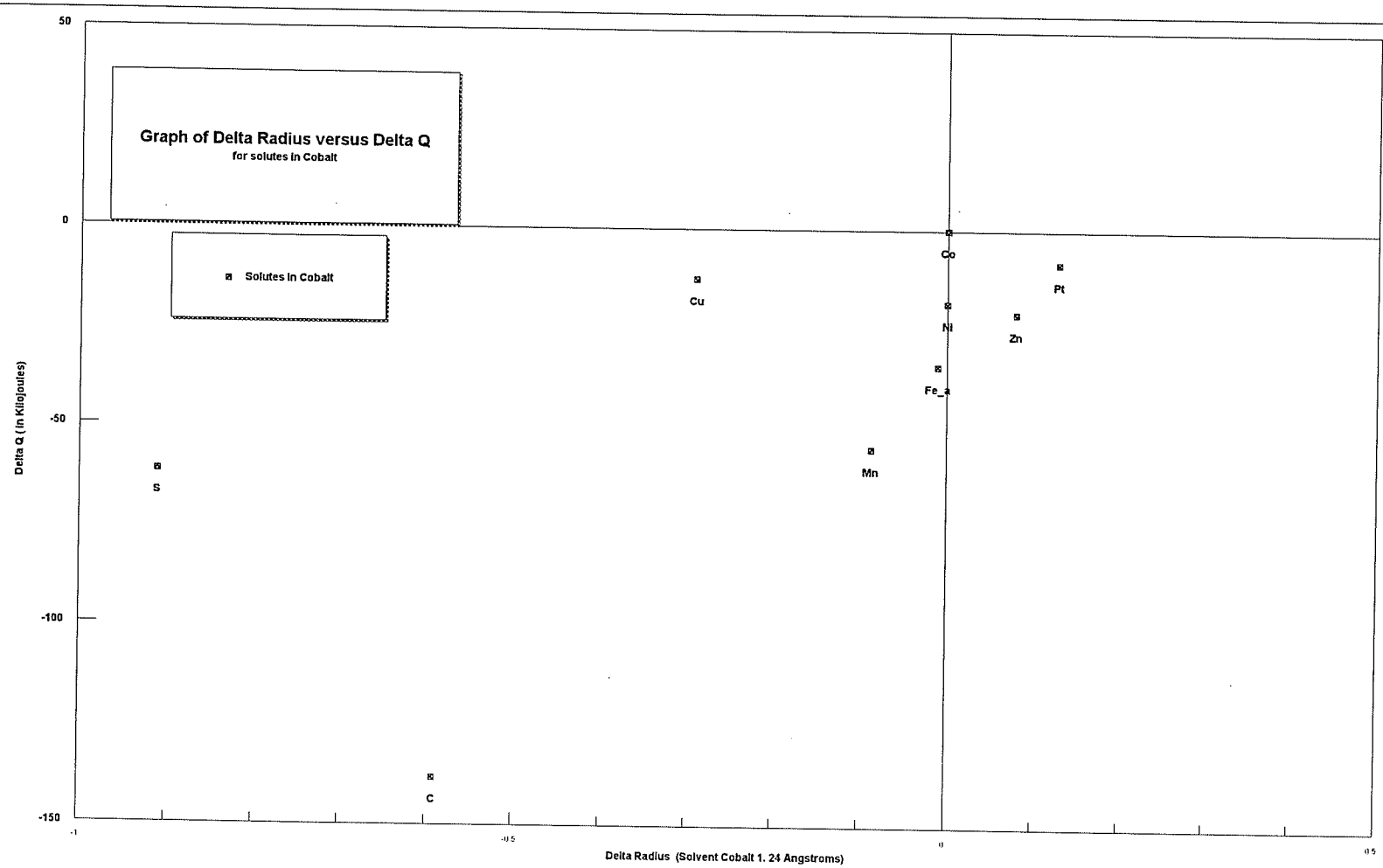
Graph of Delta Radius versus Delta Q
for solutes in Cobalt
Solutes in Cobalt
Delta Q (in Kilojoules)
50
0
-50
-100
-150
Co
Pt
Cu
Ni
Zn
Fe_a
Mn
S
C
-1
-0.5
0
0.5
Delta Radius (Solvent Cobalt 1. 24 Angstroms)

FIGURE 7

COPPER solvent system

TABLE 27

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha			0	1.28						
29	Cu	1			1.28	0.96	5.145	-16.0280	-0.0000	0	-7.453	-7.453										
SOLUTES										Le Clair U Model Predictions Difference in	Eo Values		Delta(U)	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
47	Ag	1	0		1.44	1.13	4.065	-14.2847	-1.7433	0	-7.509	-7.453	0.056	1	0.005	1.44	1.44	0.160		1	47	Ag	-16.3
79	Au	1	0		1.44	1.37	4.065	-16.6527	0.6247	1	-9.877	-7.453	2.424	1	0.222	1.44	1.44	0.160		1	79	Au	1.4
28	Ni	2	-1	0	1.25	0.78	8.564	-22.3256	6.2976	1	-8.052	-7.453	0.599	1	0.085	1.25	1.25	-0.030		0	28	Ni	88.3
26	Fe_a	2	-1	0	1.24	0.87	8.702	-22.5916	6.5636	1	-8.087	-7.453	0.634	1	0.092	1.24	1.24	-0.040		0	26	Fe_a	2.3
4	Beryllium	2	-1	0	1.14	0.54	10.296	-25.3333	9.3053	1	-8.173	-7.453	0.72	1	0.085	1.14	1.14	-0.140		0	4	Beryllium	-15.1
30	Zn	2	-1	0	1.33	0.83	7.564	-21.5560	5.5280	1	-8.948	-7.453	1.495	1	0.22	1.33	1.33	0.050		1	30	Zn	-22.1
82	Pb	2	-1	0	1.75	1.32	4.369	-16.9150	0.8870	1	-9.633	-7.453	2.18	1	0.4	1.75	1.75	0.470		1	82	Pb	-28.6
48	Cd	2	-1	0	1.5	1.03	5.947	-19.6575	3.6295	1	-9.746	-7.453	2.293	1	0.377	1.5	1.5	0.220		1	48	Cd	194
46	Pd	2	-1	0	1.37	0.5	7.129	-21.7074	5.6794	1	-9.825	-7.453	2.372	1	0.355	1.37	1.37	0.090		1	46	Pd	16.6
80	Hg	2	-1	0	1.5	1.12	5.947	-20.8905	4.8625	1	-10.979	-7.453	3.526	1	0.565	1.5	1.5	0.220		1	80	Hg	-26.8
78	Pt	2	-1	0	1.38	0.52	7.026	-22.8716	6.8436	1	-11.161	-7.453	3.708	1	0.557	1.38	1.38	0.100		1	78	Pt	22
24	Cr	3	-2	0	1.25	0.64	11.222	-21.0172	4.9892	1	-2.314	-7.453	-5.139	0	-0.945	1.1492		-0.138	1.142	0	24	Cr	-16
22	Ti_b	3	-2	0	1.47	0.69	8.114	-17.4321	1.4041	1	-3.908	-7.453	-3.545	0	-0.765	1.3769		0.063	1.343	1	22	Ti_b	-15
45	Rh	3	-2	0	1.34	0.68	9.765	-21.5496	5.5216	1	-5.274	-7.453	-2.179	0	-0.42	1.2958		-0.055	1.225	0	45	Rh	31.8
31	Ga	3	-2	0	1.35	0.62	9.621	-21.3413	5.3133	1	-5.306	-7.453	-2.147	0	-0.42	1.3055		-0.046	1.234	0	31	Ga	-18.3
33	As	3	-2	0	1.25	0.69	11.222	-24.2533	8.2253	1	-5.55	-7.453	-1.903	0	-0.345	1.2165		-0.138	1.142	0	33	As	-34.6
49	In	3	-2	0	1.57	0.92	7.113	-18.3887	2.3607	1	-6.533	-7.453	-0.92	0	-0.21	1.5448		0.155	1.435	1	49	In	-31
27	Co	3	-2	0	1.25	0.65	11.222	-26.1644	10.1364	1	-7.461	-7.453	0.008	1	0.008	1.25	1.25	-0.030		0	27	Co	101.8
51	Sb	3	-2	0	1.61	0.9	6.764	-18.7462	2.7182	1	-7.472	-7.453	0.019	1	0.008	1.61	1.61	0.330		1	51	Sb	-34
81	Tl	3	-2	0	1.71	1.06	5.996	-17.7036	1.6756	1	-7.709	-7.453	0.256	1	0.06	1.71	1.71	0.430		1	81	Tl	-29.7
25	Mn	4	-3	0	1.37	0.52	11.317	-17.9571	1.9292	1	0.905	-7.453	-8.358	0	-2.08	1.1638		-0.116	1.007	0	25	Mn	-6.7
44	Ru	4	-3	0	1.34	0.65	11.829	-20.0454	4.0174	1	-0.329	-7.453	-7.124	0	-1.72	1.1826		-0.097	1.149	0	44	Ru	46.5
14	Si	4	-3	0	1.17	0.39	15.516	-26.2355	10.2075	1	-0.374	-7.453	-7.079	0	-1.45	1.0586		-0.221	1.003	0	14	Si	-39.3
32	Ge	4	-3	0	1.22	0.44	14.271	-24.6584	8.6304	1	-0.873	-7.453	-6.58	0	-1.412	1.1074		-0.173	1.046	0	32	Ge	-24
77	Ir	4	-3	0	1.35	0.66	11.655	-25.4979	9.4699	1	-1.54	-7.453	-5.913	0	-1.427	1.2238		-0.056	1.157	0	77	Ir	65.4
74	W	4	-3	0	1.37	0.68	11.317	-22.8995	6.8715	1	-4.038	-7.453	-3.415	0	-0.827	1.3012		0.021	1.285	1	74	W	14.7
50	Sn	4	-3	0	1.58	0.74	8.508	-18.5078	2.4798	1	-4.327	-7.453	-3.126	0	-0.872	1.4959		0.216	1.482	1	50	Sn	-24
15	P	5	-4	0	1.09	0.35	20.745	-43.5539	27.5259	1	-8.977	-7.453	1.524	1	0.31	1.09	1.09	-0.190		0	15	P	-74.9
41	Nb	5	-4	0	1.43	0.74	12.053	-12.4532	-3.5748	0	-12.584	-7.453	5.131	1	1.465	1.43	1.43	0.150		1	41	Nb	40.5
29	Cu	1	0		1.28	0.96	5.145	-16.0280	null	0	-7.453	-7.453	0	0	1.28			0.000		0		CU	0
23	V	5	-4	0	1.32	0.4	14.146	-36.9440	20.9160	1	-13.367	-7.453	5.914	1	1.533	1.32	1.32	0.040		1	23	V	4
16	S	6	-5	0	1.06	0.34	24.771	-19.7943	3.7663	1	21.492	-7.453	-28.945	0		0.34		-0.940		0	16	S	-4.4
SUCCESS RATE				53.13%						18x				12x						15x			
TOTAL 32										43.75%				62.50%						53.13%			

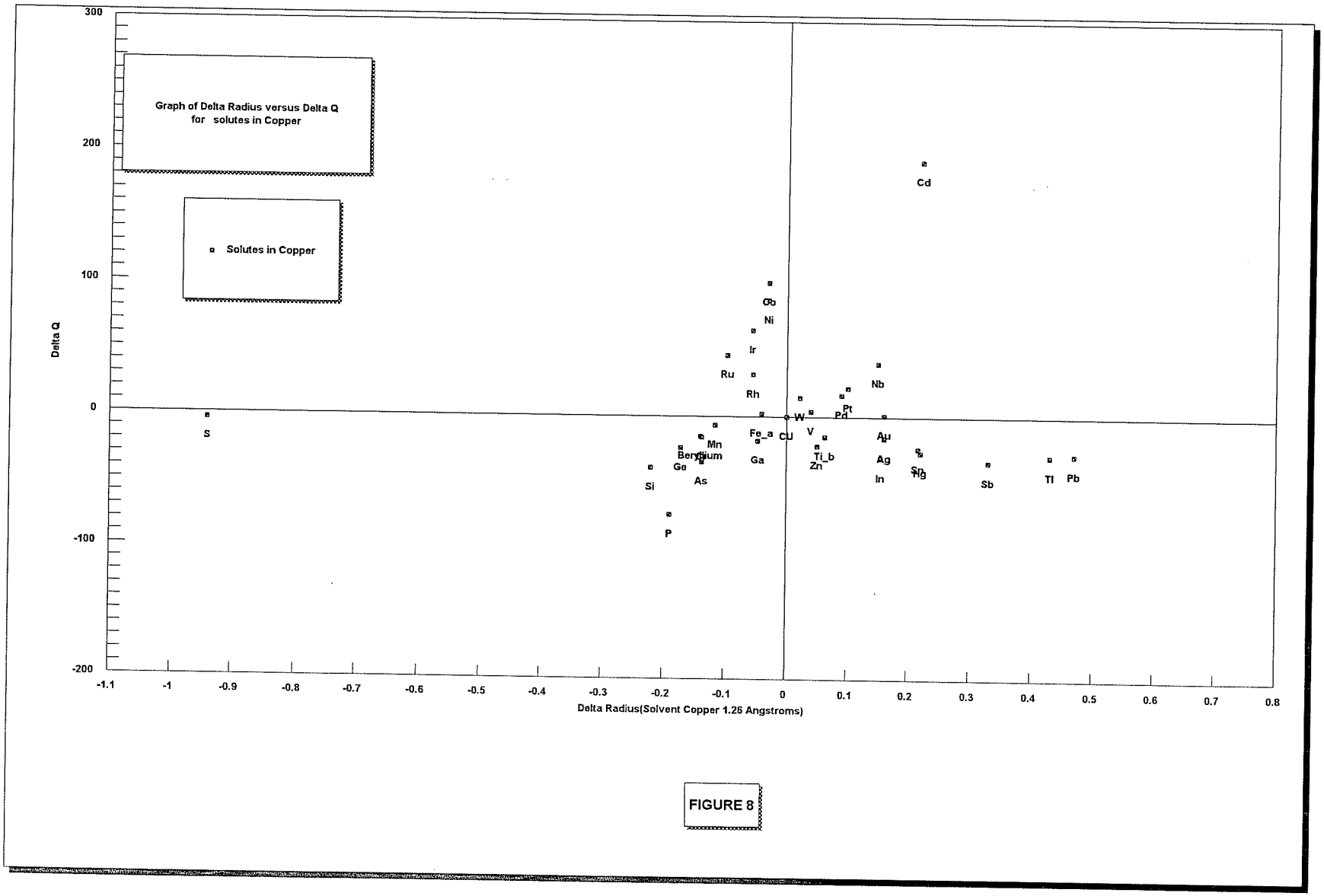
Graph of Delta Radius versus Delta Q
for solutes in Copper
Solutes in Copper
Delta Q
Delta Radius(Solvent Copper 1.26 Angstroms)
300
200
100
0
-100
-200
-1.1
-1
-0.9
-0.8
-0.7
-0.6
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
Cd
Ob
Ni
Ir
Ru
Rh
Nb
Pt
Pd
W
S
Mn
Fe_a
CU
V
Au
Ag
Sn
Ng
Ti_b
Zn
Ga
Ge
As
Si
In
Sb
Tl
Pb
P

FIGURE 8

GOLDsolvent system

TABLE 28

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha										
79	Au	1			1.44	1.37	4.065	-16.653	0.000		-9.877	-9.877			-0.003			1.4392				
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference in	Eo Values		Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions		Element	Experimental delta Q
13	Al	3	-2	0	1.43	0.57	8.574	-20.049	3.397	1	-5.758	-9.877	-4.119	0	-0.742	1.3424		-0.098	1.307	0	13	Al	-28.7
26	Fe_a	2	-1	0	1.24	0.87	8.702	-22.592	5.939	1	-8.087	-9.877	-1.79	0	-0.208	1.2102		-0.230	1.063	0	26	Fe_a	1.9
27	Co	3	-2	0	1.25	0.65	11.222	-26.164	9.512	1	-7.461	-9.877	-2.416	0	-0.382	1.2127		-0.227	1.142	0	27	Co	12.9
28	Ni	2	-1	0	1.25	0.78	8.564	-22.326	5.673	1	-8.052	-9.877	-1.825	0	-0.215	1.2188		-0.221	1.072	0	28	Ni	16.1
29	Cu	1	0		1.28	0.96	5.145	-16.028	-0.625	0	-7.453	-9.877	-2.424	0	-0.175	1.2264		-0.214	0.96	0	29	Cu	-2.1
30	Zn	2	-1	0	1.33	0.83	7.564	-21.556	4.903	1	-8.948	-9.877	-0.929	0	-0.118	1.3122		-0.128	1.140	0	30	Zn	-14.2
32	Ge	4	-3	0	1.22	0.44	14.271	-24.658	8.006	1	-0.873	-9.877	-9.004	0	-1.727	1.0759		-0.364	1.046	0	32	Ge	-27.8
46	Pd	2	-1	0	1.37	0.5	7.129	-21.707	5.055	1	-9.825	-9.877	-0.052	0	-0.005	1.3692		-0.071	1.174	0	46	Pd	22.8
47	Ag	1	0		1.44	1.13	4.065	-14.285	-2.368	0	-7.509	-9.877	-2.368	0	-0.175	1.3797		-0.060	1.13	0	47	Ag	-4
49	In	3	-2	0	1.57	0.92	7.113	-18.389	1.736	1	-6.533	-9.877	-3.344	0	-0.645	1.4877		0.048	1.435	0	49	In	-18.6
50	Sn	4	-3	0	1.58	0.74	8.508	-18.508	1.855	1	-4.327	-9.877	-5.55	0	-1.345	1.4424		0.002	1.354	0	50	Sn	-29
51	Sb	3	-2	0	1.61	0.9	6.764	-18.746	2.093	1	-7.472	-9.877	-2.405	0	-0.465	1.5508		0.111	1.471	1	51	Sb	-42.9
52	Te	4	-3	0	1.43	0.89	10.387	-22.898	6.245	1	-5.585	-9.877	-4.292	0	-0.947	1.3466		-0.093	1.341	0	52	Te	-31.2
78	Pt	2	-1	0	1.38	0.52	7.026	-22.872	6.219	1	-11.161	-9.877	1.284	1	0.167	1.38	1.38	-0.060		0	78	Pt	29.1
79	Au	1	0		1.44	1.37	4.065	-16.653	0.000	0	-9.877	-9.877	0	0	-0.003	1.4392		-0.001		0	79	Au	0
80	Hg	2	-1	0	1.5	1.12	5.947	-20.891	4.238	1	-10.979	-9.877	1.102	1	0.152	1.5	1.5	0.060		1	80	Hg	-15.8
SUCCES RATE				0.625						0.5				0.6875						0.5625			
TOTAL 16																							

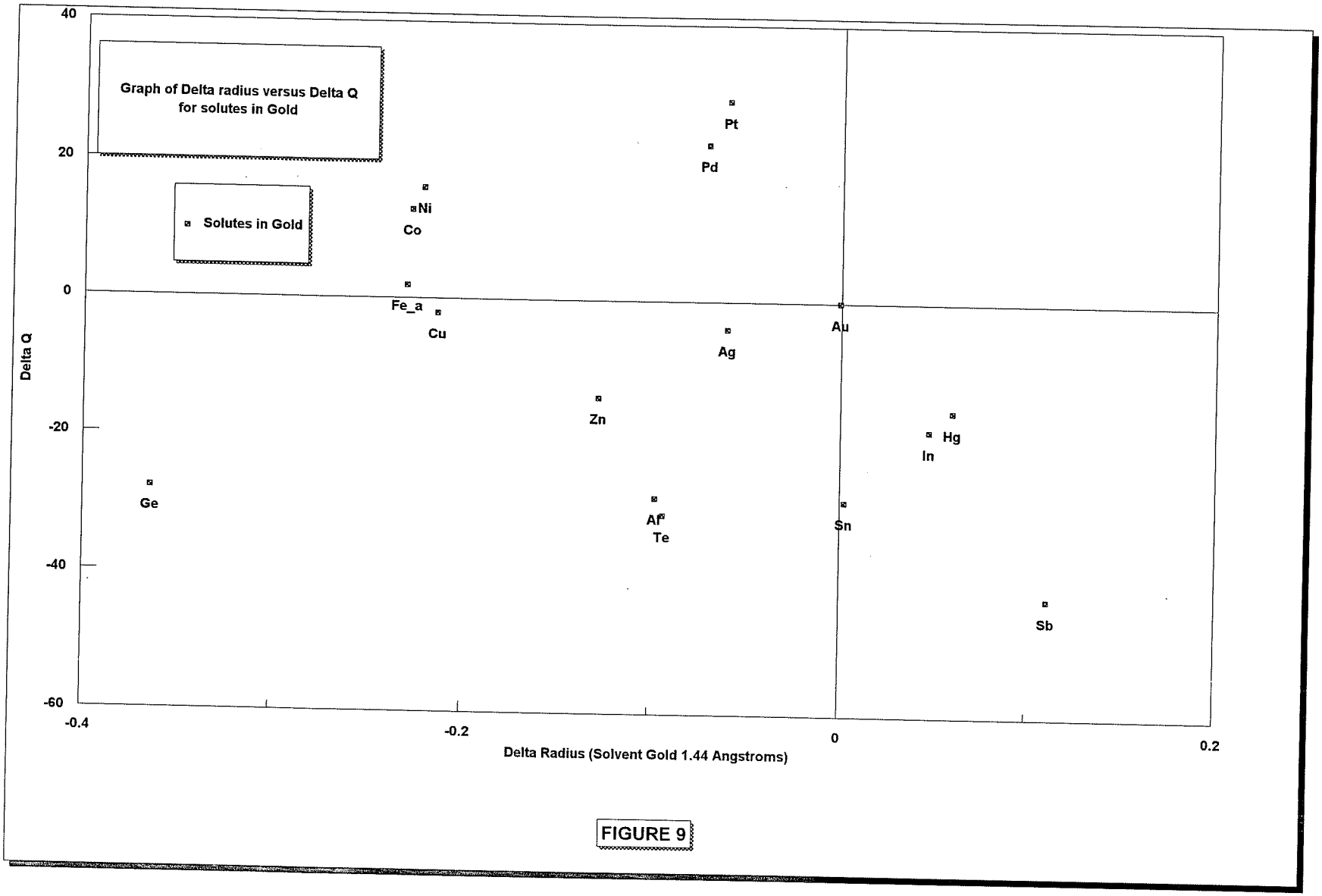
Graph of Delta radius versus Delta Q for solutes in Gold
Solutes in Gold
Delta Q
Delta Radius (Solvent Gold 1.44 Angstroms)
40
20
0
-20
-40
-60
-0.4
-0.2
0
0.2
Pt
Pd
Ni
Co
Fe_a
Cu
Au
Ag
Zn
Hg
In
Ge
Al
Te
Sn
Sb

FIGURE 9

TABLE 29

A_IRON solvent system

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha										
26	Fe_a	2			1.24	0.87	8.702	-22.592	0.000		-8.087	-8.087	0	0	0	1.24						
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference in Eo Values			Delta Emax	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions		Element	Experimental delta Q
4	Beryllium	2	0	0	1.14	0.54	10.296	-25.333	2.742	1	-8.173	-8.087	0.086	+	0.01	1.14	1.14	-0.100		0	4	Be	-22.6
13	Al	3	-1	0	1.43	0.57	8.574	-20.049	-2.542	0	-5.758	-8.087	-2.329	0	-0.465	1.3774	1.3	0.060	1.3	1	13	Al	-4.8
14	Si	4	-2	0	1.17	0.39	15.516	-26.236	3.644	1	-0.374	-8.087	-7.713	0	-1.532	1.0509	1.0509	-0.189	1	0	14	Si	-30.8
15	P	5	-3	0	1.09	0.35	20.745	-43.554	20.962	1	-8.977	-8.087	0.89	1	0.175	1.09	1.09	-0.150		0	15	P	-29.1
16	S	6	-4	0	1.06	0.34	24.771	-19.794	-2.797	0	21.492	-8.087	-29.579	0	N.S.	0.34	0.34	-0.900		0	16	S	-47.8
22	Ti_a	2	0		1.47	0.76	6.192	-46.826	24.234	1	-36.505	-8.087	28.418	1	N.S.	1.47	1.47	0.230		1	22	Ti_a	10.5
23	V	5	-3	0	1.32	0.4	14.146	-36.944	14.352	1	-13.367	-8.087	5.28	+	1.33	1.32	1.32	0.080		1	23	V	-11.3
24	Cr	3	-1	0	1.25	0.64	11.222	-21.017	-1.574	0	-2.314	-8.087	-5.773	0	-1.027	1.1388	0.97	-0.270	0.97	0	24	Cr	-11.8
25	Mn	4	-2	0	1.37	0.52	11.317	-17.957	-4.634	0	0.905	-8.087	-8.992	0	-2.162	1.1525	1.1525	-0.087	1.01	0	25	Mn	-26.1
26	Fe_a	2			1.24	0.87	8.702	-22.592	0.000	0	-8.087	-8.087	0	null				0				Fe_A	0
27	Co	3	-1	0	1.25	0.65	11.222	-26.164	3.573	1	-7.461	-8.087	-0.626	0	-0.105	1.2401	1.14	-0.100	1.14	0	27	Co	7.4
28	Ni	2	0		1.25	0.78	8.564	-22.326	-0.266	0	-8.052	-8.087	-0.035	0	-0.005	1.2493	1.07	-0.170	1.07	0	28	Ni	-8.4
29	Cu	1	1	1	1.28	0.96	5.145	-16.028	-6.564	0	-7.453	-8.087	-0.634	0	-0.048	1.2662	0.96	-0.280	0.96	0	29	Cu	-6.6
30	Zn	2	0		1.33	0.83	7.564	-21.556	-1.036	0	-8.948	-8.087	0.861	1	0.122	1.33	1.33	0.090		1	30	Zn	-19
33	As	3	-1	0	1.25	0.69	11.222	-24.253	1.662	1	-5.55	-8.087	-2.537	0	-0.442	1.2064	1.2064	-0.034	1.14	0	33	As	-27.6
41	Nb	5	-3	0	1.43	0.74	10.387	-19.462	-3.129	0	-12.584	-8.087	4.497	1	1.24	1.43	1.43	0.190		1	41	Nb	1.4
42	Mo	4	-2	0	1.36	0.68	11.484	-18.328	-4.264	0	0.813	-8.087	-8.9	0	-2.117	1.1503	0.99	-0.250	0.99	0	42	Mo	-26.4
46	Pd	2	0		1.37	0.5	7.129	-21.707	-0.884	0	-9.825	-8.087	1.738	1	0.25	1.37	1.37	0.130		1	46	Pd	30.3
47	Ag	1	1	1	1.44	1.13	4.065	-14.285	-8.307	0	-7.509	-8.087	-0.578	0	-0.048	1.4245	1.13	-0.110	1.13	0	47	Ag	-17.6
50	Sn	4	-2	0	1.58	0.74	8.508	-18.508	-4.084	0	-4.327	-8.087	-3.76	0	-1.015	1.4805	1.35	0.110	1.35	1	50	Sn	-28.4
51	Sb	3	-1	0	1.61	0.9	6.764	-18.746	-3.845	0	-7.472	-8.087	-0.615	0	-0.135	1.5936	1.47	0.230	1.47	1	51	Sb	8.8
72	Hf_b	4	-2	0	1.59	0.84	8.402	-19.365	-3.227	0	-5.361	-8.087	-2.726	0	-0.737	1.5196	1.49	0.250	1.49	1	72	Hf_b	39.4
74	W	4	-2	0	1.37	0.68	11.317	-22.899	0.308	1	-4.038	-8.087	-4.049	0	-0.947	1.2901	1.28	0.040	1.28	1	74	W	-4.4
78	Pt	2	0		1.38	0.52	7.026	-22.872	0.280	1	-11.161	-8.087	3.074	1	0.445	1.38	1.38	0.140		1	78	Pt	45.4
79	Au	1	1	1	1.44	1.37	4.065	-16.653	-5.939	0	-9.877	-8.087	1.79	1	0.155	1.44	1.44	0.200		1	79	Au	6.4
				R.V.M.						U Model				Mod L.C.						R.C.M.		
SUCCESS RATE				0.44						0.6				0.76						0.76		

Prediction positive Delta Q

0 negative Delta Q * or null in case of self-diffusion Empty cell no prediction possible

total 25

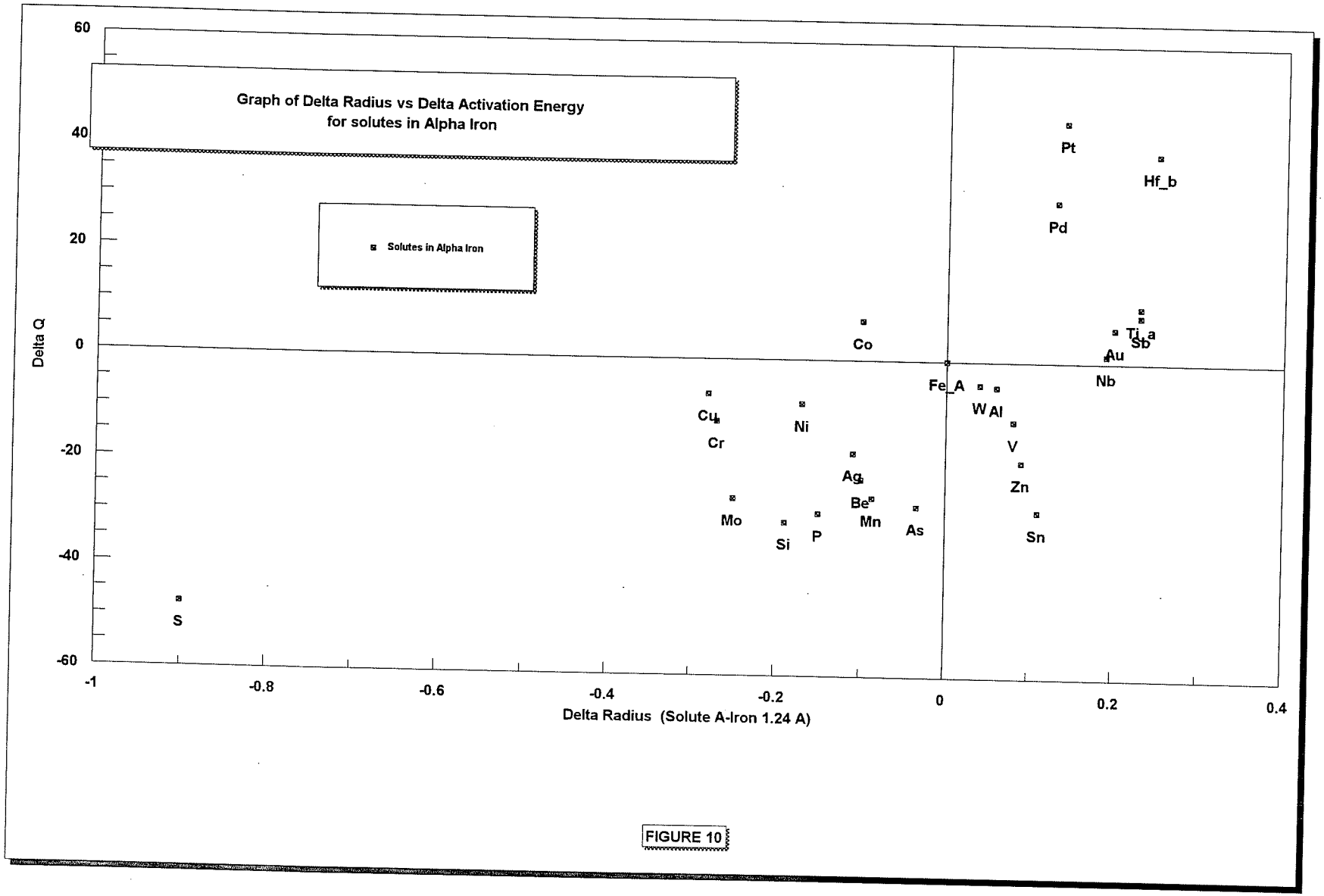
Graph of Delta Radius vs Delta Activation Energy
for solutes in Alpha Iron
Solutes in Alpha Iron
Delta Q
Delta Radius (Solute A-Iron 1.24 A)
60
40
20
0
-20
-40
-60
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
Pt
Hf_b
Pd
Co
Ti_a
Sb
Au
Nb
Fe_A
W
Al
V
Zn
Sn
Cu
Ni
Cr
Ag
Be
Mn
As
Mo
Si
P
S

FIGURE 10

G-IRON solvent system

TABLE 30

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha										
26	Fe_g	3			1.26	0.67	11.044	-21.473			-3.066	-3.066			0	1.26						
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference in Eo Values			Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
26	Fe_g	3			1.26	0.67	11.044	-21.473	0.000	null	-3.066	-3.066		null	0	1.26		0		0	26	Fe_g	0
29	Cu	1	2	1	1.28	0.96	5.145	-16.028	-5.445	0	-7.453	-3.066	4.387	1	0.59	1.28	1.28	0.02		1	29	Cu	-18.7
28	Ni	2	1	1	1.25	0.78	8.564	-22.326	0.852	1	-8.052	-3.066	4.986	1	0.97	1.25	1.25	-0.01		0	28	Ni	-18.3
4	Beryllium	2	1	1	1.14	0.54	13.381	-12.618	-8.856	0	-8.173	-3.066	5.107	1	0.865	1.14	1.14	-0.12		0	4	Be	-35.3
30	Zn	2	1	1	1.33	0.83	7.564	-21.556	0.083	1	-8.948	-3.066	5.882	1	1.232	1.33	1.33	0.07		1	30	Zn	-17.2
46	Pd	2	1	1	1.37	0.5	7.129	-21.707	0.234	1	-9.825	-3.066	6.759	1	1.465	1.37	1.37	0.11		1	46	Pd	-12.7
78	Pt	2	1	1	1.38	0.52	7.026	-22.872	1.398	1	-11.161	-3.066	8.095	1	1.75	1.38	1.38	0.12		1	78	Pt	-8.3
22	Ti_a	2	1	1	1.47	0.76	6.192	-46.826	25.352	1	-36.505	-3.066	33.439	1			1.47			nan	22	Ti_a	-30.2
24	Cr	3	0		1.25	0.64	11.222	-21.017	-0.456	0	-2.314	-3.066	-0.752	0	-0.18	1.2329		-0.0271	1.142	0	24	Cr	-27.4
33	As	3	0		1.25	0.69	11.222	-24.253	2.780	1	-5.55	-3.066	2.484	1	0.6	1.25	1.25	-0.01		0	33	As	-46.3
27	Co	3	0		1.25	0.65	11.222	-26.164	4.691	1	-7.461	-3.066	4.395	1	1.05	1.25	1.25	-0.01		0	27	Co	-7.3
25	Mn	4	-1	0	1.37	0.52	11.317	-17.957	-3.516	0	0.905	-3.066	-3.971	0	-1.33	1.2523		-0.0077	1.174	0	25	Mn	-27.3
42	Mo	4	-1	0	1.36	0.68	11.484	-18.328	-3.145	0	0.813	-3.066	-3.879	0	-1.285	1.2477		-0.0123	1.276	0	42	Mo	-51.5
74	W	4	-1	0	1.37	0.68	11.317	-22.899	1.426	1	-4.038	-3.066	0.972	1	0.32	1.37	1.37	0.11		1	74	W	-19.3
50	Sn	4	-1	0	1.58	0.74	8.508	-18.508	-2.965	0	-4.327	-3.066	1.261	1	0.508	1.58	1.58	0.32		1	50	Sn	-100.3
72	Hf_b	4	-1	0	1.59	0.84	8.402	-19.365	-2.109	0	-5.361	-3.066	2.295	1	0.92	1.59	1.59	0.33		1	72	Hf_b	115.7
15	P	5	-2	0	1.09	0.35	20.745	-43.554	22.081	1	-8.977	-3.066	5.911	1	1.443	1.09	1.09	-0.17		0	15	P	-18.3
41	Nb	5	-2	0	1.43	0.74	12.053	-32.673	11.200	1	-12.584	-3.066	9.518	1	3.52	1.43	1.43	0.17		1	41	Nb	-5.3
23	V	5	-2	0	1.32	0.4	14.146	-36.944	15.471	1	-13.367	-3.066	10.301	1	3.363	1.32	1.32	0.06		1	23	V	-27.3
16	S	6	-3	0	1.06	0.34	24.771	-19.794	-1.679	0	21.492	-3.066	-24.558	0						0	16	S	-54.9
SUCCESS RATE				40.00%						35.00%				30.00%						55.00%			
TOTAL 20																				0.55			

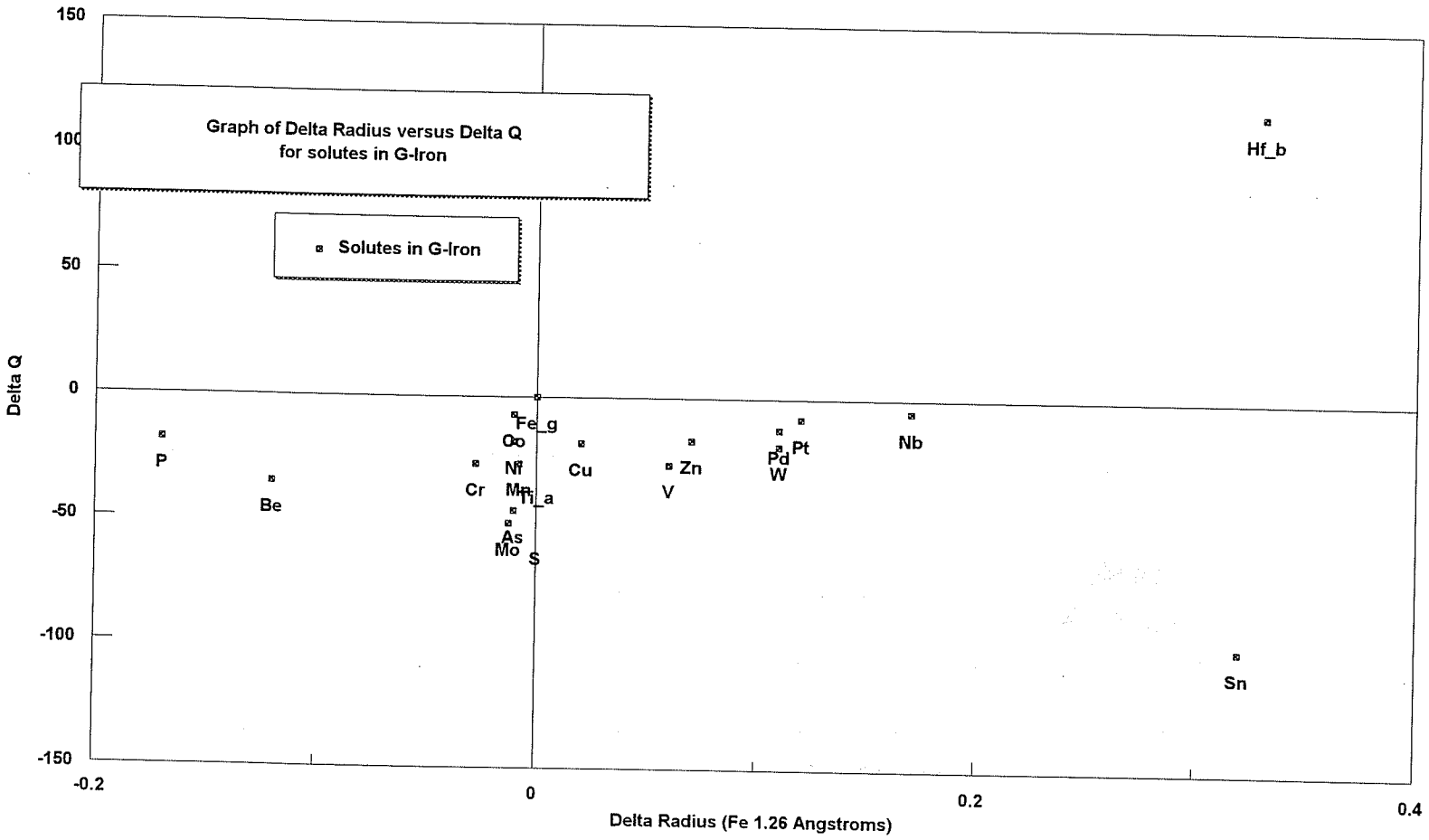
Graph of Delta Radius versus Delta Q
for solutes in G-Iron
Solutes in G-Iron
Delta Q
Delta Radius (Fe 1.26 Angstroms)
150
100
50
0
-50
-100
-150
-0.2
0
0.2
0.4
Hf_b
Sn
Nb
Pt
Pd
W
Zn
V
Cu
Fe_g
Co
Ni
Cr
Mn
Ti_a
As
Mo
S
P
Be

FIGURE 11

LEAD solvent system

TABLE 31

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha											
82	Pb	2			1.75	1.32	4.369	-16.915	0.000	1	-9.633	-9.633	0	0	0.002	1.7504							
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference In Eo Values			Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
11	Na	1	1	1	1.86	0.98	2.437	-8.498	-8.417	0	-4.437	-9.633	-5.196	0	-0.453	1.6269		-0.123	0.98	0	11	Na	9.5
29	Cu	1	1	1	1.28	0.96	5.145	-16.028	-0.887	0	-7.453	-9.633	-2.18	0	-0.16	1.2313		-0.519	0.96	0	29	Cu	-75.4
47	Ag	1	1	1	1.44	1.13	4.065	-14.285	-2.630	0	-7.509	-9.633	-2.124	0	-0.168	1.3825		-0.620	1.130	0	47	Ag	-48.2
79	Au	1	1	1	1.44	1.37	4.065	-16.653	-0.262	0	-9.877	-9.633	0.244	1	0.02	1.44	1.44	-0.310		0	79	Au	-69.9
28	Ni	2	0		1.25	0.78	8.564	-22.326	5.411	1	-8.052	-9.633	-1.581	0	-0.193	1.2222		-0.678	1.072	0	28	Ni	-63.6
30	Zn	2	0		1.33	0.83	7.564	-21.556	4.641	1	-8.948	-9.633	-0.685	0	-0.088	1.3168		-0.610	1.140	0	30	Zn	-61.2
82	Pb	2	0		1.75	1.32	4.369	-16.915	0.000	1	-9.633	-9.633	0	0	0.002	1.7504		0.000		null	82	Pb	0
48	Cd	2	0		1.5	1.03	5.947	-19.658	2.743	1	-9.746	-9.633	0.113	1	0.017	1.5	1.5	-0.250		0	48	Cd	-16.2
46	Pd	2	0		1.37	0.5	7.129	-21.707	4.792	1	-9.825	-9.633	0.192	1	0.025	1.37	1.37	-0.380		0	46	Pd	-73.6
80	Hg	2	0		1.5	1.12	5.947	-20.891	3.976	1	-10.979	-9.633	1.346	1	0.182	1.5	1.5	-0.250		0	80	Hg	-14
78	Pt	2	0		1.38	0.52	7.026	-22.872	5.957	1	-11.161	-9.633	1.528	1	0.197	1.38	1.38	-0.370		0	78	Pt	-66.7
49	In	3	-1	0	1.57	0.92	7.113	-18.389	1.474	1	-6.533	-9.633	-3.1	0	-0.607	1.493		-0.315	1.435	0	49	In	3.2
27	Co	3	-1	0	1.25	0.65	11.222	-26.164	9.249	1	-7.461	-9.633	-2.172	0	-0.352	1.2157		-0.608	1.142	0	27	Co	-62.6
51	Sb	3	-1	0	1.61	0.9	6.764	-18.746	1.831	1	-7.472	-9.633	-2.161	0	-0.435	1.5549		-0.279	1.471	0	51	Sb	-16.1
81	Tl	3	-1	0	1.71	1.06	5.996	-17.704	0.789	1	-7.709	-9.633	-1.924	0	-0.397	1.6568		-0.187	1.563	0	81	Tl	-7.1
50	Sn	4	-2	0	1.58	0.74	8.508	-18.508	1.593	1	-4.327	-9.633	-5.306	0	-1.3	1.4478		-0.396	1.354	0	50	Sn	-9.6

16

SUCCESS RATE 37.50% 25.00% 56.25% 87.50%

Total 16

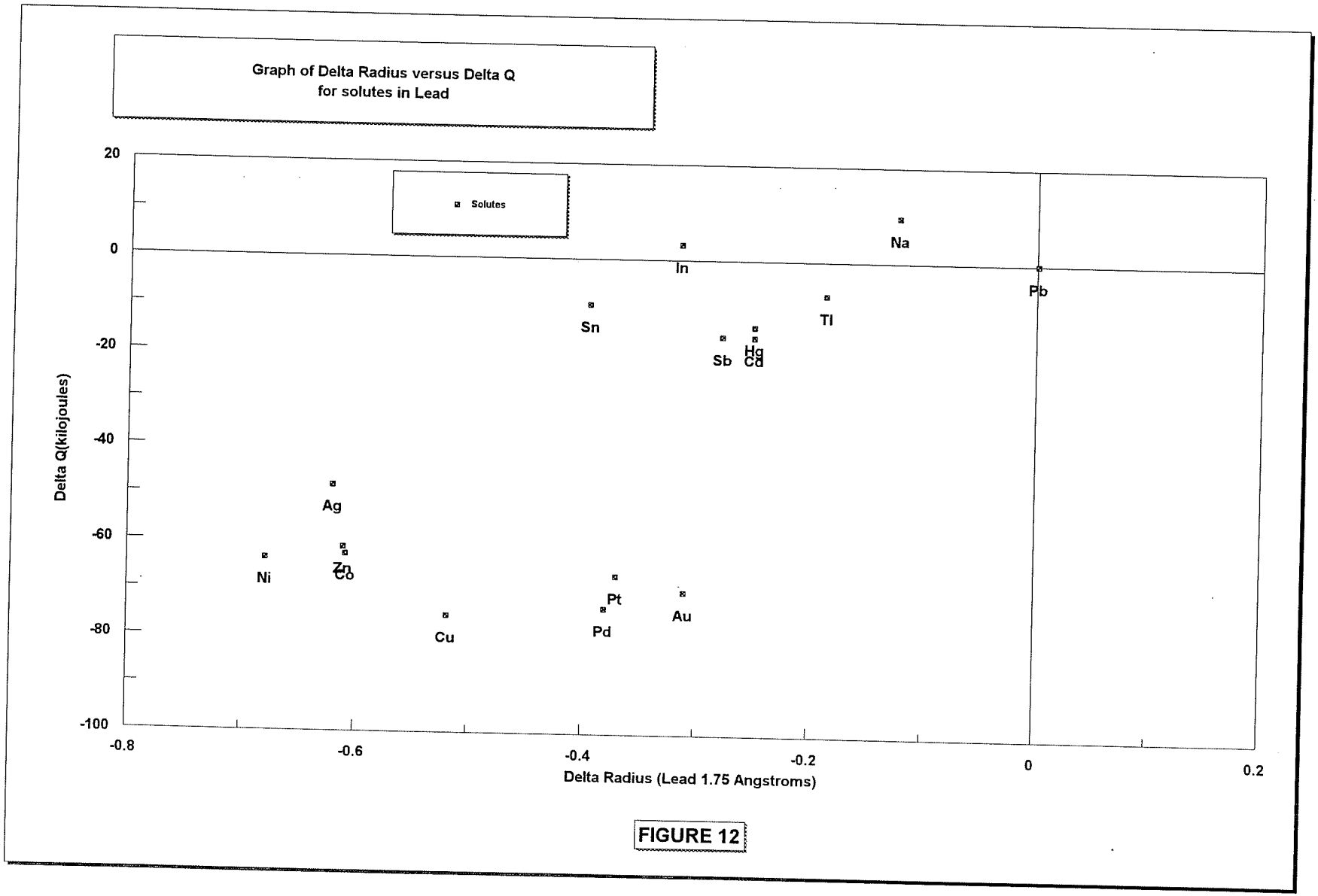
Graph of Delta Radius versus Delta Q
for solutes in Lead
Solutes
20
0
-20
-40
-60
-80
-100
Delta Q(kilojoules)
-0.8
-0.6
-0.4
-0.2
0
0.2
Delta Radius (Lead 1.75 Angstroms)
Na
In
Pb
Sn
Tl
Sb
Hg
Cd
Ag
Ni
Zn
Co
Pt
Au
Cu
Pd

FIGURE 12

LITHIUM solvent system

TABLE 32

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha				1.52						
3	Lithium	1			1.52	0.78	3.648	-10.436	0.000		-4.355	-4.355										
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference in	Eo Values		Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
3	Lithium	1	0		1.52	0.78	3.648	-10.436	0.000	1	-4.355	-4.355	0	0	0.005	1.52		0		0	3	Lithium	0
11	Na	1	0		1.86	0.98	2.437	-8.498	-1.938	0	-4.437	-4.355	0.082	1	0.02	1.86	1.86	0.34		1	11	Na	-1
29	Cu	1	0		1.28	0.96	5.145	-16.028	5.592	1	-7.453	-4.355	3.098	1	0.357	1.28	1.28	-0.24		0	29	Cu	-11.93
47	Ag	1	0		1.44	1.13	4.065	-14.285	3.848	1	-7.509	-4.355	3.154	1	0.41	1.44	1.44	-0.08		0	47	Ag	-0.08
79	Au	1	0		1.44	1.37	4.065	-16.653	6.216	1	-9.877	-4.355	5.522	1	0.702	1.44	1.44	-0.08		0	79	Au	-7.79
30	Zn	2	-1	0	1.33	0.83	7.564	-21.556	11.120	1	-8.948	-4.355	4.593	1	0.857	1.33	1.33	-0.19		0	30	Zn	0.54
48	Cd	2	-1	0	1.5	1.03	5.947	-19.658	9.221	1	-9.746	-4.355	5.391	1	1.142	1.5	1.5	-0.02		0	48	Cd	9
80	Hg	2	-1	0	1.5	1.12	5.947	-20.891	10.454	1	-10.979	-4.355	6.624	1	1.397	1.5	1.5	-0.02		0	80	Hg	5.57
31	Ga	3	-2	0	1.35	0.62	9.621	-21.341	10.905	1	-5.306	-4.355	0.951	1	0.233	1.35	1.35	-0.17		0	31	Ga	0.25
49	In	3	-2	0	1.57	0.92	7.113	-18.389	7.952	1	-6.533	-4.355	2.178	1	0.645	1.57	1.57	0.05		1	49	In	12.64
51	Sb	3	-2	0	1.61	0.9	6.764	-18.746	8.310	1	-7.472	-4.355	3.117	1	0.938	1.61	1.61	0.09		1	51	Sb	120
50	Sn	4	-3	0	1.58	0.74	8.508	-18.508	8.071	1	-4.327	-4.355	-0.028	0	-0.01	1.5791		-0.038	1.482	1	50	Sn	12.52
SUCCESS RATE				0.00%						66.67%				58.33%						58.33%			
TOTAL 12																							

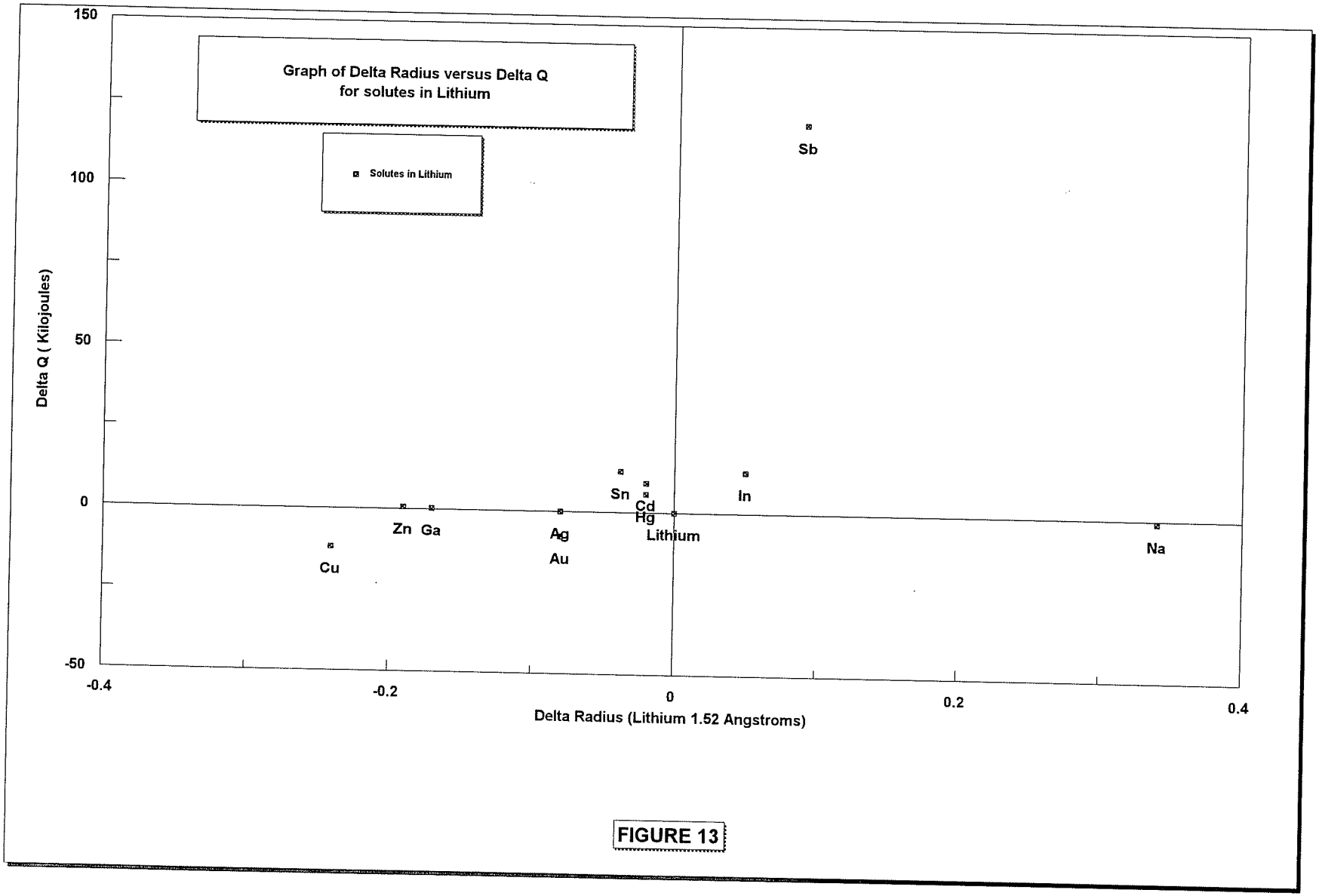
Graph of Delta Radius versus Delta Q
for solutes in Lithium
Solutes in Lithium
Delta Q (Kilojoules)
150
100
50
0
-50
-0.4
-0.2
0
0.2
0.4
Delta Radius (Lithium 1.52 Angstroms)
Sb
Sn
Cd
Hg
In
Zn
Ga
Ag
Au
Lithium
Cu
Na

FIGURE 13

MAGNESIUM solvent system

TABLE 33

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha										
12	Mg	2			1.6	0.78	5.227	-17.740	-0.000	0	-9.028	-9.028	0	0	0.002	1.6004						
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference In	Eo Values		Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
47	Ag	1	1	1	1.44	1.13	4.065	-14.285	-3.455	0	-7.509	-9.028	-1.519	0	-0.123	1.3987		-0.47	1.130	0	47	Ag	14.3 , -0.8
28	Ni	2	0		1.25	0.78	8.564	-22.326	4.586	1	-8.052	-9.028	-0.976	0	-0.118	1.2333		-0.52845	1.072	0	28	Ni	-38
26	Fe_a	2	0		1.24	0.87	8.702	-22.592	4.852	1	-8.087	-9.028	-0.941	0	-0.118	1.2234		-0.53702	1.063	0	26	Fe_a	-45.1
30	Zn	2	0		1.33	0.83	7.564	-21.556	3.816	1	-8.948	-9.028	-0.08	0	-0.005	1.3292		-0.45987	1.140	0	30	Zn	-14.2
12	Mg	2	0		1.6	0.78	5.227	-17.740	-0.000	null	-9.028	-9.028	0	null	0.002	1.6	1.6	0		null	12	Mg	0
48	Cd	2	0		1.5	1.03	5.947	-19.658	1.918	1	-9.746	-9.028	0.718	1	0.107	1.5	1.5	-0.1		0	48	Cd	-1.2 , 6.8
49	In	3	-1	0	1.57	0.92	7.113	-18.389	0.649	1	-6.533	-9.028	-2.495	0	-0.51	1.5063		-0.16528	1.435	0	49	In	8.5
51	Sb	3	-1	0	1.61	0.9	6.764	-18.746	1.007	1	-7.472	-9.028	-1.556	0	-0.322	1.5698		-0.12872	1.471	0	51	Sb	3.4
6	Carbon	4	-2	0	0.77	0.2	35.825	-49.566	31.826	1	10.144	-9.028	-19.172	0	-2.125	0.6507		-1.03415	0.566	0	6	C	-81.6
50	Sn	4	-2	0	1.58	0.74	8.508	-18.508	0.768	1	-4.327	-9.028	-4.701	0	-1.195	1.4602		-0.24555	1.354	0	50	Sn	16
SUCCESS RATE				0.2						0.6				0.7						0.7			
TOTAL 10																							

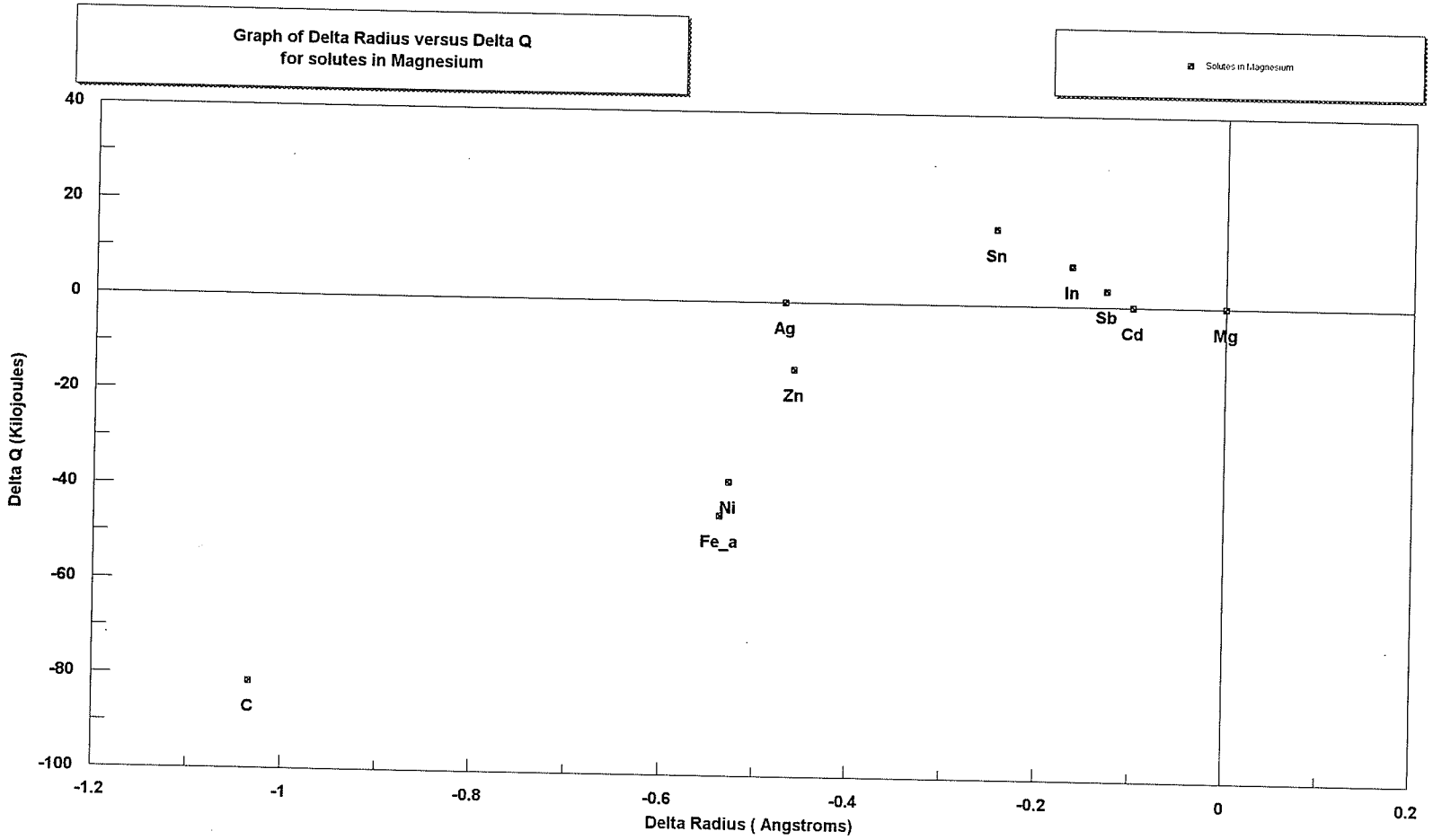
Graph of Delta Radius versus Delta Q
for solutes in Magnesium
Solutes in Magnesium
Delta Q (Kilojoules)
40
20
0
-20
-40
-60
-80
-100
-1.2
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
Delta Radius (Angstroms)
Sn
In
Sb
Cd
Mg
Ag
Zn
Ni
Fe_a
C

FIGURE 14

MOLYBDENUM solvent system

TABLE 34

SELF Q = 405 from CAHOON and SHERBY

		val			at rad	Ion rad	Ef	Eo	U		Emax	Alpha												
42	Mo	4			1.36	0.68	11.484	-18.328	0.000	1	0.813	0.813	0	0	0.005	1.3603								
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference in Eo Values			Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q	
3	Lithium	1	3	1	1.52	0.78	3.648	-10.436	-7.891	0	-4.355	0.813	5.168	1	N.S.	1.52	1.52	0.16		1	3	Li	64.9	
24	Cr	3	1	1	1.25	0.64	11.222	-21.017	2.689	1	-2.314	0.813	3.127	1	1.088	1.25	1.25	-0.11		0	24	Cr	-63.2	-179.6
26	Fe_g	3	1	1	1.26	0.67	11.044	-21.473	3.145	1	-3.066	0.813	3.879	1	1.358	1.26	1.26	-0.1		0	26	Fe_g	-59.5	-113.9
39	Y	3	1	1	1.81	1.06	5.352	-15.684	-2.644	0	-6.764	0.813	7.577	1	N.S.	1.81	1.81	0.45		1	39	Y	-190.9	
27	Co	3	1	1	1.25	0.65	11.222	-26.164	7.837	1	-7.461	0.813	8.274	1	2.738	1.25	1.25	-0.11		0	27	Co	-81.2	41
6	Carbon	4	0		0.77	0.2	35.825	-49.566	31.238	1	10.144	0.813	-9.331	0	-1.375	0.7012		-0.6999	0.660	0	6	Carbon	-284.8	-266.7
42	Mo	4	0		1.36	0.68	11.484	-18.328	0.000	null	0.813	0.813	0	null	0.005	1.3603		null		0	42	Mo	0	
74	W	4	0		1.37	0.68	11.317	-22.899	4.572	1	-4.038	0.813	4.851	1	2.188	1.37	1.37	0.01		1	74	W	54.8	163.7
15	P	5	-1	0	1.09	0.35	20.745	-43.554	25.226	1	-8.977	0.813	9.79	1	2.875	1.09	1.09	-0.27		0	15	P	-68.7	-81.2
41	Nb	4	0	0	1.43	0.74	10.387	-19.462	1.134	1	-12.584	0.813	13.397	1	N.S.		1.43	0.07		1	41	Nb	46.9	163.7
23	V	5	-1	0	1.32	0.4	14.146	-36.944	18.616	1	-13.367	0.813	14.18	1	N.S.		1.32	-0.04		0	23	V	67.4	
73	Ta	5	-1	0	1.47	0.68	11.406	-41.159	22.831	1	-22.148	0.813	22.961	1	N.S.		1.47	0.11		0	73	Ta	67.4	-58.2
16	S	6	-2	0	1.06	0.34	24.771	-19.794	1.467	1	21.492	0.813	-20.679	0	N.S.			-1.02	0.34	0	16	S	-108.4	17.2
SUCCESS RATE				30.77%						53.85%				69.23%	9					84.62%	11			
TOTAL 13														% correct	13					% correct	13			

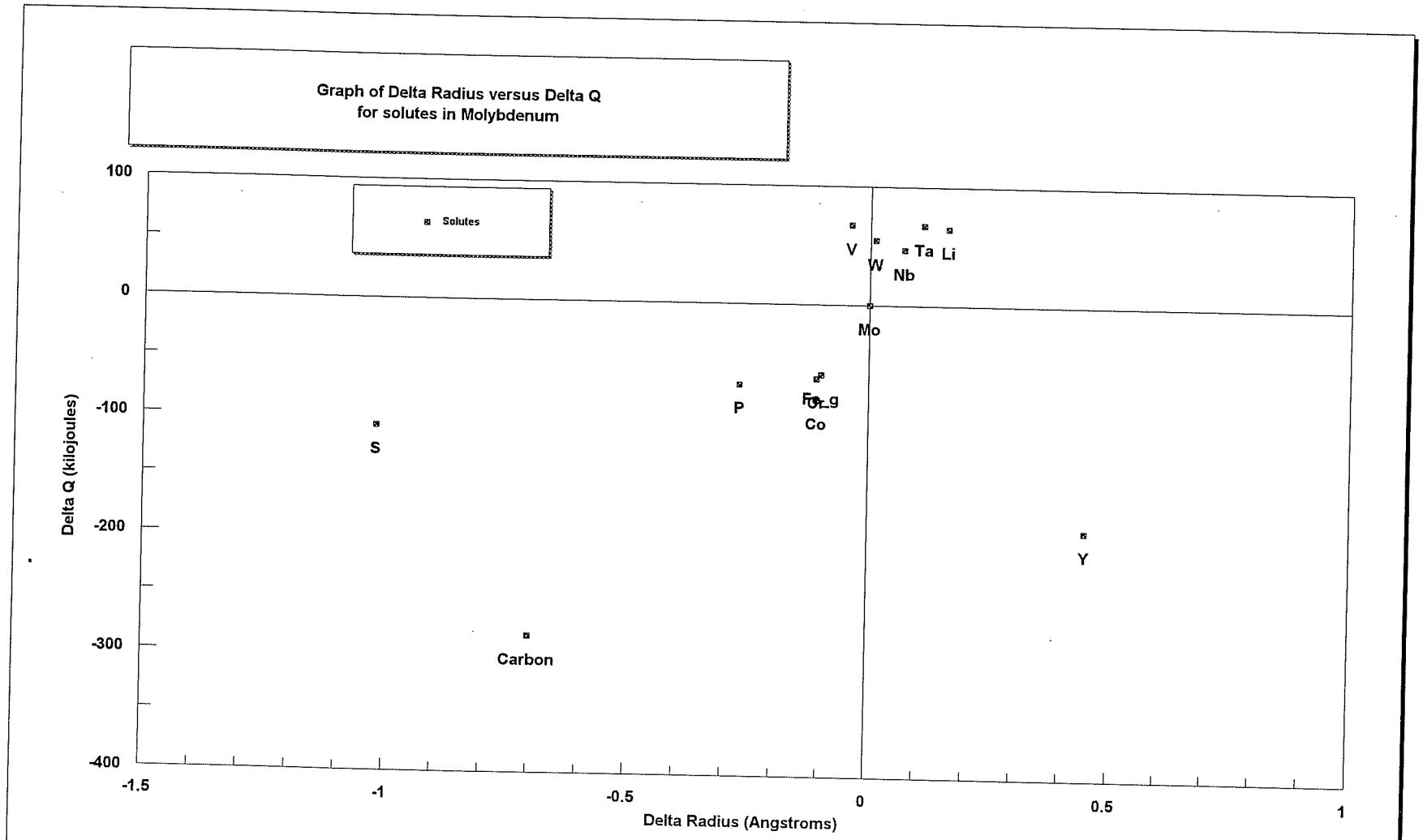
Graph of Delta Radius versus Delta Q
for solutes in Molybdenum
Solutes
100
0
-100
-200
-300
-400
Delta Q (kilojoules)
-1.5
-1
-0.5
0
0.5
1
Delta Radius (Angstroms)
V
W
Ta
Li
Nb
Mo
P
Fe
Cr
Co
S
Y
Carbon

FIGURE 15

NICKEL solvent system

TABLE 35

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha			0	1.25							
28	Ni	2			1.25	0.78	8.564	-22.326	-0.000	0	-8.052	-8.052											
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference_in	Eo Values		Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
29	Cu	1	1	1	1.28	0.96	5.145	-16.028	-5.298	0	-7.453	-8.052	-0.599	0	-0.048	1.2662		-0.27	0.98	0	29	Cu	-20
47	Ag	1	1	1	1.44	1.13	4.065	-14.285	-8.041	0	-7.509	-8.052	-0.543	0	-0.048	1.4245		-0.12	1.13	0	47	Ag	4.4
79	Au	1	1	1	1.44	1.37	8.429	-2.747	-19.578	0	-9.877	-8.052	1.825	1	0.162	1.44	1.44	0.19		1	79	Au	-4.9
28	Ni	2	0		1.25	0.78	8.564	-22.326	-0.000	null	-8.052	-8.052	0	null	-0.005	1.2493		0	1.250	null	28	Ni	0
26	Fe_a	2	0		1.24	0.87	8.702	-22.592	0.266	1	-8.087	-8.052	0.035	1	0.01	1.24	1.24	-0.01		0	26	Fe_a	-5.6
4	Beryllium	2	0		1.14	0.54	10.296	-25.333	3.008	1	-8.173	-8.052	0.121	1	0.017	1.14	1.14	-0.11		0	4	Be	-82
78	Pt	2	0		1.38	0.52	7.026	-22.872	0.546	1	-11.161	-8.052	3.109	1	0.445	1.38	1.38	0.13		1	78	Pt	11.8
24	Cr	3	-1	0	1.25	0.64	11.222	-21.017	-1.308	0	-2.314	-8.052	-5.738	0	-1.02	1.1397		-0.2708	0.979	0	24	Cr	-2.4
26	Fe_g	3	-1	0	1.26	0.67	11.044	-21.473	-0.852	0	-3.066	-8.052	-4.986	0	-0.892	1.1649		-0.0986	1.151	0	26	Fe_g	-22.1
58	Ce_g	3	-1	0	1.82	1.18	5.293	-13.924	-8.401	0	-5.102	-8.052	-2.95	0	-0.727	1.711		0.41318	1.663	1	58	Ce_g	-20.4
60	Nd	3	-1	0	1.82	1.15	5.293	-14.088	-8.237	0	-5.266	-8.052	-2.786	0	-0.682	1.7185		0.41318	1.663	1	60	Nd	-24.5
33	As	3	-1	0	1.25	0.69	11.222	-24.253	1.928	1	-5.55	-8.052	-2.502	0	-0.442	1.2064		-0.1077	1.142	0	33	As	-23.2
13	Al	3	-1	0	1.43	0.57	8.574	-20.049	-2.276	0	-5.758	-8.052	-2.294	0	-0.465	1.3774		0.05679	1.307	1	13	Al	-15
27	Co	3	-1	0	1.25	0.65	11.222	-26.164	3.839	1	-7.461	-8.052	-0.591	0	-0.105	1.2401		-0.1077	1.142	0	27	Co	-5.4
51	Sb	3	-1	0	1.61	0.9	6.764	-18.746	-3.579	0	-7.472	-8.052	-0.58	0	-0.127	1.5945		0.22128	1.471	1	51	Sb	-11
6	Carbon	4	-2	0	0.77	0.2	35.825	-49.566	27.240	1	10.144	-8.052	-18.196	0	-2.065	0.6552		-0.6842	0.566	0	6	C	-137.7
32	Ge	4	-2	0	1.22	0.44	14.271	-24.658	2.333	1	-0.873	-8.052	-7.179	0	-1.495	1.0995		-0.2042	1.046	0	32	Ge	-11
74	W	4	-2	0	1.37	0.68	11.317	-22.899	0.574	1	-4.038	-8.052	-4.014	0	-0.947	1.2901		0.03516	1.285	1	74	W	24.4
50	Sn	4	-2	0	1.58	0.74	8.508	-18.508	-3.818	0	-4.327	-8.052	-3.725	0	-1	1.4821		0.23215	1.482	1	50	Sn	-7.8
72	Hf_b	4	-2	0	1.59	0.84	8.402	-19.365	-2.961	0	-5.361	-8.052	-2.691	0	-0.722	1.5211		0.24153	1.492	1	72	Hf_b	-24
52	Te	4	-2	0	1.43	0.89	10.387	-22.898	0.572	1	-5.585	-8.052	-2.467	0	-0.595	1.3797		0.09144	1.341	1	52	Te	-21
23	V	5	-3	0	1.32	0.4	14.146	-36.944	14.618	1	-13.367	-8.052	5.315	1	1.338	1.3914	1.32	0.07		1	23	V	3.4
16	S	6	-4	0	1.06	0.34	24.771	-19.794	-2.531	0	21.492	-8.052	-29.544	0				-0.91	0.34	0	16	S	-56
SUCCESS RATE				23																			
TOTAL 23				65.22%						65.22%				78.26%						60.87%			

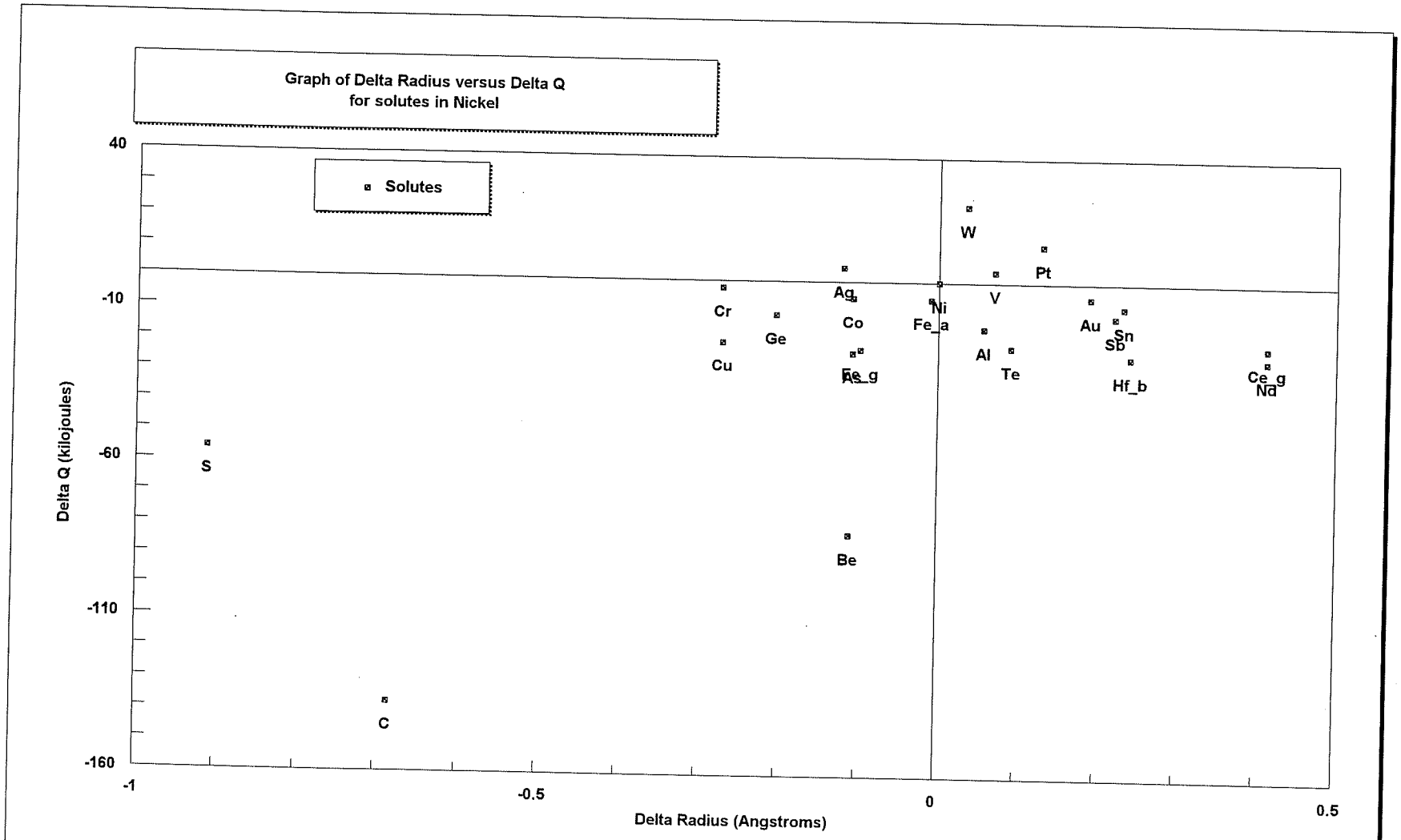
Graph of Delta Radius versus Delta Q
for solutes in Nickel
Solutes
40
-10
-60
-110
-160
Delta Q (kilojoules)
-1
-0.5
0
0.5
Delta Radius (Angstroms)
W
Pt
V
Ag
Cr
Co
Ni
Fe_a
Au
Sn
Sb
Ge
Al
Te
Cu
Fe_g
Hf_b
Ce_g
Nd
S
Be
C

FIGURE 16

NIOBIUM solvent system

TABLE 36

		val			at rad	Ion rad	Ef	Eo	U		Emax	Alpha											
41	Nb	5			1.43	0.74	12.053	-32.673	-0.000		-12.584	-12.584	0	0	0	1.43							
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference in Eo Values			Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
28	Ni	2	3	1	1.25	0.78	8.564	-22.326	-10.348	0	-8.052	-12.584	-4.532	0	-0.463	1.179		-0.251		0	28	Ni	-65.3
26	Fe_a	2	3	1	1.24	0.87	8.702	-22.592	-10.082	0	-8.087	-12.584	-4.497	0	-0.463	1.1696		-0.2604		0	26	Fe_a	-76.6
24	Cr	3	2	1	1.25	0.64	11.222	-21.017	-11.656	0	-2.314	-12.584	-10.27	0	-1.462	1.0774		-0.4508	0.979	0	24	Cr	-64.4
13	Al	3	2	1	1.43	0.57	8.574	-20.049	-12.624	0	-5.758	-12.584	-6.826	0	-1.065	1.2972		-0.3098	1.120	0	13	Al	28.2
39	Y	3	2	1	1.81	1.06	5.352	-15.684	-16.989	0	-6.764	-12.584	-5.82	0	-1.042	1.6461		-0.0121	1.418	0	39	Y	-169.1
27	Co	3	2	1	1.25	0.65	11.222	-26.164	-6.509	0	-7.461	-12.584	-5.123	0	-0.712	1.1769		-0.2877	1.142	0	27	Co	-127.2
81	Tl	3	2	1	1.71	1.06	5.996	-17.704	-14.970	0	-7.709	-12.584	-4.875	0	-0.84	1.5896		0.13266	1.563	1	81	Tl	-31.4
6	Carbon	4	1	1	0.77	0.2	35.825	-49.566	16.892	1	10.144	-12.584	-22.728	0	-2.297	0.6369		-0.8642	0.566	0	6	Carbon	-259.98
42	Mo	4	1	1	1.36	0.68	11.484	-18.328	-14.345	0	0.813	-12.584	-13.397	0	-2.537	1.0875		-0.4306	0.999	0	42	Mo	-51
44	Ru	4	1	1	1.34	0.65	11.829	-20.045	-12.628	0	-0.329	-12.584	-12.255	0	-2.282	1.1105		-0.4453	0.985	0	44	Ru	58.2
40	Zr_a	4	1	1	1.58	0.87	8.508	-17.625	-15.048	0	-3.444	-12.584	-9.14	0	-1.907	1.3681		-0.0756	1.354	0	40	Zr_a	-22.5
74	W	4	1	1	1.37	0.68	11.317	-22.899	-9.774	0	-4.038	-12.584	-8.546	0	-1.6	1.223		-0.2556	1.174	0	74	W	-18
50	Sn	4	1	1	1.58	0.74	8.508	-18.508	-14.165	0	-4.327	-12.584	-8.257	0	-1.727	1.3934		-0.0756	1.354	0	50	Sn	-71.6
15	P	5	0		1.09	0.35	20.745	-43.554	10.881	1	-8.977	-12.584	-3.607	0	-0.612	1.0588		-0.3927	1.037	0	15	P	-186.3
41	Nb	5	0		1.43	0.74	12.053	-32.673	-0.000	null	-12.584	-12.584	0	null	0.003	1.43		0		null	41	Nb	0
23	V	5	0		1.32	0.4	14.146	-36.944	4.271	1	-13.367	-12.584	0.783	1	0.16	1.32		-0.11		0	23	V	-46
73	Ta	5	0		1.47	0.68	11.406	-41.159	8.486	1	-22.148	-12.584	9.564	1	2.148	1.47		0.04		1	73	Ta	13.8
16	S	6	-1	0	1.06	0.34	24.771	-19.794	-12.879	0	21.492	-12.584	-34.076	0				-1.09	0.34	0	16	S(approx)	-95.9

SUCCESS RATE 16.67% 72.22% 83.33% 83.33%

TOTAL 18

109.1

251

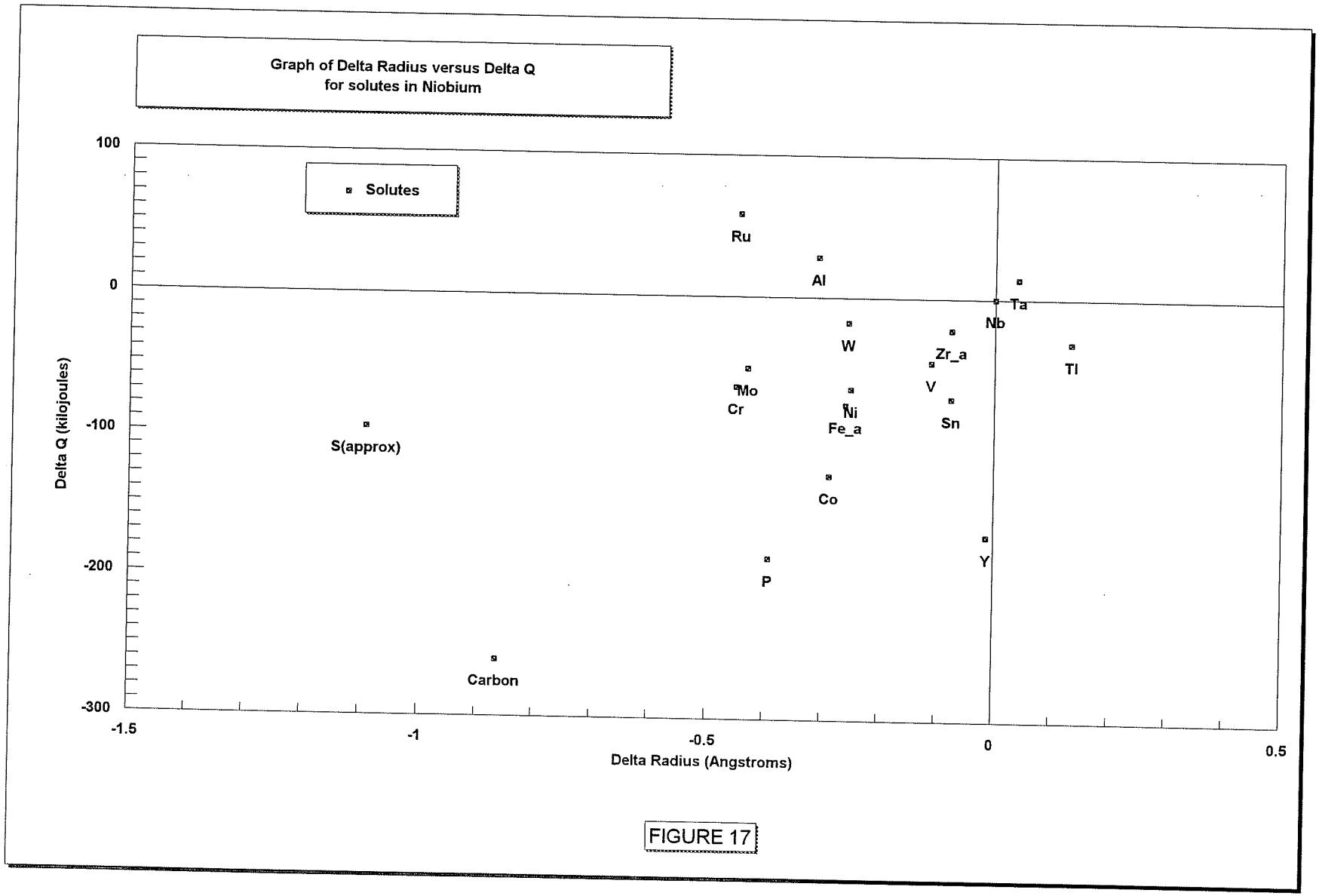
Graph of Delta Radius versus Delta Q
for solutes in Niobium
Solutes
Ru
Al
Ta
Nb
W
Zr_a
Tl
Mo
V
Cr
Ni
Fe_a
Sn
S(approx)
Co
Y
P
Carbon
100
0
-100
-200
-300
Delta Q (kilojoules)
-1.5
-1
-0.5
0
0.5
Delta Radius (Angstroms)

FIGURE 17

Praseodymium solvent system

TABLE 37

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha											
59	Pr	4			1.83	1	6.343	-9.824	-0.000	0	0.747	0.747		0	0	1.83							
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference In Eo Values			Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
29	Cu	1	3	1	1.28	0.96	5.145	-16.028	6.204	1	-7.453	0.747	8.2	1	N.S.	1.28	1.28	-0.55		0	29	Cu	-47.2
47	Ag	1	3	1	1.44	1.13	4.065	-14.285	4.460	1	-7.509	0.747	8.256	1	N.S.	1.44	1.44	-0.39		0	47	Ag	-16.7
79	Au	1	3	1	1.44	1.37	4.065	-16.653	6.828	1	-9.877	0.747	10.624	1	N.S.	1.44	1.44	-0.39		0	79	Au	-40.5
26	Fe_a	2	2	1	1.24	0.87	3.345	-4.654	-5.171	0	-8.087	0.747	8.834	1	N.S.	1.24	1.24	-0.59		0	26	Fe_a	-83.6
30	Zn	2	2	1	1.33	0.83	7.564	-21.556	11.732	1	-8.948	0.747	9.695	1	N.S.	1.33	1.33	-0.5		0	30	Zn	-19.2
67	Ho	3	1	1	1.76	1.05	5.660	-15.416	5.592	1	-5.982	0.747	6.729	1	N.S.	1.76	1.76	-0.07		0	67	Ho	-12.9
57	La_g	3	1	1	1.87	1.22	5.014	-14.494	4.670	1	-6.137	0.747	6.884	1	N.S.	1.87	1.87	0.04		1	57	La_g	-15.4
49	In	3	1	1	1.57	0.92	7.113	-18.389	8.564	1	-6.533	0.747	7.28	1	N.S.	1.57	1.57	-0.26		0	49	In	-3
27	Co	3	1	1	1.25	0.65	11.222	-26.164	16.340	1	-7.461	0.747	8.208	1	2.7	1.25	1.25	-0.58		0	27	Co	-54.3
59	Pr	4	0		1.83	1	6.343	-9.824	-0.000	0	0.747	0.747	0	0	0	1.83		NULL		0	59	Pr	0
25	Mn	4	0		1.37	0.52	11.317	-17.957	8.133	1	0.905	0.747	-0.158	0	-0.07		1.3645	-0.54484	1.285	0	25	Mn	-109.7

SUCCESS RATE 0.00% 18.18% 18.18% 90.91%

TOTAL 11

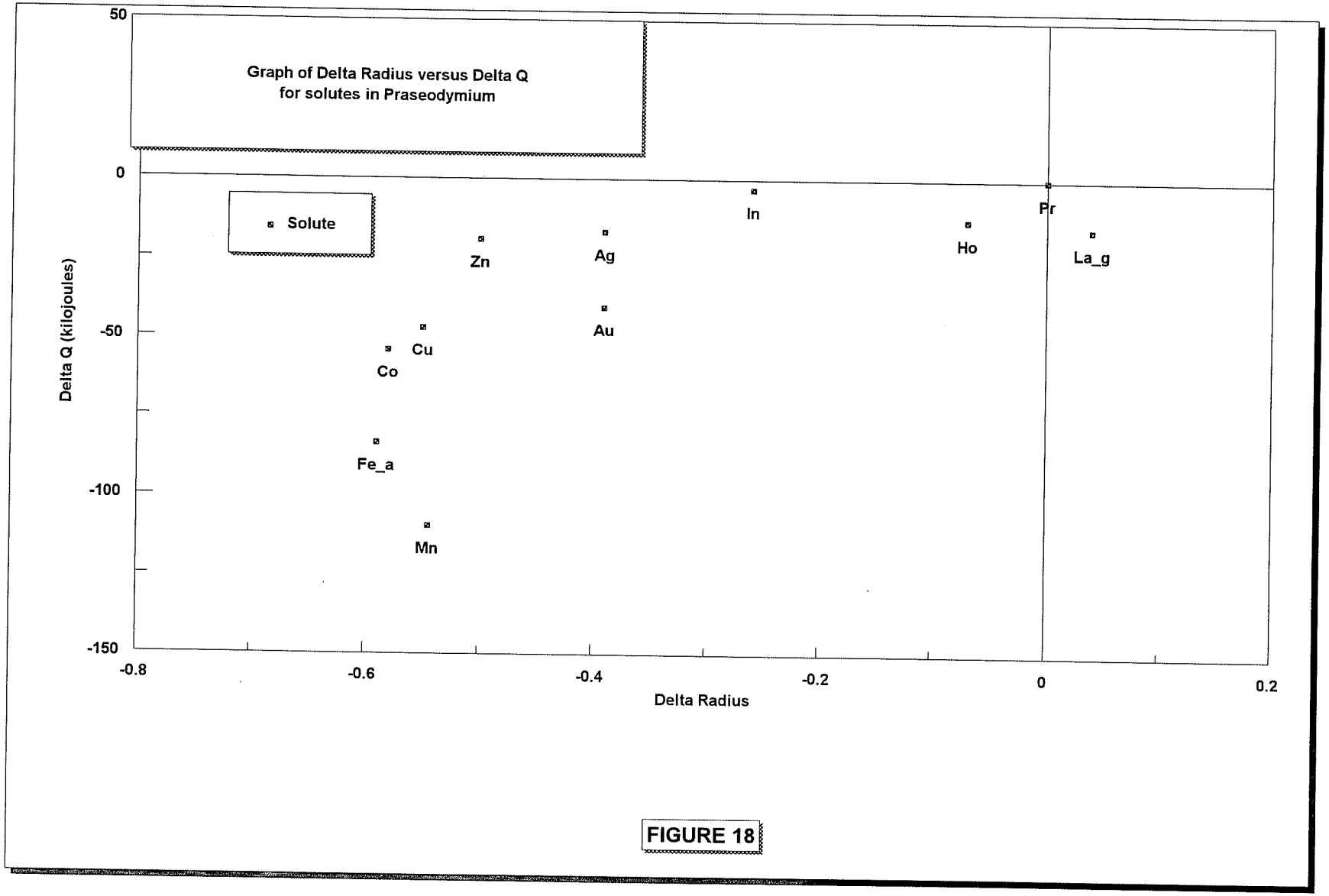
Graph of Delta Radius versus Delta Q
for solutes in Praseodymium
Solute
Delta Q (kilojoules)
50
0
-50
-100
-150
-0.8
-0.6
-0.4
-0.2
0
0.2
Delta Radius
In
Pr
Ho
La_g
Zn
Ag
Au
Cu
Co
Fe_a
Mn

FIGURE 18

SILVER solvent system

TABLE 38

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha										
47	Ag	1			1.44	1.13	4.065	-14.285	-0.000		-7.509	-7.509	0	0	0	1.440						
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference in	Eo Values		Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
47	Ag	1	0		1.44	1.13	4.065	-14.285	-0.000	0	-7.509	-7.509	0	0	0	1.440		Null		0	47	Ag	0
29	Cu	1	0		1.28	0.96	5.145	-16.028	1.743	1	-7.453	-7.509	-0.056	0	-0.05	1.265		-0.175	0.960	0	29	Cu	-11.2
30	Zn	2	-1	0	1.33	0.83	7.564	-21.556	7.271	1	-8.948	-7.509	1.439	1	0.125	1.348	1.33	-0.110		0	30	Zn	-17.2
78	Pt	2	-1	0	1.38	0.52	7.026	-22.872	8.587	1	-11.161	-7.509	3.652	1	0.437	1.442	1.38	-0.060		0	78	Pt	4.7
4	Beryllium	2	-1	0	1.14	0.54	10.296	-25.333	11.049	1	-8.173	-7.509	0.664	1	0.012	1.142	1.14	-0.300		0	4	Be	-50.1
46	Pd	2	-1	0	1.37	0.5	7.129	-21.707	7.423	1	-9.825	-7.509	2.316	1	0.25	1.406	1.37	-0.070		0	46	Pd	-12.7
28	Ni	2	-1	0	1.25	0.78	8.564	-22.326	8.041	1	-8.052	-7.509	0.543	1	-0.013	1.248		-0.192	1.072	0	28	Ni	-18.3
27	Co	3	-2	0	1.25	0.65	11.222	-26.164	11.880	1	-7.461	-7.509	-0.048	0	-0.112	1.239		-0.201	1.142	0	27	Co	-43.9
24	Cr	3	-2	0	1.25	0.64	4.383	-2.094	-12.191	0	-2.314	-7.509	-5.195	0	-1.037	1.138		-0.302	1.142	0	24	Cr	-27.4
22	Ti_b	3	-2	0	1.47	0.69	8.114	-17.432	3.147	1	-3.908	-7.509	-3.601	0	-0.862	1.363		-0.077	1.343	0	22	Ti_b	-30.2
33	As	3	-2	0	1.25	0.69	11.222	-24.253	9.969	1	-5.55	-7.509	-1.959	0	-0.45	1.206		-0.234	1.142	0	33	As	-44.7
50	Sn	4	-3	0	1.58	0.74	8.508	-18.508	4.223	1	-4.327	-7.509	-3.182	0	-1.012	1.481		0.041	1.354	1	50	Sn	-100.3
72	Hf_b	4	-3	0	1.59	0.84	8.402	-19.365	5.080	1	-5.361	-7.509	-2.148	0	-0.725	1.521		0.081	1.492	1	72	Hf_b	115.7
74	W	4	-3	0	1.37	0.68	11.317	-22.899	8.615	1	-4.038	-7.509	-3.471	0	-0.95	1.290		-0.150	1.285	0	74	W	-19.3
25	Mn	4	-3	0	1.37	0.52	11.317	-17.957	3.672	1	0.905	-7.509	-8.414	0	-2.162	1.153		-0.287	0.52	0	25	Mn	-27.3
42	Mo	4	-3	0	1.36	0.68	11.484	-18.328	4.043	1	0.813	-7.509	-8.322	0	-2.112	1.151		-0.289	0.68	0	42	Mo	-51.5
15	P	5	-4	0	1.09	0.35	20.745	-43.554	29.269	1	-8.977	-7.509	1.468	1	0.175	1.098	1.09	-0.350		0	15	P	-18.3
41	Nb	4	-3	0	1.43	0.74	10.387	-19.462	5.177	1	-12.584	-7.509	5.075	1	1.25	1.519	1.43	-0.010		0	41	Nb	-5.3
23	V	5	-4	0	1.32	0.4	14.146	-36.944	22.659	1	-13.367	-7.509	5.858	1	1.338	1.391	1.32	-0.120		0	23	V	-27.3
16	S	6	-5	0	1.06	0.34			-14.285	0	21.492	-7.509	-29.001	0		0.34		-1.100	0.34	0	16	S	-54.9

SUCCESS RATE 0.9 0.2 0.65 0.9

TOTAL 20 % correct % correct

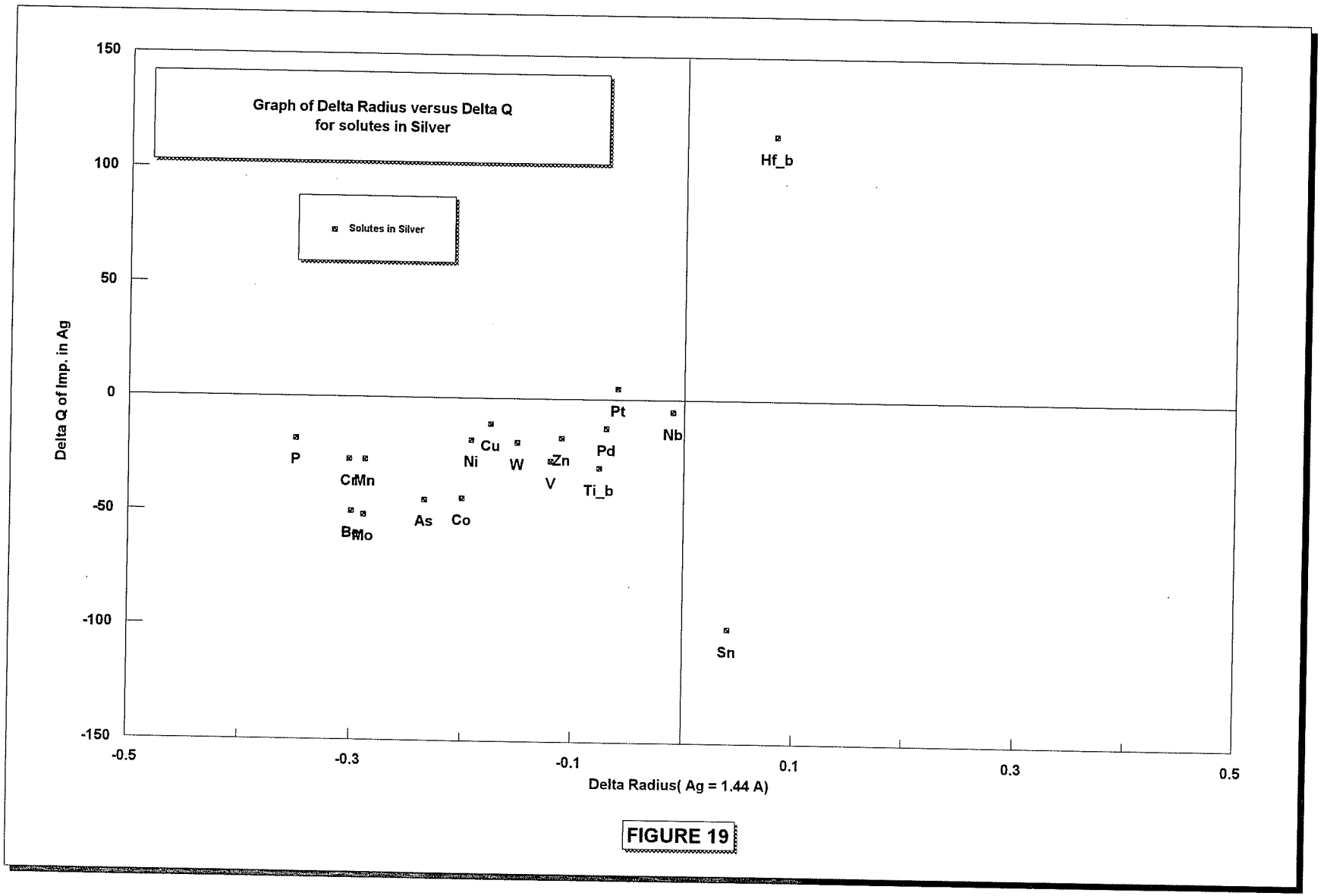
Graph of Delta Radius versus Delta Q
for solutes in Silver
Solutes in Silver
Delta Q of Imp. in Ag
Delta Radius(Ag = 1.44 A)
150
100
50
0
-50
-100
-150
-0.5
-0.3
-0.1
0.1
0.3
0.5
Hf_b
Pt
Nb
P
Cu
Ni
W
Zn
Pd
Cr
Mn
V
Ti_b
As
Co
Mo
Sn

FIGURE 19

TIN solvent system

TABLE 39

		val			at rad	Ion rad					Emax	Alpha												
50	Sn	4			1.58	0.74	8.508	-18.508	-0.000	0	-4.327	-4.327	0	0	0	1.58								
SOLUTES			Delta Valence	Relative Valence Model Predictions									Delta E	Mod. LeClaire Model Predictions	Charge Transfer	*equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q	Alt.value delta Q
29	Cu	1	3	1	1.28	0.96	5.145	-16.028	-2.480	0	-7.453	-4.327	3.126	1	0.357	1.28	1.28	-0.3		0	29	Cu	-73.1	
47	Ag	1	3	1	1.44	1.13	4.065	-14.285	-4.223	0	-7.509	-4.327	3.182	1	0.41	1.44	1.44	-0.14		0	47	Ag	-54.6	
79	Au	1	3	1	1.44	1.37	4.065	-16.653	-1.855	0	-9.877	-4.327	5.55	1	0.71	1.44	1.44	-0.14		0	79	Au	-60	
28	Ni	2	2	1	1.25	0.78	8.564	-22.326	3.818	1	-8.052	-4.327	3.725	1	0.647	1.25	1.25	-0.33		0	28	Ni	-88	
26	Fe_a	2	2	1	1.24	0.87	8.702	-22.592	4.084	1	-8.087	-4.327	3.76	1	0.647	1.24	1.24	-0.34		0	26	Fe_a	-55	
30	Zn	2	2	1	1.33	0.83	7.564	-21.556	3.048	1	-8.948	-4.327	4.621	1	0.857	1.33	1.33	-0.25		0	30	Zn	-55.9	
48	Cd	2	2	1	1.5	1.03	5.947	-19.658	1.150	1	-9.746	-4.327	5.419	1	1.15	1.5	1.5	-0.08		0	48	Cd	-29	12
80	Hg	2	2	1	1.5	1.12	5.947	-20.891	2.383	1	-10.979	-4.327	6.652	1	1.405	1.5	1.5	-0.08		0	80	Hg	-0.2	6.1
49	In	3	1	1	1.57	0.92	17.534	-16.731	-1.777	0	-6.533	-4.327	2.206	1	0.645	1.57	1.57	-0.01		0	49	In	1.1	
27	Co	3	1	1	1.25	0.65	11.222	-26.164	7.657	1	-7.461	-4.327	3.134	1	0.69	1.25	1.25	-0.33		0	27	Co	-14	
51	Sb	3	1	1	1.61	0.9	6.764	-18.746	0.238	1	-7.472	-4.327	3.145	1	0.945	1.61	1.61	0.03		1	51	Sb	15.7	
81	Tl	3	1	1	1.71	1.06	5.996	-17.704	-0.804	0	-7.709	-4.327	3.382	1	1.088	1.71	1.71	0.13		1	81	Tl	-44.6	
50	Sn	4	0		1.58	0.74	8.508	-18.508	-0.000	null	-4.327	-4.327	0	null	0.005	1.58	1.58	0		null	50	Sn	0	
SUCCESS RATE				38.46%						69.23%				38.46%						84.62%				
TOTAL 13																								

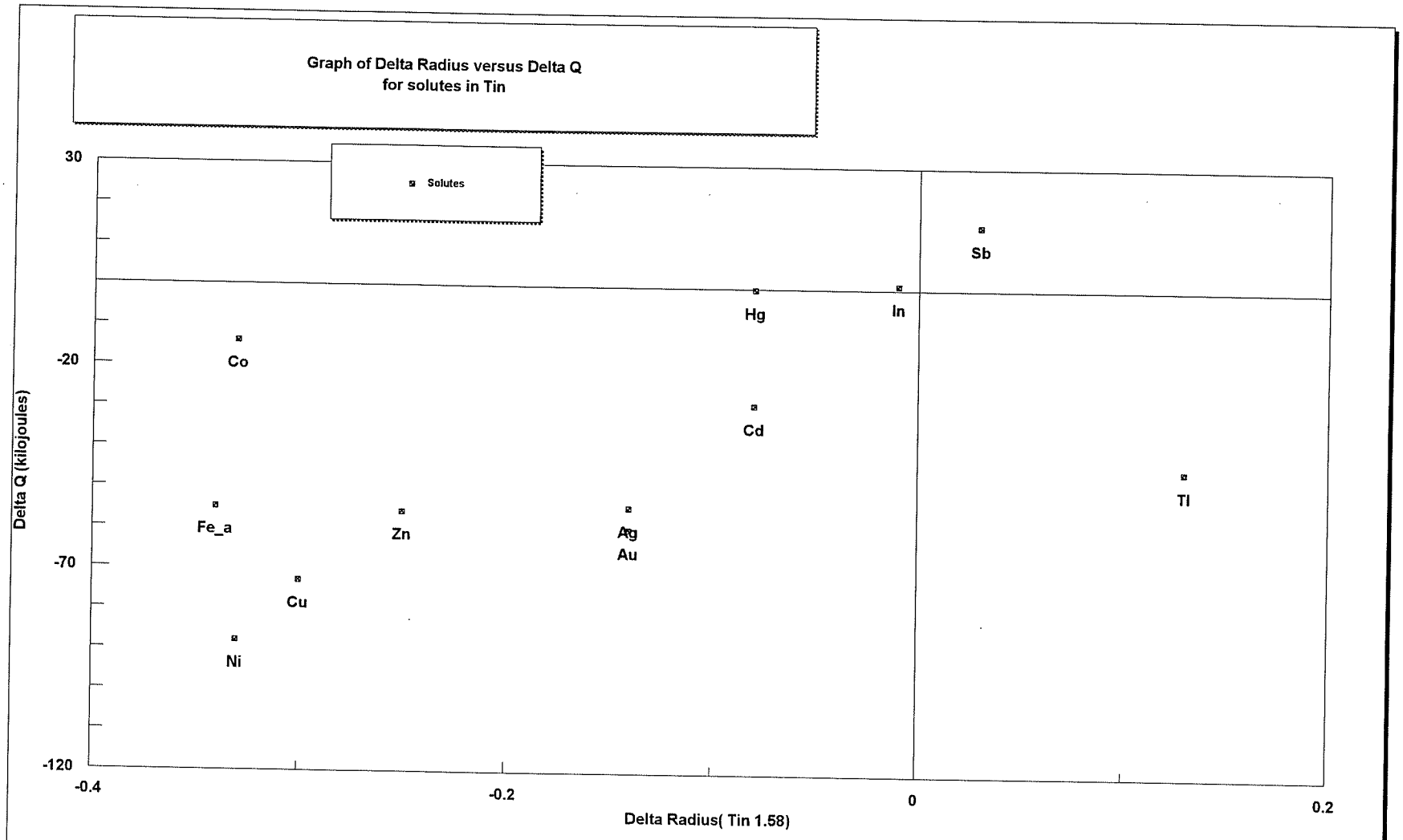
Graph of Delta Radius versus Delta Q
for solutes in Tin
Solutes
30
-20
-70
-120
Delta Q (kilojoules)
-0.4
-0.2
0
0.2
Delta Radius(Tin 1.58)
Sb
Hg
In
Co
Cd
Tl
Fe_a
Zn
Ag
Au
Cu
Ni

FIGURE 20

beta THORIUM solvent system

TABLE 40

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha										
90	Th	4			1.8	1.1	6.556	-15.655	-0.000	0	-5.138	-5.138			0	1.8						
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference in Eo Values			Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
28	Ni	2	2	1	1.25	0.78	8.564	-22.326	6.671	1	-8.052	-5.138	2.914	1	0.475	1.25	1.25	-0.55		0	28	Ni	-380.3
26	Fe_g	3	1	1	1.26	0.67	11.044	-21.473	5.818	1	-3.066	-5.138	-2.072	0	-0.442	1.2161		-0.64857	1.151	0	26	Fe_g	-346.8
27	Co	3	1	1	1.25	0.65	11.222	-26.164	10.509	1	-7.461	-5.138	2.323	1	0.48	1.25	1.25	-0.55		0	27	Co	-353.1
6	Carbon	4	0		0.77	0.2	35.825	-49.566	33.911	1	10.144	-5.138	-15.282	0	-1.877	0.6689		-1.13992	0.660	0	6	C	-305.4
42	Mo	4	0		1.36	0.68	11.484	-18.328	2.673	1	0.813	-5.138	-5.951	0	-1.705	1.202		-0.63415	1.166	0	42	Mo	-202.4
40	Zr_a	4	0		1.58	0.87	8.508	-17.625	1.970	1	-3.444	-5.138	-1.694	0	-0.565	1.5274		-0.31785	1.482	0	40	Zr_a	-34.4
75	Re	4	0		1.38	0.72	11.153	-22.448	6.793	1	-3.858	-5.138	-1.28	0	-0.362	1.3511		-0.50546	1.295	0	75	Re	-334.4
74	W	4	0		1.37	0.68	11.317	-22.899	7.245	1	-4.038	-5.138	-1.1	0	-0.302	1.3462		-0.51484	1.285	0	74	W	-258.4
41	Nb	5	-1	0	1.43	0.74	12.053	-32.673	17.018	1	-12.584	-5.138	7.446	1	2.41	1.43	1.43	-0.37		0	41	Nb	-216.6
23	V	5	-1	0	1.32	0.4	14.146	-36.944	21.289	1	-13.367	-5.138	8.229	1	2.395	1.32	1.32	-0.48		0	23	V	-288.6
73	Ta	5	-1	0	1.47	0.68	11.406	-41.159	25.504	1	-22.148	-5.138	17.01	1	N.S.	1.47	1.47	-0.33		0	73	Ta	-207.8
90	Th	4	0		1.8	1.1	6.556	-15.655	-0.000	null	-5.138	-5.138	0	null	0	1.8		0		null	90	Th	0

SUCCESS RATE 27.27% 9.09% 63.64% 100.00%

TOTAL 11

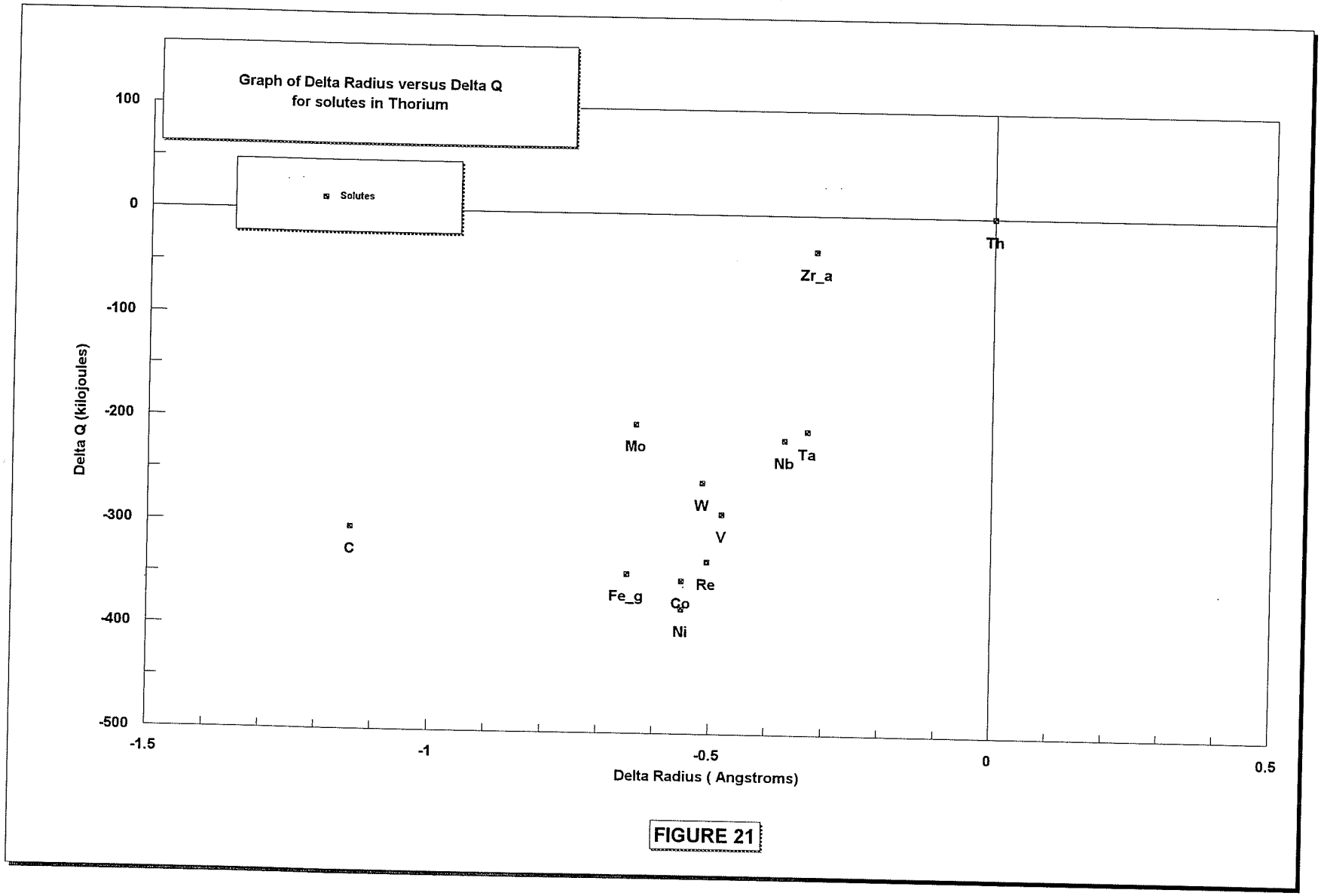
Graph of Delta Radius versus Delta Q
for solutes in Thorium
Solutes
100
0
-100
-200
-300
-400
-500
Delta Q (kilojoules)
-1.5
-1
-0.5
0
0.5
Delta Radius (Angstroms)
Th
Zr_a
Mo
Nb
Ta
W
V
C
Re
Fe_g
Co
Ni

FIGURE 21

TUNGSTEN solvent system

TABLE 41

		val			at rad	Ion rad	Eo	Er	U		Emax	Alpha			0	1.37							
74	W	4			1.37	0.68	11.317	-22.899	-0.000	0	-4.038	-4.038											
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference In	Eo Values		Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q	
26	Fe_a	2	2	1	1.24	0.87	8.702	-22.592	-0.308	0	-8.087	-4.038	4.049	1	0.715	1.24	1.24	-0.130		0	26	Fe_a	-126.7	
39	Y	3	1	1	1.81	1.06	5.352	-15.684	-7.215	0	-6.764	-4.038	2.726	1	0.968	1.81	1.81	0.440		1	39	Y	-117.9	
6	Carbon	4	0		0.77	0.2	35.825	-49.566	26.666	1	10.144	-4.038	-14.182	0	-1.802	0.674		-0.696	0.660	0	6	Carbon	-233.9	
42	Mo	4	0		1.36	0.68	11.484	-18.328	-4.572	0	0.813	-4.038	-4.851	0	-1.495	1.2256		-0.144	1.166	0	42	Mo	-81.5	
77	Ir	4	0		1.35	0.66	11.655	-25.498	2.598	1	-1.54	-4.038	-2.498	0	-0.745	1.2895		-0.081	1.266	0	77	Ir	-101.5	103.2
75	Re	4	0		1.38	0.72	11.153	-22.448	-0.452	0	-3.858	-4.038	-0.18	0	-0.047	1.3763		-0.075	1.295	0	75	Re	-177.1	92.5
74	W	4	0		1.37	0.68	11.317	-22.899	-0.000	null	-4.038	-4.038	0	0	-0.002	1.3698		0.000	1.285	null	74	W	0	
76	Os	4	0		1.35	0.67	11.655	-25.506	2.606	1	-6.081	-4.038	2.043	1	0.598	1.35	1.35	-0.020		0	76	Os	33.9	
15	P	5	-1	0	1.09	0.35	20.745	-43.554	20.654	1	-8.977	-4.038	4.939	1	1.165	1.09	1.09	-0.280		0	15	P	5.5	
41	Nb	5	-1	0	1.43	0.74	12.053	-32.673	9.774	1	-12.584	-4.038	8.546	1	2.965	1.43	1.43	0.060		1	41	Nb	71.6	
73	Ta	5	-1	0	1.47	0.68	11.406	-41.159	18.259	1	-22.148	-4.038	18.11	1	N.S.	1.47	1.47	0.100		1	73	Ta	81.2	
16	S	6	-2	0	1.06	0.34	24.771	-19.794	-3.105	0	21.492	-4.038	-25.53	0	N.S.			-1.030	0.34	0	16	S	-110.8	

SUCCESS RATE 16.67% 91.67% 91.67% 75.00%

TOTAL 12

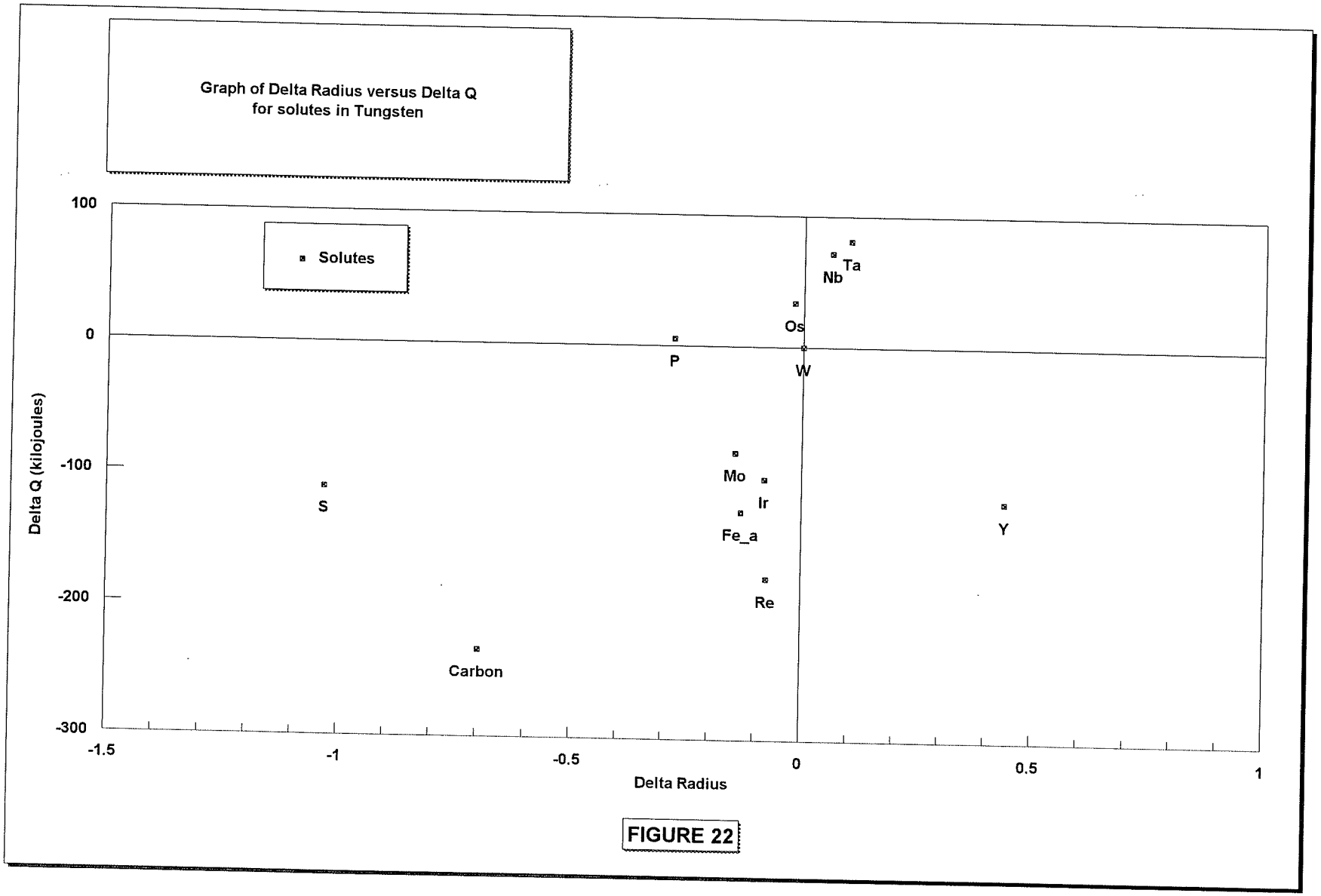
Graph of Delta Radius versus Delta Q
for solutes in Tungsten
Solutes
100
0
-100
-200
-300
Delta Q (kilojoules)
-1.5
-1
-0.5
0
0.5
1
Delta Radius
Ta
Nb
Os
P
W
Mo
Ir
S
Fe_a
Y
Re
Carbon

FIGURE 22

gamma URANIUM solvent system

TABLE 42

		val			at rad	ion rad	Ef	Eo	U		Emax	Alpha											
92	U	4			1.38	1.05	11.153	-19.993	0.000	0	-1.759	-1.759			0	1.38							
Electron configuration parameters taken from PERIOD																							
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference In	Eo Values		Delta E	LE CLAIRE Mod. LeClaire Model Predictions	charge transfer Charge Transfer	equil.Ro 'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
29	Cu	1	3	1	1.28	0.96	5.145	-16.028	-3.965	0	-7.453	-1.759	5.694	1	0.897	1.28	1.28	-0.100		0	29	Cu	-18.5
79	Au	1	3	1	1.44	1.37	4.065	-16.653	-3.341	0	-9.877	-1.759	8.118	1		1.44	1.44	0.060		1	79	Au	8.1
28	Ni	2	2	1	1.25	0.78	8.564	-22.326	2.332	1	-8.052	-1.759	6.293	1	1.375	1.25	1.25	-0.130		0	28	Ni	-53.6
26	Fe_a	2	2	1	1.24	0.87	8.702	-22.592	2.598	1	-8.087	-1.759	6.328	1	1.367	1.24	1.24	-0.140		0	26	Fe_a	-68.9
24	Cr	3	1	1	1.25	0.64	11.222	-21.017	1.024	1	-2.314	-1.759	0.555	1	0.158	1.25	1.25	-0.130		0	24	Cr	-16.8
27	Co	3	1	1	1.25	0.65	11.222	-26.164	6.171	1	-7.461	-1.759	5.702	1	1.508	1.25	1.25	-0.130		0	27	Co	-66.6
6	Carbon	4	0		0.77	0.2	35.825	-49.566	29.572	1	10.144	-1.759	-11.903	0	-1.615	0.6864		-0.720	0.660	0	6	Carbon	3.8
25	Mn	4	0		1.37	0.52	11.317	-17.957	-2.036	0	0.905	-1.759	-2.664	0	-0.992	1.2858		-0.095	1.285	0	25	Mn	-61.1
92	U	4	0		1.38	1.05	11.153	-19.993	0.000	null	-1.759	-1.759	0	null	0.005	1.38	1.38	0.000		null	92	U	0
41	Nb	5	-1	0	1.43	0.74	12.053	-32.673	12.680	1	-12.584	-1.759	10.825	1	4.383	1.43	1.43	0.050		1	41	Nb	46.8

SUCCESS RATE 10.00% 50.00% 40.00% 90.00%

TOTAL 10

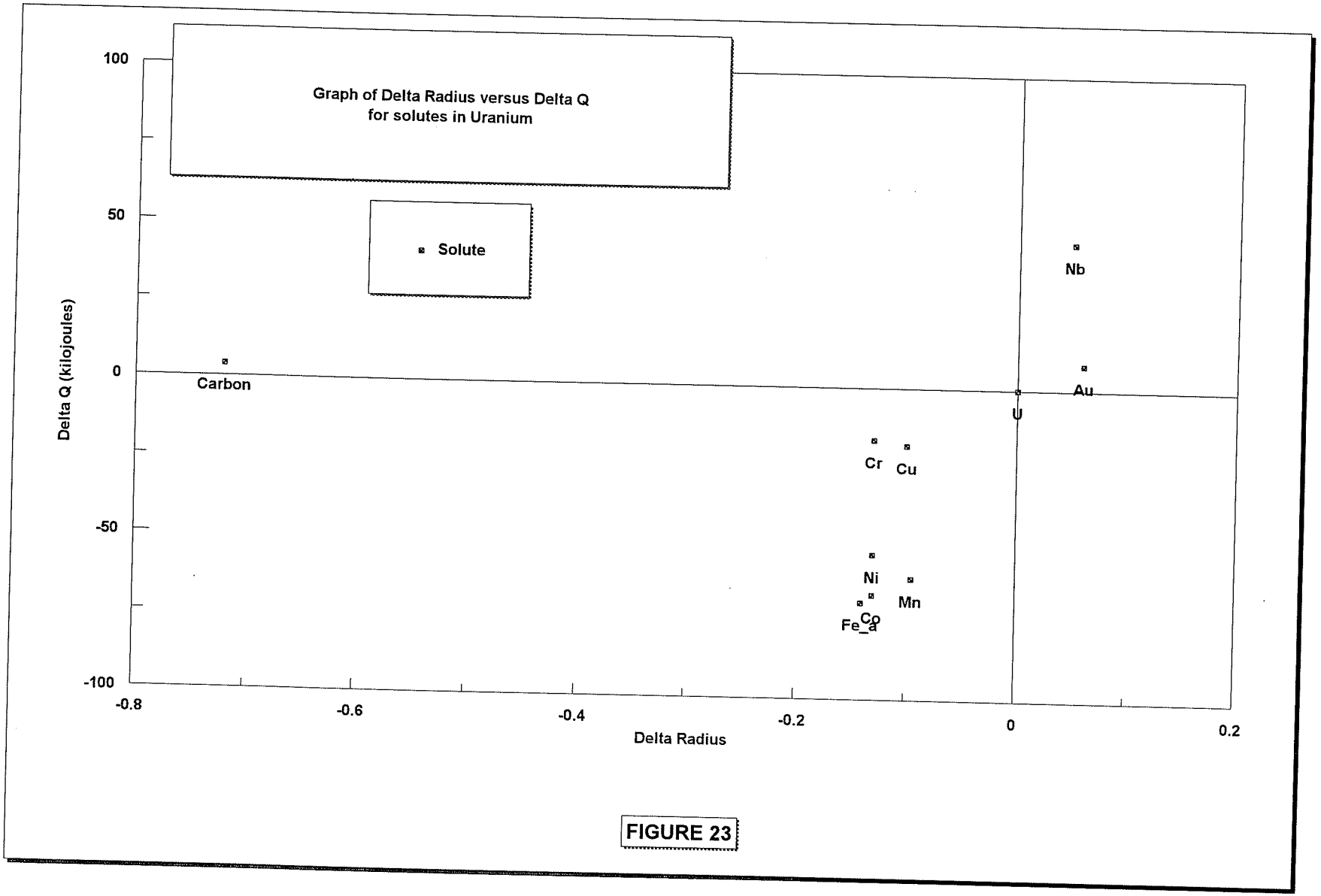
Graph of Delta Radius versus Delta Q
for solutes in Uranium
Solute
Delta Q (kilojoules)
100
50
0
-50
-100
-0.8
-0.6
-0.4
-0.2
0
0.2
Delta Radius
Carbon
Nb
Au
U
Cr
Cu
Ni
Mn
Co
Fe

FIGURE 23

ZINC solvent system

TABLE 43

		val			at rad	ion rad	Eo	Ef	U		Emax	Alpha											
30	Zn	2			1.33	0.83	7.564	-21.556	-0.000	0	-8.948	-8.948	0	0	0	1.33							
SOLUTES			Delta Valence	Relative Valence Model Predictions						Le Clair U Model Predictions Difference in	Eo Values		Delta E	Mod. LeClaire Model Predictions	Charge Transfer	'equil.Ro from iter.cpp	Acceptors fixed at atomic dia.	Delta Radius	Next full Charge Radius	Rad. Comp. Model Predictions	Atomic Number	Element	Experimental delta Q
29	Cu	1	1	1	1.28	0.96	5.145	-16.028	-5.528	0	-7.453	-8.948	-1.495	0	-0.115	1.2457		-0.37	0.960	0	29	Cu	29.2
47	Ag	1	1	1	1.44	1.13	4.065	-14.285	-7.271	0	-7.509	-8.948	-1.439	0	-0.123	1.3987		-0.2	1.130	1	47	Ag	15
79	Au	1	1	1	1.44	1.37	4.065	-16.653	-4.903	0	-9.877	-8.948	0.929	1	0.08	1.44	1.44	0.11		1	79	Au	30.4
28	Ni	2	0		1.25	0.78	8.564	-22.326	0.770	1	-8.052	-8.948	-0.896	0	-0.11	1.2344		-0.2584	1.072	0	28	Ni	42.7
30	Zn	2	0		1.33	0.83	7.564	-21.556	-0.000	NULL	-8.948	-8.948	0	NULL	0	1.33		-0.1899	1.140	NULL	30	Zn	0
48	Cd	2	0		1.5	1.03	5.947	-19.658	-1.898	0	-9.746	-8.948	0.798	1	0.122	1.5	1.5	0.17		1	48	Cd	-7.9
80	Hg	2	0		1.5	1.12	5.947	-20.891	-0.665	0	-10.979	-8.948	2.031	1	0.295	1.5	1.5	0.17		1	80	Hg	-11.5
31	Ga	3	-1	0	1.35	0.62	9.621	-21.341	-0.215	0	-5.306	-8.948	-3.642	0	-0.66	1.2775		-0.0963	1.234	0	31	Ga	-16.9
49	In	3	-1	0	1.57	0.92	7.113	-18.389	-3.167	0	-6.533	-8.948	-2.415	0	-0.495	1.5083		0.10472	1.435	1	49	In	-13.9
6	Carbon	4	-2	0	0.77	0.2	35.825	-49.566	28.010	1	10.144	-8.948	-19.092	0	-2.11	0.6518		-0.7642	0.566	0	6	Carbon	-43.7
50	Sn	4	-2	0	1.58	0.74	8.508	-18.508	-3.048	0	-4.327	-8.948	-4.621	0	-1.18	1.4619		0.02445	1.354	1	50	Sn	-12.7
SUCCESS RATE										8 /11													
TOTAL 11				54.55%						72.73%				63.64%						45.45%			

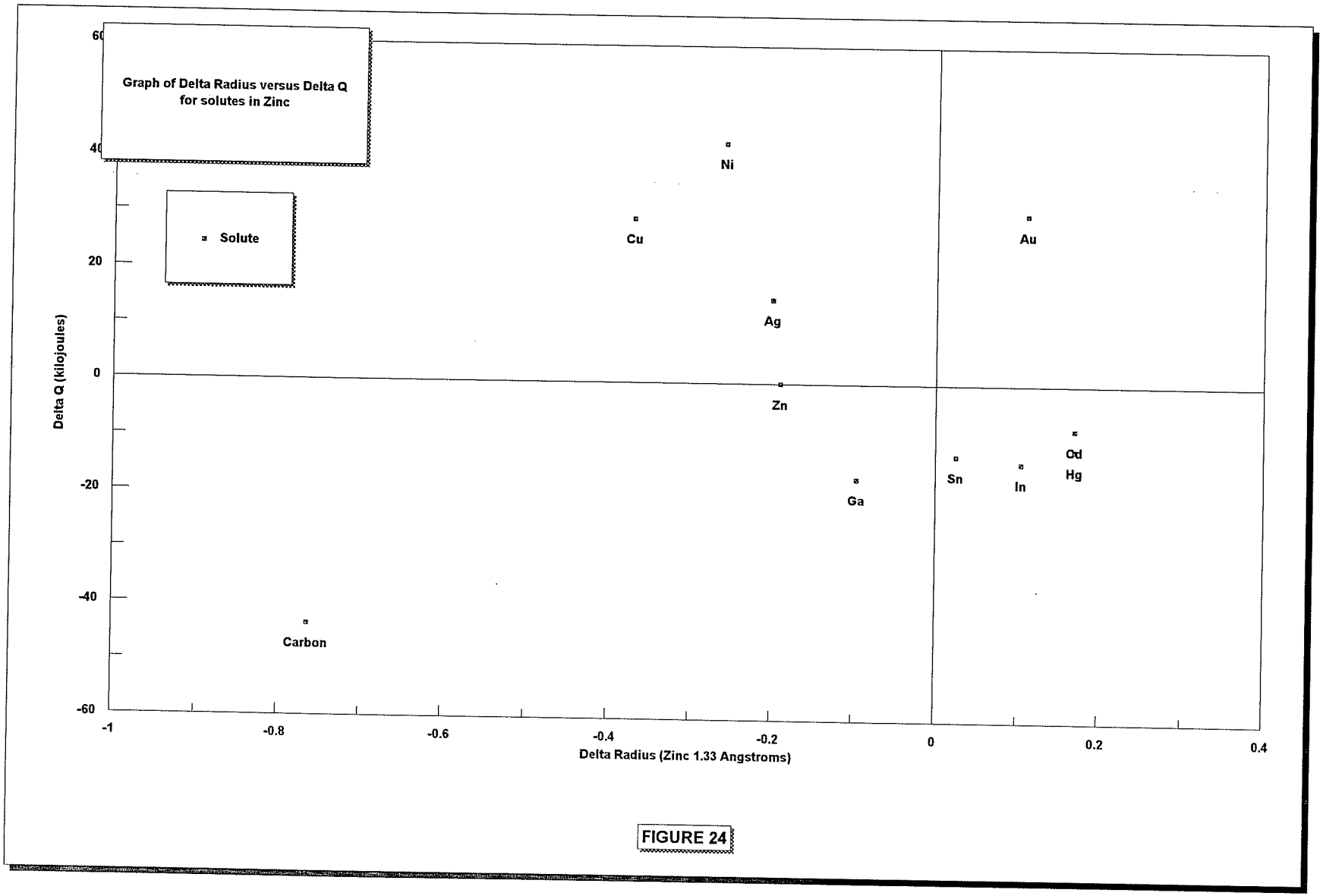
Graph of Delta Radius versus Delta Q
for solutes in Zinc
Solute
Ni
Cu
Au
Ag
Zn
Cd
Hg
Sn
In
Ga
Carbon
Delta Q (kilojoules)
60
40
20
0
-20
-40
-60
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
Delta Radius (Zinc 1.33 Angstroms)

FIGURE 24

APPENDIX A4

Tables 44-49 **Tables of Results for the Radius Compensating Model , modified to force large solutes to accomodate to the Solvent Lattice Parameters**

Figures 25-30 **Scatterplots of ΔQ versus Δ Radius for Systems forcing large solutes to accomodate to the Solvent Lattice Parameters**

TABLE 44

Solutes in Aluminium - Squeezed to 5% greater than Lattice Parameter (1.43 Angstroms x 1.05)

Element		Valence	At.Rad	Ion Rad	Emax	Alpha	Delta Emax	Charge transfer	Status	Equil. Radius	Delta Radius	R.C.M. Test	Prediction	Element	Experimental Delta Q
1	H	1	0.46	1.54	12.95	-5.76	-18.71	-0.53	Hill	0.39	-1.06	0	neg	H	-95.96
3	Li	1	1.52	0.78	-4.30	-5.76	-1.46	-0.05	Hill	1.41	-0.04	0	neg	Li	-16.00
4	Be	2	1.14	0.54	-8.17	-5.76	2.42	0.43	Well	1.19	-0.31	0	neg	Be	25.44
11	Na	1	1.86	0.98	-3.57	-5.76	-2.19	-0.15	Hill	1.38	-0.08	0	neg	Na	-44.90
12	Mg	2	1.60	0.78	-8.56	-5.76	2.80	0.73	Well	1.53	0.15	1	pos	Mg	-27.00
13	Al	3	1.43	0.57	-5.76	-5.76	0.00	0.18		1.45	-0.00	0	null	Al	0.00
14	Si	4	1.17	0.39	-0.37	-5.76	-5.38	-1.13	Hill	1.09	-0.36	0	neg	Si	-18.10
23	V	5	1.32	0.40	-13.37	-5.76	7.61	2.33	Well	1.44	-0.13	0	neg	V	-59.00
24	Cr	3	1.25	0.64	-2.31	-5.76	-3.44	-0.63	Hill	1.19	-0.26	0	neg	Cr	-58.70
25	Mn	4	1.37	0.52	0.91	-5.76	-6.66	-1.75	Hill	1.20	-0.25	0	neg	Mn	-21.40
27	Co	3	1.25	0.65	-7.46	-5.76	1.70	0.48	Well	1.29	-0.20	0	neg	Co	32.00
28	Ni	2	1.25	0.78	-8.05	-5.76	2.29	0.48	Well	1.31	-0.20	0	neg	Ni	-58.28
29	Cu	1	1.28	0.96	-7.45	-5.76	1.69	0.28	Well	1.35	-0.17	0	neg	Cu	-15.00
30	Zn	2	1.33	0.83	-8.95	-5.76	3.19	0.68	Well	1.42	-0.12	0	neg	Zn	-23.00
31	Ga	3	1.35	0.62	-5.31	-5.76	-0.45	0.05	Well	1.35	-0.10	0	neg	Ga	-18.90
32	Ge	4	1.22	0.44	-0.87	-5.76	-4.89	-1.05	Hill	1.14	-0.31	0	neg	Ge	-58.28
41	Nb	5	1.43	0.74	-12.58	-5.76	6.83	2.38	Well	1.56	-0.02	0	neg	Nb	-58.28
42	Mo	4	1.36	0.68	0.81	-5.76	-6.57	-1.70	Hill	1.20	-0.25	0	neg	Mo	-87.00
46	Pd	2	1.37	0.50	-9.83	-5.76	4.07	0.85	Well	1.48	-0.08	0	neg	Pd	-58.00
47	Ag	1	1.44	1.13	-7.51	-5.76	1.75	0.33	Well	1.52	-0.01	0	neg	Ag	-25.00
48	Cd	2	1.50	1.03	-9.75	-5.76	3.99	0.93	Well	1.55	0.05	1	pos	Cd	-17.00
49	In	3	1.57	0.92	-6.09	-5.76	0.33	0.28	Well	1.46	0.12	1	pos	In	-26.00
50	Sn	4	1.58	0.74	-3.72	-5.76	-2.04	-0.43	Hill	1.39	-0.06	0	neg	Sn	-22.00
51	Sb	3	1.61	0.90	-6.80	-5.76	1.04	0.45	Well	1.47	0.16	1	pos	Sb	-20.30
53	I	5	1.36	0.94	-21.21	-5.76	15.45	4.03	Well	1.55	-0.09	0	neg	I	-19.70
55	Cs	1	2.65	1.65	-2.08	-5.76	-3.67	-0.35	Hill	1.29	-0.16	0	neg	Cs	-42.80
59	Pr	3	1.83	1.00	-2.80	-5.76	-2.95	-0.60	Hill	1.36	-0.09	0	neg	Pr	-41.54
79	Au	1	1.44	1.37	-9.88	-5.76	4.12	0.53	Well	1.57	-0.01	0	neg	Au	-25.00
80	Hg	2	1.50	1.12	-10.98	-5.76	5.22	1.18	Well	1.58	0.05	1	pos	Hg	-0.02
81	Tl	3	1.71	1.06	-6.52	-5.76	0.76	0.40	Well	1.47	0.26	1	pos	Tl	10.70
82	Pb	2	1.75	1.32	-8.59	-5.76	2.83	0.73	Well	1.53	0.30	1	pos	Pb	3.60

Success rate	with squeezing	77.42%
	without	67.74%

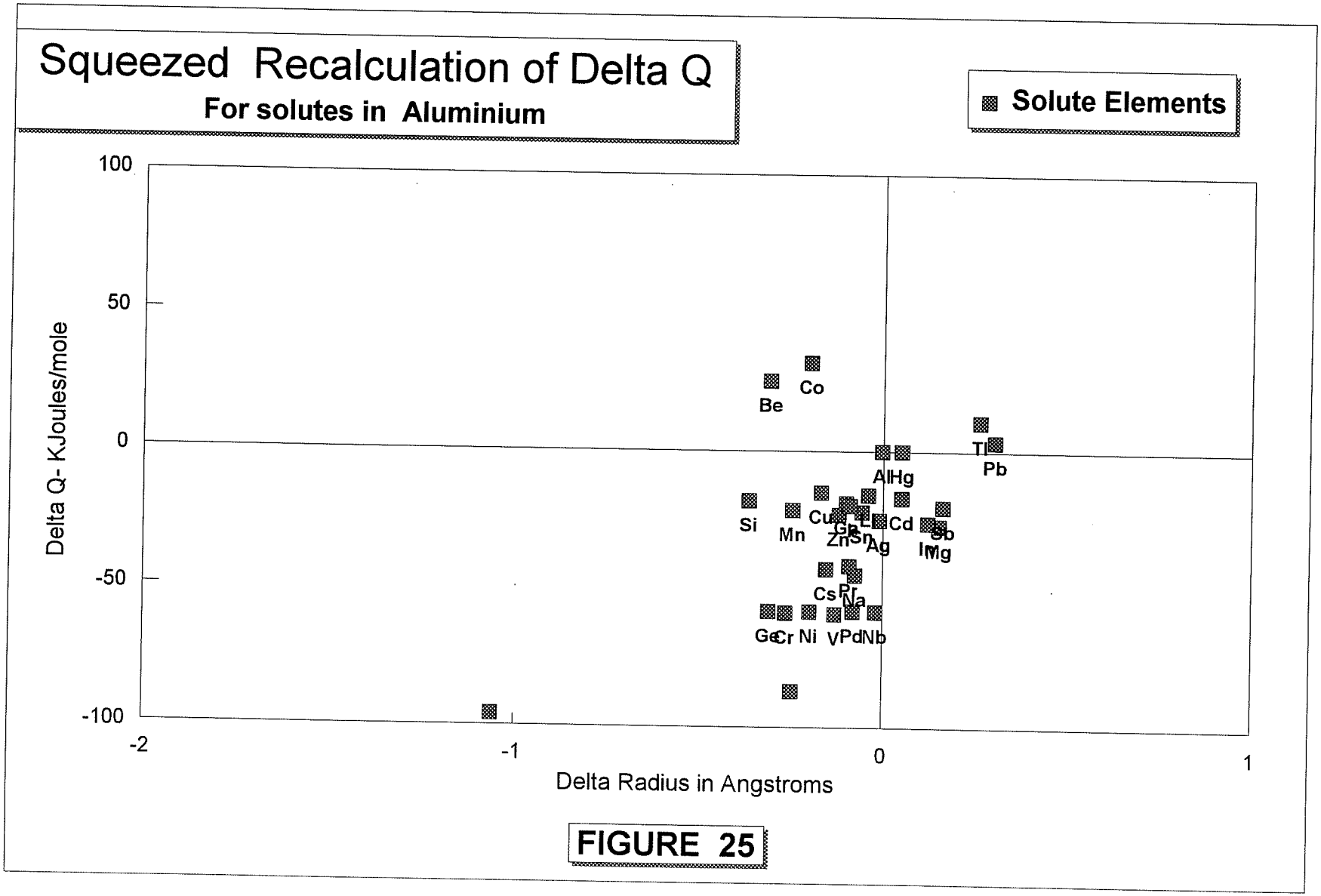
Squeezed Recalculation of Delta Q
For solutes in Aluminium
Solute Elements
Delta Q- KJoules/mole
100
50
0
-50
-100
-2
-1
0
1
Delta Radius in Angstroms
Be
Co
Si
Mn
Cu
Zn
Ga
Sn
Ag
Cd
Sb
Mg
Tl
Pb
Al
Hg
Cs
Na
Ge
Cr
Ni
V
Pd
Nb

FIGURE 25

TABLE 45

Solutes in Copper- Squeezed to 5% greater than Lattice Parameter (1.28 Angstroms x 1.05)

	Element	Valence	At.Rad	Ion Rad	Emax	Alpha	Delta	Ema	Charge trar	Status	Equil. Radi	Delta Radiu	R.C.M. Test	Prediction	Element	Experiment Delta Q
4	Beryllium	2	1.14	0.54	-8.173	-7.453	0.72	0.175		Well	1.1603	-0.1311	0	neg	Beryllium	-15.1
14	Si	4	1.17	0.39	-0.374	-7.453	-7.079	-1.4		Hill	1.0624	-0.229	0	neg	Si	-39.3
15	P	5	1.09	0.35	-8.977	-7.453	1.524	0.375		Well	1.1072	-0.1842	0	neg	P	-74.9
16	S	6	1.06	0.34	21.492	-7.453	-28.945			Hill				neg	S	-4.4
22	Ti_b	2	1.47	0.76	-35.695	-7.453	28.242			Well	N.S.			pos	Ti_b	-15
23	V	5	1.32	0.4	-13.367	-7.453	5.914	1.675		Well	1.364	0.0726	1	pos	V	4
24	Cr	3	1.25	0.64	-2.314	-7.453	-5.139	-0.875		Hill	1.1566	-0.1348	0	neg	Cr	-16
25	Mn	4	1.37	0.52	1.2	-7.453	-8.653	-2.05		Hill	1.0899	-0.2015	0	neg	Mn	-6.7
26	Fe_a	2	1.24	0.87	-8.087	-7.453	0.634	0.175		Well	1.2618	-0.0296	0	neg	Fe_a	2.3
27	Co	3	1.25	0.65	-7.461	-7.453	0.008	0.1		Well	1.2579	-0.0335	0	neg	Co	101.8
28	Ni	2	1.25	0.78	-8.052	-7.453	0.599	0.175		Well	1.2719	-0.0195	0	neg	Ni	88.3
29	Cu	1	1.28	0.96	-7.453	-7.453	0	0.05		Well	1.2914	0	0	null	CU	0
30	Zn	2	1.33	0.83	-8.948	-7.453	1.495	0.325		Well	1.3218	0.0304	1	pos	Zn	-22.1
31	Ga	3	1.35	0.62	-5.249	-7.453	-2.204	-0.35		Hill	1.2438	-0.0476	0	neg	Ga	-18.3
32	Ge	4	1.22	0.44	-0.873	-7.453	-6.58	-1.35		Hill	1.1125	-0.1789	0	neg	Ge	-24
33	As	3	1.25	0.69	-5.55	-7.453	-1.903	-0.275		Hill	1.2224	-0.069	0	neg	As	-34.6
41	Nb	5	1.43	0.74	-11.523	-7.453	4.07	1.225		Well	1.3429	0.0515	1	pos	Nb	40.5
44	Ru	4	1.34	0.65	-0.329	-7.453	-7.124	-1.65		Hill	1.1362	-0.1552	0	neg	Ru	46.5
45	Rh	3	1.34	0.68	-5.274	-7.453	-2.179	-0.35		Hill	1.2438	-0.0476	0	neg	Rh	31.8
46	Pd	2	1.37	0.5	-9.639	-7.453	2.186	0.45		Well	1.3373	0.0459	1	pos	Pd	16.6
47	Ag	1	1.44	1.13	-7.108	-7.453	-0.345	0.05		Well	1.2914	0	0	neg	Ag	-16.3
48	Cd	2	1.5	1.03	-8.772	-7.453	1.319	0.3		Well	1.3184	0.027	1	pos	Cd	194
49	In	3	1.57	0.92	-4.804	-7.453	-2.649	-0.425		Hill	1.2359	-0.0555	0	neg	In	-31
50	Sn	4	1.58	0.74	-2.159	-7.453	-5.294	-1.175		Hill	1.1837	-0.1077	0	neg	Sn	-24
51	Sb	3	1.61	0.9	-5.51	-7.453	-1.943	-0.275		Hill	1.2515	-0.0399	0	neg	Sb	-34
74	W	4	1.37	0.68	-3.743	-7.453	-3.71	-0.8		Hill	1.2169	-0.0745	0	neg	W	14.7
77	Ir	4	1.35	0.66	-1.47	-7.453	-5.983	-1.35		Hill	1.167	-0.1244	0	neg	Ir	65.4
78	Pt	2	1.38	0.52	-10.907	-7.453	3.454	0.625		Well	1.358	0.0666	1	pos	Pt	22
79	Au	1	1.44	1.37	-9.476	-7.453	2.023	0.25		Well	1.3424	0.051	1	pos	Au	1.4
80	Hg	2	1.5	1.12	-10.005	-7.453	2.552	0.475		Well	1.3401	0.0487	1	pos	Hg	-26.8
81	Tl	3	1.71	1.06	-5.236	-7.453	-2.217	-0.35		Hill	1.2438	-0.0476	0	neg	Tl	-29.7
82	Pb	2	1.75	1.32	-7.607	-7.453	0.154	0.125		Well	1.2957	0.0043	1	pos	Pb	-28.6

Success rate	with squeezing	67.74%
	without	54.84%

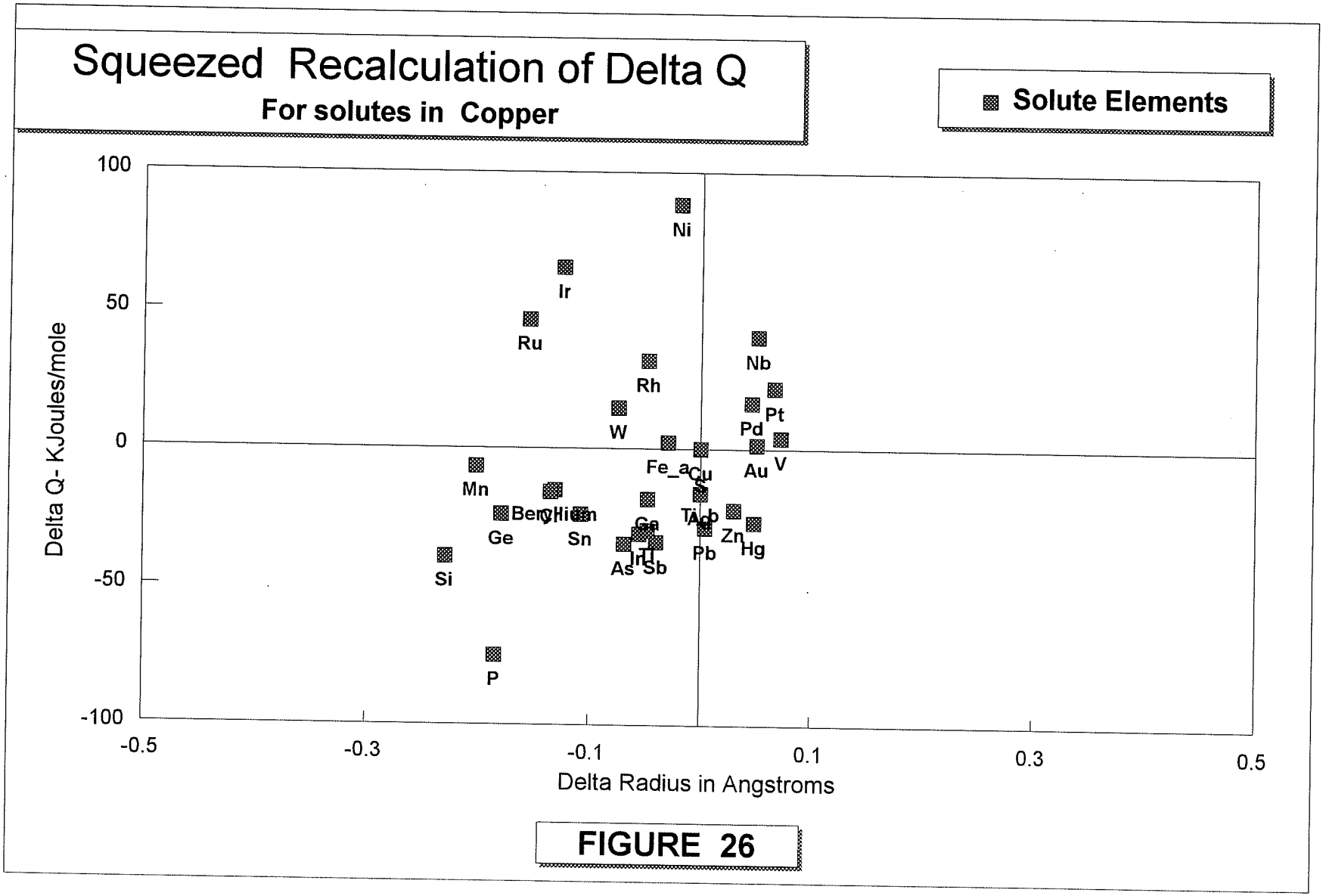
Squeezed Recalculation of Delta Q
For solutes in Copper
Solute Elements
Delta Q- KJoules/mole
100
50
0
-50
-100
-0.5
-0.3
-0.1
0.1
0.3
0.5
Delta Radius in Angstroms
Ni
Ir
Ru
Nb
Rh
W
Pt
Pd
V
Au
Fe_a
Cu
Mn
Ge
Sn
Zn
Hg
Pb
As
Sb
Si
P

FIGURE 26

TABLE 46

Solutes in Gold - Squeezed to 5% greater than Lattice Parameter (1.44 Angstroms x 1.05)

Element		Valence	At.Rad	Ion Rad	Emax	Alpha	Delta Emax	Charge Transfer	Status	Equil. Radius	Delta Radius	R.C.M. Test	Prediction	Element	Experimen Delta Q
13	Al	3	1.43	0.57	-5.758	-9.877	-4.119	-0.65	Hill	1.3532	-0.0868	0	neg	Al	-28.7
26	Fe_a	2	1.24	0.87	-8.087	-9.877	-1.79	-0.15	Hill	1.2176	-0.2224	0	neg	Fe_a	1.9
27	Co	3	1.25	0.65	-7.461	-9.877	-2.416	-0.3	Hill	1.2202	-0.2198	0	neg	Co	12.9
28	Ni	2	1.25	0.78	-8.052	-9.877	-1.825	-0.15	Hill	1.2274	-0.2126	0	neg	Ni	16.1
29	Cu	1	1.28	0.96	-7.453	-9.877	-2.424	-0.125	Hill	1.2407	-0.1993	0	neg	Cu	-2.1
30	Zn	2	1.33	0.83	-8.948	-9.877	-0.929	-0.05	Hill	1.3211	-0.1189	0	neg	Zn	-14.2
32	Ge	4	1.22	0.44	-0.873	-9.877	-9.004	-1.675	Hill	1.0807	-0.3593	0	neg	Ge	-27.8
46	Pd	2	1.37	0.5	-9.825	-9.877	-0.052	0.075	Hill	1.3798	-0.0602	0	neg	Pd	22.8
47	Ag	1	1.44	1.13	-7.509	-9.877	-2.368	-0.125	Hill	1.3958	-0.0442	0	neg	Ag	-4
49	In	3	1.57	0.92	-6.162	-9.877	-3.715	-0.625	Hill	1.3657	-0.0743	0	neg	In	-18.6
50	Sn	4	1.58	0.74	-3.805	-9.877	-6.072	-1.35	Hill	1.3129	-0.1271	0	neg	Sn	-29
51	Sb	3	1.61	0.9	-6.869	-9.877	-3.008	-0.5	Hill	1.3814	-0.0586	0	neg	Sb	-42.9
52	Te	4	1.43	0.89	-5.585	-9.877	-4.292	-0.85	Hill	1.355	-0.085	0	neg	Te	-31.2
78	Pt	2	1.38	0.52	-11.161	-9.877	1.284	0.25	well	1.4151	-0.0249	0	neg	Pt	29.1
79	Au	1	1.44	1.37	-9.877	-9.877	0	0.05	null	1.4538	0.0138	null	null	Au	0
80	Hg	2	1.5	1.12	-10.979	-9.877	1.102	0.225	Well	1.4728	0.0328	1	pos	Hg	-15.8

Success rate	with squeezing	62.50%
	without	56.25%

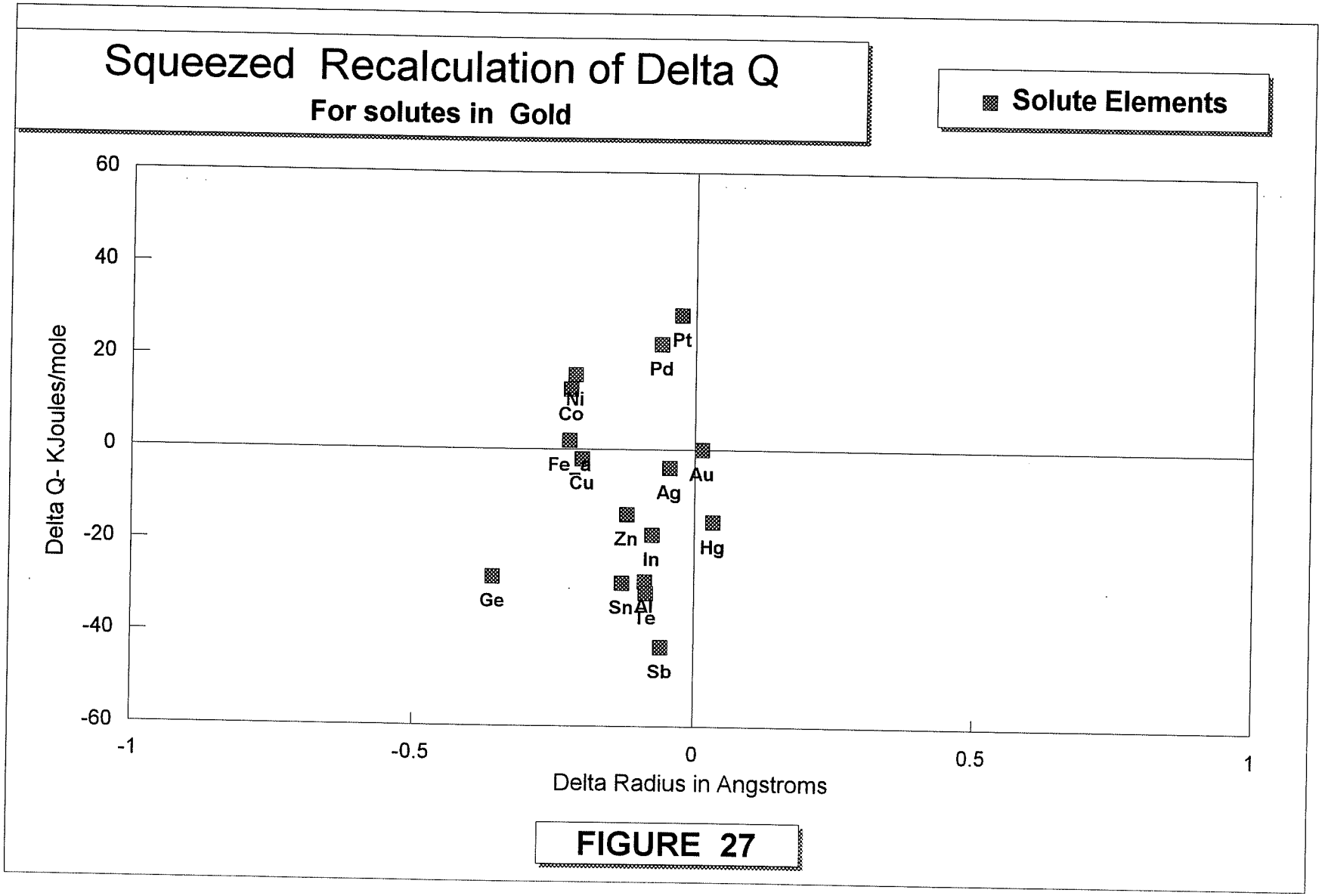
Squeezed Recalculation of Delta Q
For solutes in Gold
Solute Elements
Delta Q- KJoules/mole
60
40
20
0
-20
-40
-60
-1
-0.5
0
0.5
1
Delta Radius in Angstroms
Pt
Pd
Ni
Co
Fe
Cu
Au
Ag
Zn
In
Hg
Ge
Sn
Al
Te
Sb

FIGURE 27

TABLE 47

Solutes in Nickel - Squeezed to 5% greater than Lattice Parameter (1.25 Angstroms x 1.05)

	Element	Valence	At.Rad	Ion Rad	Emax	Alpha	Delta Emax	Charge transfer	Status	Equil. Radius	Delta Radius	R.C.M. Test	Prediction	Element	Experimental Delta Q
4	Beryllium	2	1.14	0.54	-8.173	-8.052	0.121	0.1	Well	1.1514	-0.1075	0	neg	Be	-82
6	Carbon	4	0.77	0.2	10.144	-8.052	-18.196	-2.05	HIII	0.6562	-0.6027	0	neg	C	-137.7
13	Al	3	1.43	0.57	-4.689	-8.052	-3.363	-0.55	HIII	1.1937	-0.0652	0	neg	Al	-15
16	S	6	1.06	0.34	21.492	-8.052	-29.544		HIII		-0.1989		neg	S	-56
23	V	5	1.32	0.4	-13.259	-8.052	5.207	1.425	Well	1.3208	0.0619	1	pos	V	3.4
24	Cr	3	1.25	0.64	-2.314	-8.052	-5.738	-0.95	HIII	1.1475	-0.1114	0	neg	Cr	-2.4
26	Fe_g	2	1.24	0.87	-8.087	-8.052	0.035	0.075	Well	1.2488	-0.0101	0	neg	Fe_g	-22.1
26	Fe_a	3	1.26	0.67	-3.066	-8.052	-4.986	-0.825	HIII	1.1626	-0.0963	0	neg	Fe_a	-5.6
27	Co	3	1.25	0.65	-7.461	-8.052	-0.591	0	HIII	1.2489	-0.01	0	neg	Co	-5.4
28	Ni	2	1.25	0.78	-8.052	-8.052	0	0.075		1.2589	0	0	null	Ni	0
29	Cu	1	1.28	0.96	-7.453	-8.052	-0.599	0.025	HIII	1.2547	-0.0042	0	neg	Cu	-20
32	Ge	4	1.22	0.44	-0.873	-8.052	-7.179	-1.45	HIII	1.103	-0.1559	0	neg	Ge	-11
33	As	3	1.25	0.69	-5.55	-8.052	-2.502	-0.35	HIII	1.2149	-0.044	0	neg	As	-23.2
47	Ag	1	1.44	1.13	-6.957	-8.052	-1.095	-0.025	HIII	1.2406	-0.0183	0	neg	Ag	4.4
50	Sn	4	1.58	0.74	-1.779	-8.052	-6.273	-1.35	HIII	1.1396	-0.1193	0	neg	Sn	-7.8
51	Sb	3	1.61	0.9	-5.196	-8.052	-2.856	-0.45	HIII	1.2044	-0.0545	0	neg	Sb	-11
52	Te	4	1.43	0.89	-4.29	-8.052	-3.762	-0.775	HIII	1.1906	-0.0683	0	neg	Te	-21
58	Ce_g	3	1.82	1.18	-1.845	-8.052	-6.207	-1.1	HIII	1.1281	-0.1308	0	neg	Ce_g	-20.4
60	Nd	3	1.82	1.15	-2.009	-8.052	-6.043	-1.05	HIII	1.1347	-0.1242	0	neg	Nd	-24.5
72	Hf_b	4	1.59	0.84	-2.742	-8.052	-5.31	-1.125	HIII	1.1605	-0.0984	0	neg	Hf_b	-24
74	W	4	1.37	0.68	-3.362	-8.052	-4.69	-0.975	HIII	1.1738	-0.0851	0	neg	W	24.4
78	Pt	2	1.38	0.52	-10.667	-8.052	2.615	0.475	Well	1.3091	0.0502	1	pos	Pt	11.8
79	Au	1	1.44	1.37	-9.325	-8.052	1.273	0.175	Well	1.2932	0.0343	1	pos	Au	-4.9

Success rate	with squeezing	77.42%
	without	67.74%

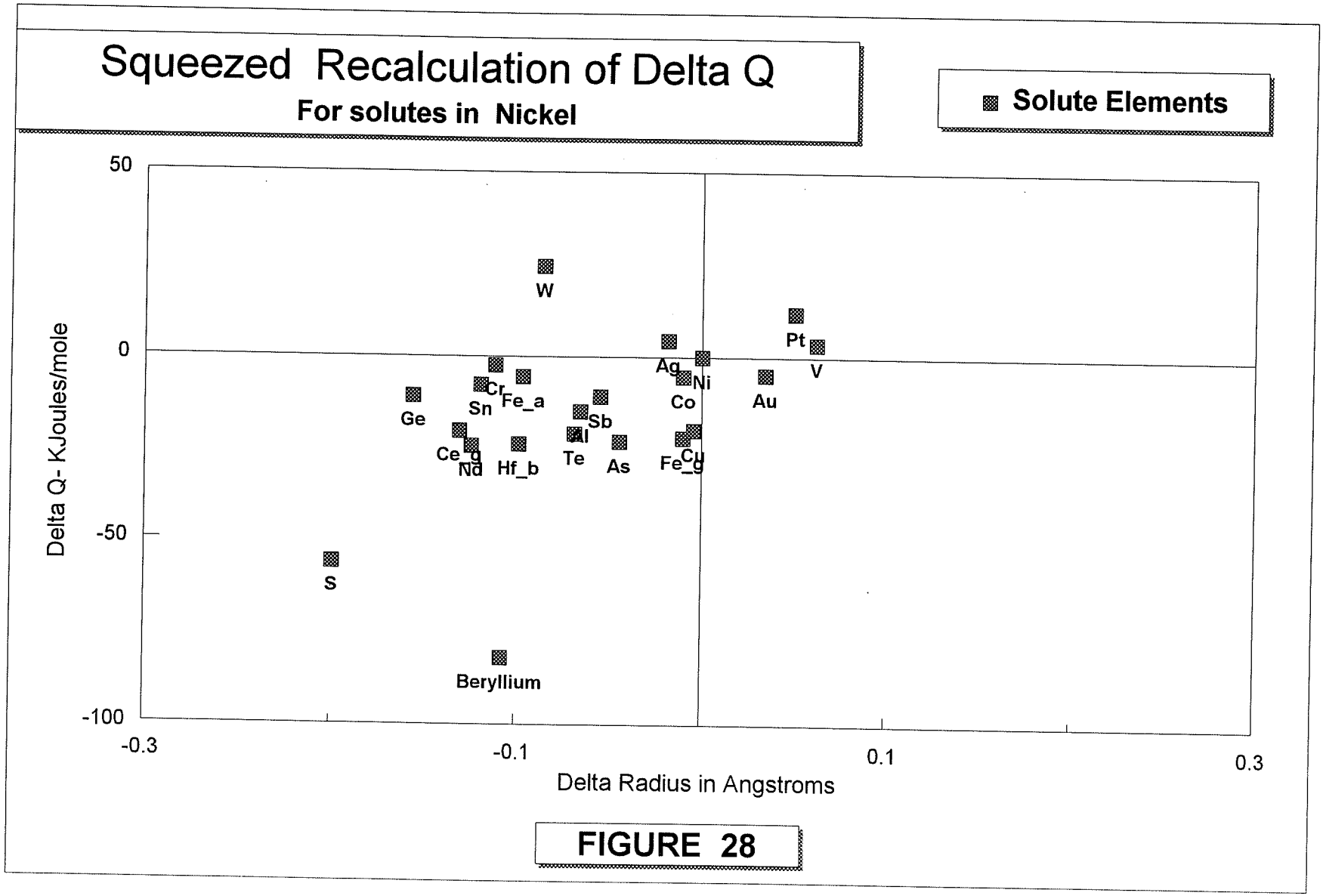
Squeezed Recalculation of Delta Q
For solutes in Nickel
Solute Elements
50
0
-50
-100
-0.3
-0.1
0.1
0.3
Delta Q- KJoules/mole
Delta Radius in Angstroms
W
Pt
V
Ag
Ni
Au
Co
Cr
Fe_a
Sn
Ge
Sb
Al
Te
As
Hf_b
Nd
Ce_g
Fe_g
Cu
S
Beryllium

FIGURE 28

TABLE 48

Solutes in a -Iron , Squeezed to 5% greater than Lattice Parameter (1.26 Angstroms x 1.05)

	Element	Valence	At.Rad	Ion Rad	Emax	Alpha	Delta Emax	Charge transfer	Status	Equil. Radius	Delta Radius	R.C.M. Test	Prediction	Element	Experimental Delta Q
4	Be	2	1.140	0.540	-8.173	-8.087	0.086	0.075	Well	1.148	-0.101	0	neg	Be	-22.600
13	Al	3	1.430	0.570	-4.579	-8.087	-3.508	-0.575	Hill	1.182	-0.067	0	neg	Al	-4.800
14	Si	4	1.170	0.390	-0.374	-8.087	-7.713	-1.475	Hill	1.056	-0.194	0	neg	Si	-30.800
15	P	5	1.090	0.350	-8.977	-8.087	0.890	0.250	Well	1.101	-0.148	0	neg	P	-29.100
22	Ti_a	2	1.470	0.760	-35.371	-8.087	-29.579	N.S.	Hill	N.S	-0.180		neg	S	-47.800
23	V	5	1.320	0.400	-13.105	-8.087	27.284	N.S.	Well	N.S	0.230		pos	Ti_a	10.500
24	Cr	3	1.250	0.640	-2.314	-8.087	5.018	1.350	Well	1.307	0.058	1	pos	V	-11.300
25	Mn	4	1.370	0.520	1.713	-8.087	-9.800	-0.950	Hill	1.138	-0.111	0	neg	Cr	-11.800
26	Fe	2	1.240	0.870	-8.087	-8.087	0.000	-2.200	Hill	1.037	-0.212	0	neg	Mn	-26.100
27	Co	3	1.250	0.650	-7.461	-8.087	-0.626	0.075	NULL	1.249	-0.000	0	null	Fe_A	0.000
28	Ni	2	1.250	0.780	-8.052	-8.087	-0.035	-0.025	Hill	1.237	-0.012	0	neg	Co	7.400
29	Cu	1	1.280	0.960	-7.453	-8.087	-0.634	0.075	Hill	1.249	-0.000	0	neg	Ni	-8.400
30	Zn	2	1.330	0.830	-8.729	-8.087	0.642	0.025	Hill	1.245	-0.004	0	neg	Cu	-6.600
33	As	3	1.250	0.690	-5.550	-8.087	-2.537	0.175	Well	1.262	0.013	1	pos	Zn	-19.000
41	Nb	5	1.430	0.740	-10.926	-8.087	2.839	-0.375	Hill	1.203	-0.046	0	neg	As	-27.600
42	Mo	4	1.360	0.680	1.510	-8.087	-9.597	0.825	Well	1.282	0.033	1	pos	Nb	1.400
46	Pd	2	1.370	0.500	-9.316	-8.087	1.229	-2.125	Hill	1.047	-0.202	0	neg	Mo	-26.400
47	Ag	1	1.440	1.130	-6.904	-8.087	-1.183	0.250	Well	1.271	0.022	1	pos	Pd	30.300
50	Sn	4	1.580	0.740	-1.646	-8.087	-6.441	-0.050	Hill	1.224	-0.025	0	neg	Ag	-17.600
51	Sb	3	1.610	0.900	-5.086	-8.087	-3.001	-1.375	Hill	1.128	-0.121	0	neg	Sn	-28.400
72	Hf	4	1.590	0.840	-2.609	-8.087	-5.478	-0.475	Hill	1.192	-0.057	0	neg	Sb	8.800
74	W	4	1.370	0.680	-3.229	-8.087	-4.858	-1.150	Hill	1.149	-0.100	0	neg	Hf_b	39.400
78	Pt	2	1.380	0.520	-10.583	-8.087	2.496	-1.000	Hill	1.162	-0.087	0	neg	W	-4.400
79	Au	1	1.440	1.370	-9.272	-8.087	1.185	0.425	Well	1.293	0.044	1	pos	Pt	45.400
								0.150	Well	1.277	0.028	1	pos	Au	6.400

N.S. No Solution found within iteration range

Success rate	with squeezing	80.00%
	without	76.00%

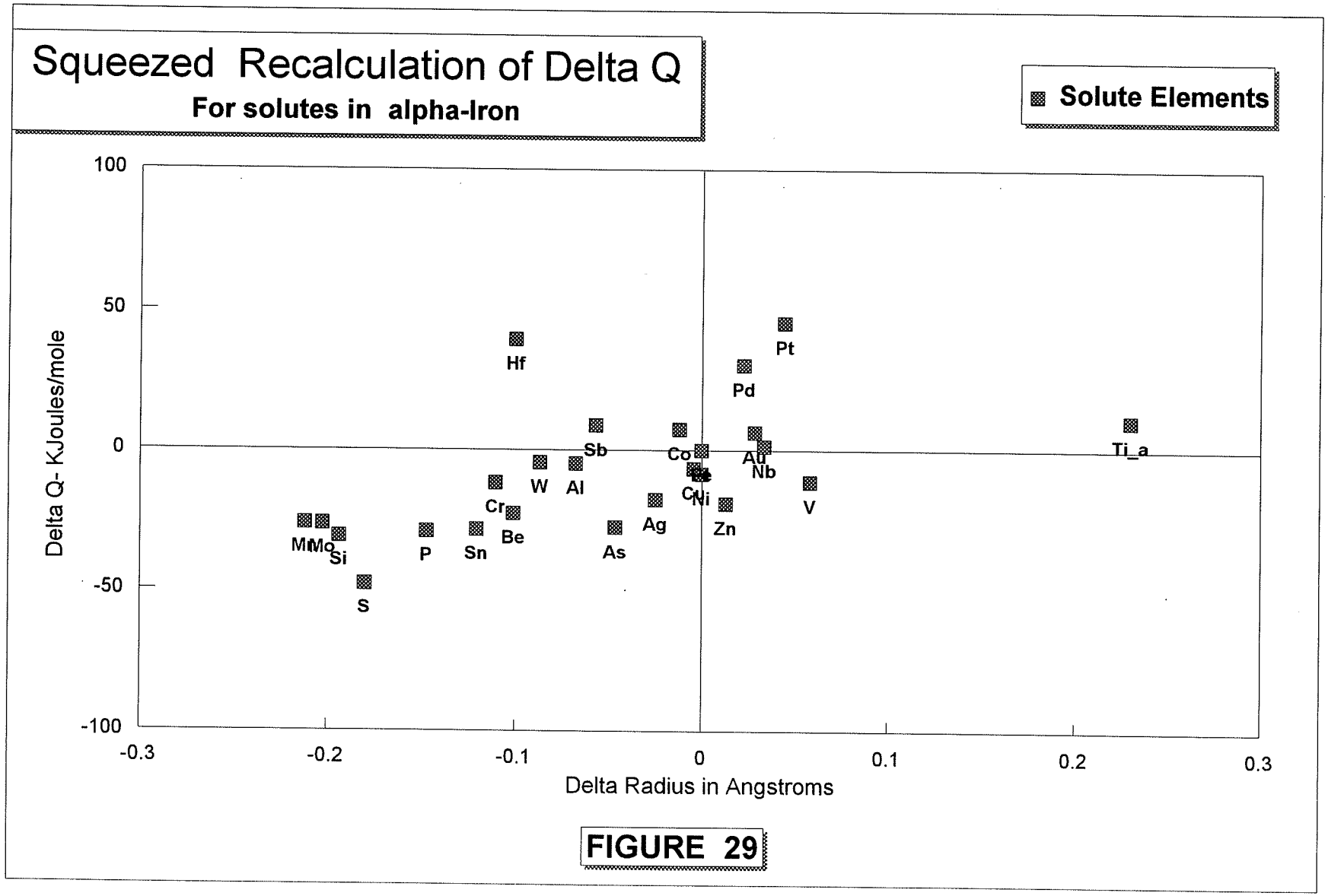
Squeezed Recalculation of Delta Q
For solutes in alpha-Iron
Solute Elements
Delta Q- KJoules/mole
Delta Radius in Angstroms
100
50
0
-50
-100
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
Hf
Pt
Pd
Sb
Co
Au
Nb
Ti_a
W
Al
Cr
Ni
V
Ag
Zn
Be
As
P
Sn
Mn
Mo
Si
S

FIGURE 29

TABLE 49

Solutes in Zinc - Squeezed to 5% greater than Lattice Parameter (1.33 Angstroms x 1.05)

Element		Valence	At.Rad	Ion Rad	Emax	Alpha	Delta Emax	Charge transfer	Status	Equil. Radius	Delta Radius				
6	Carbon	4	0.77	0.2	10.144	-8.948	-19.092	-2.1	Hill	0.6524	-0.6871	0	neg	Carbon	-43.7
28	Ni	2	1.25	0.78	-8.052	-8.948	-0.896	-0.05	Hill	1.2417	-0.0978	0	neg	Ni	42.7
29	Cu	1	1.28	0.96	-7.453	-8.948	-1.495	-0.075	Hill	1.2563	-0.0832	0	neg	Cu	29.2
30	Zn	2	1.33	0.83	-8.948	-8.948	0	0.075	null	1.3395	0	0	null	Zn	0
31	Ga	3	1.35	0.62	-5.306	-8.948	-3.642	-0.575	Hill	1.2673	-0.0722	0	neg	Ga	-16.9
47	Ag	1	1.44	1.13	-7.338	-8.948	-1.61	-0.1	Hill	1.2969	-0.0426	0	neg	Ag	15
48	Cd	2	1.5	1.03	-9.136	-8.948	0.188	0.1	Well	1.3429	0.0866	1	pos	Cd	-7.9
49	In	3	1.57	0.92	-5.281	-8.948	-3.667	-0.625	Hill	1.2614	-0.0781	0	neg	In	-13.9
50	Sn	4	1.58	0.74	-2.738	-8.948	-6.21	-1.35	Hill	1.2126	-0.1269	0	neg	Sn	-12.7
79	Au	1	1.44	1.37	-9.706	-8.948	0.758	0.125	Well	1.3633	0.0238	1	pos	Au	30.4
80	Hg	2	1.5	1.12	-10.369	-8.948	1.421	0.3	Well	1.3703	0.0308	1	pos	Hg	-11.5

Success rate	with squeezing	54.55%
	without	45.45%

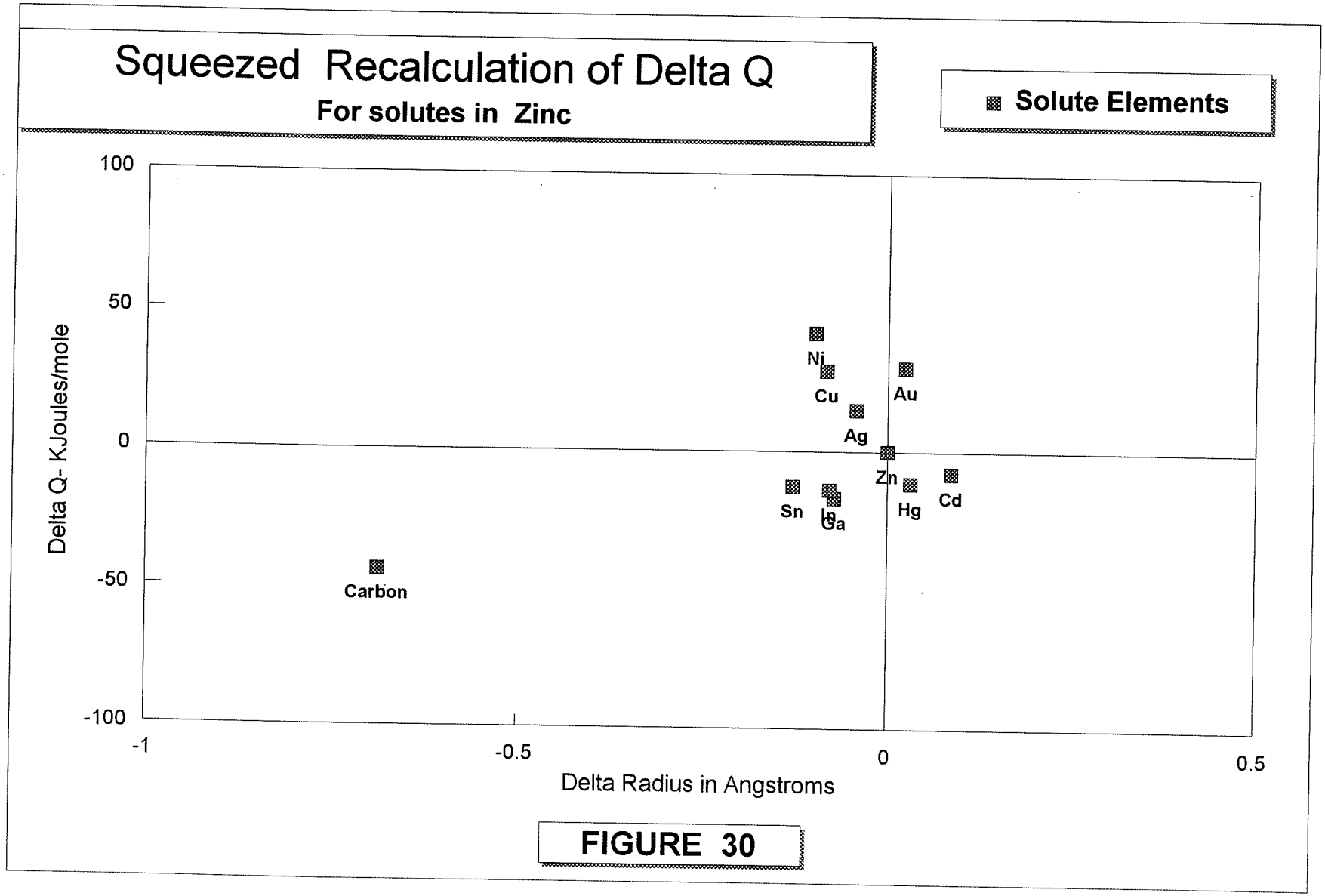
Squeezed Recalculation of Delta Q
For solutes in Zinc
Solute Elements
100
50
0
-50
-100
Delta Q- KJoules/mole
-1
-0.5
0
0.5
Delta Radius in Angstroms
Ni
Cu
Au
Ag
Zn
Cd
Hg
Sn
In
Ga
Carbon

FIGURE 30

APPENDIX A5

Iter.cpp C++ Source Code for the Iterative Solution Algorithm Determining the Charge Transfer and Equilibrium Radii for Impurity Atoms.

ION.dat Data File Supportting the Iterative Solution Routine.

// **Iter.cpp**

C++ program to iteratively solve for the charge transfer required to equilibrate solute Emax energy values with those of the solvent. Program reads raw atomic data and calculates relevant variables such as Eo , Emax, Ef, charge transfer, equilibrium radius. The
primary output permits the detailed examination of the iteration solutions . Secondary output to a file in a format compatible with a Lotus Spreadsheet Application. In the primary output a print out of predictions based on the combination of energy difference and equilibrium radius is presented. The program can also search for the radius of the full integral value of charge transfer.

Originally compiled using ZORTECH version 3.0 compiler.

```
#include<stdio.h>
//#include<iostream.h>
#include <stream.hpp>
#include<stdlib.h>
#include<math.h>
#include<conio.h>

void o_lotus(void);
void open_datfile(int sol_num);
void open_outfile(void);
void error(const char *s);
// Variable Declarations follow
int val,atnum;
     float atrad,irad,Qf,sumi,Qm,hv,sol_emax,beta,gamma,delta;
     float ii, N,NN,out,new_rad,term,imp_emax,vEf,gamma2,full_rad,term2;
     char atname[8];
 char filename[128];
 char filename2[128];
 float Sol_atrad,alpha,F,Limit;
int  counter,solv_num,count,count1;
float av_rad,charge_t;
 FILE *ifp;
 FILE *ifl;
int main(void)
{
     int i,ti,tti;
     char nDQ[45]=  "possible  LeClaire       ***neg delta Q";
     char pDQ[45]=  "possible  LeClaire       ***pos delta Q";
     char ronDQ[45]="Ro  smaller than solvent  ***neg delta Q";
```

```
      char eonDQ[45]="ERo smaller than solvent  ***neg delta Q";
      char ropDQ[45]="Ro  greater than solvent  ***pos delta Q";
      char not[50]=  "NOT GOING TO DILATE ENOUGH***neg delta Q";
      char cpos[50]= "CLASSIC BIG IMPURITY defin   pos delta Q";

        cout << "\n What is the  element # of the solvent\n";
        cin >> solv_num;
        open_datfile(solv_num);
        open_outfile();
        o_lotus();

 // open the data file ion.DAT
          FILE *inpc;
            inpc = fopen("ion.dat","r");
          if (!inpc)
        {
          puts("Can't open ion.DAT");
          exit(1);
        }
// read number of entries from  data file ion.DAT which was extracted
// from the LOTUS 123 data table ATOMT.wk1, which contains almost
everything!
         fscanf(inpc, " %i ", &count);
          if (count <= 0)
          {
            printf("Bad count value of %d\n", count);
            exit(2);
          }
   cout << "\n The total number of entries in \n"
        << " ion.DAT( Table of Elements) is ...\n" << count;


// set up loop to read the values of each line
          for (i = 0; i < count; i++)
          {

          fscanf(inpc, "%i %s %i %e %e %e %e %e  %e " ,
             &atnum,&atname,&val,&hv,&sumi,&atrad,&irad,&Qm,&Qf);
// Output  to data file Values.dat
       cout<< "\n the value of i...."<<i;
      fprintf(ifp,"\n\n% 2i %10s %2i %4f  %4f %4f
%4f\n",atnum,atname,val,hv,sumi,atrad,irad);

// the basic polynomial expression alpha+beta(x)+gamma(x^(-2/9))=0
```

```
    alpha=sol_emax;
    beta=(hv+sumi+Qm-Qf);
// Squeeze routine, Making the solute smaller forces the Ef higher
     if( atrad > (Limit))
     {
       gamma2=((5.62)*pow(val,.6666666667)/(Limit*Limit)) ;
       imp_emax=-(beta/val)+gamma2;
       gamma=(5.62)*pow(val,.44444444444)/(Sol_atrad*Sol_atrad);
     }
   if( atrad <= (Limit))
// under this condition the  smaller solutes are not modified
     {

       gamma2=((5.62)*pow(val,.6666666667)/(atrad*atrad)) ;
       imp_emax=-(beta/val)+gamma2;
       gamma=(5.62)*pow(val,.44444444444)/(atrad*atrad);

   }

   delta=imp_emax-alpha;

   fprintf(ifp," \n %4f %4f %4f %4f %4f \n",imp_emax,alpha, delta,
           beta,gamma);
   counter=0;
   av_rad=0;
   charge_t=0;
   for (ii =-val; ii<=val ; )
   {

   N=ii;
   NN= (1/(val+N));
   out =-alpha-(beta*NN)+(gamma*pow(NN,-.22222222));
   term=(1+(N/val));

       if (atrad>(Sol_atrad))
      {
      new_rad=Sol_atrad*pow(term,.222222);
       }

  if(atrad <= Sol_atrad)
   {
   new_rad=atrad*pow(term,.222222);
   }
```

```
// Displays  iterative output as out gets near zero
          if((out >= -3) && (out <=3))
          {
          charge_t=charge_t+N;
          av_rad=av_rad+new_rad;
          counter = counter+1;
          fprintf(ifp," %12.4f  %12.4f %12.4f\n",out,N,new_rad);
          }

      ii=ii+.05;
      }
// potential hill situation
      if (delta > 0)
        {


        fprintf(ifp,"%50s\n", nDQ);
        if (atrad<Sol_atrad) fprintf(ifp,"%50s\n",ronDQ);
            if ((av_rad/counter)< Sol_atrad) fprintf(ifp,"%50s\n",eonDQ);

// check routine to see if radius at full charge gets small enough only
// needed if the initial atrad was too big
// evaluate on the basis that N are negative values -1,-2,-3, to val


             for (ti=0;ti<=val;ti++)
      {
      F=ti;
      term2=(1-(F/val));

      full_rad=atrad*pow(term2,.222222);
      fprintf(ifp,"%4.2f %6.4f ",F,full_rad);

      }

   }

// potential well situation
      if (delta < 0)
            {
      fprintf(ifp,"%50s\n", pDQ);
      if (atrad<Sol_atrad)
         fprintf(ifp,"%50s\n",ronDQ);
      if ((atrad>Sol_atrad) && (av_rad/counter)> Sol_atrad)
```

```
            fprintf(ifp,"%50s\n",cpos);


        if ((atrad<Sol_atrad) && (av_rad/counter)< Sol_atrad)
         {
           fprintf(ifp,"%50s\n",not);
             for (tti=0;tti<=val;tti++)
            {
             F=tti;
             term2=(1+(F/val));
             full_rad=atrad*pow(term2,.222222);
             fprintf(ifp,"%4.2f %6.4f %6.4f ",F,term2,full_rad);

              }
            }



         }

       fprintf(ifl,"\n%1i %4s %2i %6.4f %6.4f %4.2f %4.2f %6.3f %6.3f %6.3f
                %6.4f", atnum, atname, val, hv, sumi, atrad,irad,imp_emax,
                alpha,  (charge_t/counter),(av_rad/counter) );
  }
          fclose(ifp);
          fclose(ifl);
          return (0);
}


void open_datfile(int atnum)
{
           int i;
           FILE *inp;
             inp = fopen("ion.dat","r");
           if (!inp)
        {
           puts("Can't open ion.DAT");
           exit(1);
        }
```

```
            fscanf(inp, " %i ", &count1);
            if (count1 <= 0)
             {
               printf("Bad count value of %d\n", count);
               exit(2);
             }
          for (i = 0; i < count1; i++)
          {

           fscanf(inp, "%i %s %i %e %e %e %e %e %e %e " ,
 &atnum,&atname,&val,&hv,&sumi,&ferm , &atrad,&irad,&Qm,&Qf);
 //(calculate sol_emax and set as alpha)
           if(solv_num ==atnum)
           {
           Sol_atrad=atrad;
           beta=(hv+sumi+Qm-Qf);
           gamma2=((5.62)*pow(val,.6666666667)/(atrad*atrad)) ;
           sol_emax=-(beta/val)+gamma2;
           alpha=sol_emax;
           }

       }
            fclose(inp);

}

void o_lotus(void)
{

      cout << "\n  lotus Output Filename include ext .txt   ??? ( use the
solvent's atomic  name)\n";
      cin >> filename2;

      ifl = fopen(filename2,"w");
      if (!ifl) error("Error Opening LOTUS DUMP file");
}


void open_outfile(void)
{

      cout << "\n Output Filename   ??? ( use the solvent's atomic
name)\n";
      cin >> filename;
```

```
        ifp= fopen(filename,"w");
        if (!ifp) error("Error Opening ionize file");
 }


void error(const char *s)
{
  cout << "\nERROR:" << s;
  exit(1);
}
```

ION.dat **Data file for the program Iter.cpp**

77(*Number of Entries*)

Atomic Number	*Symbol*	*Valence*	*Ev*	*ΣIp*	*Ef*	*Radii Atom*	*Radii Ion*	*Qm*	*Qf*
1	H	1	0.0093	13.598	38.9319	0.46	1.54	0	0
3	Li	1	1.3959	5.392	3.5656	1.52	0.78	0	
4	Be	2	3.0307	27.533	10.2895	1.14	0.54	0.4	.889
5	B	3	5.5856	71.382	18.2121	0.97	0.2	2.2	4.408
6	C	4	3.6878	148.022	35.0118	0.77	0.2	5.2	101.94
11	Na	1	0.9229	5.139	2.4396	1.86	0.98	0	0
12	Mg	2	1.3335	22.681	5.1082	1.6	0.78	0.4	-0.611
13	Al	3	3.0444	53.261	8.3797	1.43	0.57	2.2	24.08
14	Si	4	3.9824	103.129	15.1643	1.17	0.39	5.2	69.435
15	P	5	0.1257	176.784	20.2744	1.09	0.35	9.2	72.066
16	S	6	0.0997	115.82	18.475	1.06	0.34	14.2	159.98
19	K	1	0.8036	4.341	1.5438	2.31	1.33	0	0
20	Ca	2	1.5542	17.984	3.3696	1.97	1.06	0.4	-2.242
21	Sc	2	3.1592	19.34	5.2335	1.6	0.83	0.4	-1.74
22	Ti_a	2	4.4451	47.891	6.2	1.47	0.76	0.2	-28.731
22	Ti_b	3	4.4451	47.891	7.9299	1.47	0.69	2.2	26.582
23	V	5	4.753	162.637	13.8246	1.32	0.4	9.5	62.898
24	Cr	3	3.615	54.226	14.7066	1.25	0.64	2.2	30.654
25	Mn	4	2.2776	107.942	11.06	1.37	0.52	5.2	88.858
26	Fe	2	3.6385	24.05	8.5048	1.24	0.87	0.4	0.31
26	Fe_g	3	3.6385	54.701	10.7935	1.26	0.67	2.2	29.252
27	Co	3	3.9637	44.095	10.7935	1.25	0.65	2.2	5.43
28	Ni	2	3.854	25.803	8.3693	1.25	0.78	0.4	2.533
29	Cu	3	3.1571	7.726	5.1416	1.28	0.96	0	0
30	Zn	2	1.1952	27.358	7.3927	1.33	0.83	0	0.57
31	Ga	3	2.654	57.219	9.4023	1.35	0.62	2.2	26.911
32	Ge	4	3.465	103.763	13.9468	1.22	0.44	5.4	71.077
33	As	3	0.3603	56.794	5.4164	1.25	0.69	2.2	20.259
34	Se	6	0.2728	173.006	20.215	1.16	0.35	14.2	76.658
37	Rb	1	0.7172	4.177	1.3076	2.51	1.49	0	0
38	Sr	2	1.4398	16.725	2.829	2.15	1.27	0.4	-2.665
39	Y	3	4.0765	39.14	5.2305	1.81	1.06	2.2	14.42
40	Zr_a	4	6.028	77.3	8.0084	1.58	0.87	5.2	52.06
40	Zr_b	4	6.028	77.3	8.0084	1.58	0.87	5.2	52.06
41	Nb	5	7.2206	135.09	10.1513	1.43	0.74	9.2	48.41
42	Mo	4	6.1581	96.809	11.2232	1.36	0.68	5.2	80.791
44	Ru	4	5.8848	98.31	11.5607	1.34	0.65	5.2	76.53
45	Rh	3	5.1346	56.6	9.5432	1.34	0.68	2.2	28.58
46	Pd	2	4.0765	27.68	6.9673	1.37	0.5	0.4	3
47	Ag	1	2.6437	7.576	3.9728	1.44	1.13	0	0
48	Cd	2	1.0351	25.901	5.812	1.5	1.03	0.4	-0.085

49 In	3	2.3461	52.685	6.9519	1.57	0.92	2.2	23.405
50 Sn	4	3.0096	93.212	8.3154	1.58	0.74	5.5	61.724
51 Sb	3	0.7039	50.471	6.6108	1.61	0.9	2.2	17.429
52 Te	4	0.5248	92.979	10.1513	1.43	0.89	5.2	48.661
53 I	5	0.4323	180.692	13.0234	1.36	0.94	9.2	39.858
55 Cs	1	0.683	3.894	1.1731	2.65	1.65	0	0
56 Ba	2	1.5643	15.216	2.7771	2.17	1.43	0.4	-3.208
57 La_g	3	4.1415	35.812	4.9003	1.87	1.22	2.2	13.713
58 Ce_g	3	3.2525	36.52	5.3	1.82	1.18	2.2	16.08
58 Ce_d	4	3.2525	73.24	6.2669	1.82	1.02	5.2	65.64
59 Pr	3	3.4477	37.59	5.2423	1.83	1	2.2	19.27
59 Pr	4	3.4477	76.54	6.1986	1.83	1	5.2	71.26
60 Nd	3	2.9403	35.385	5.1732	1.82	1.15	2.2	14.14
62 Sm	3	1.9862	35.875	5.2305	1.81	1.13	2.2	13.65
63 Eu	3	1.8214	36.095	4.1176	2.04	1.13	2.2	13.43
64 Gd	3	3.2308	37.415	5.4696	1.8	1.11	2.2	12.11
65 Tb	4	3.4297	74.29	6.626	1.77	0.89	5.2	64.59
66 Dy	3	2.3932	36.775	5.4696	1.77	1.07	2.2	12.75
67 ho	3	2.602	36.995	5.5319	1.76	1.05	2.2	12.53
68 Er	3	3.0357	37.205	5.5953	1.75	1.04	2.2	12.32
69 Tm	3	1.9797	41.94	5.6598	1.74	1.04	2.2	21.19
70 Yb	3	1.336	43.624	4.6003	1.93	1	2.2	23.976
71 Lu	3	3.6888	38.501	5.7255	1.73	0.99	2.2	11.024
72 Hf_b	4	6.8519	78.5	8.2111	1.59	0.84	5.2	46.7
73 Ta	5	7.806	176.154	11.1472	1.47	0.68	9.2	44.396
74 W	4	8.283	103.844	11.06	1.37	0.68	5.2	70.996
75 Re	4	7.329	103.744	10.9003	1.38	0.72	5.2	71.096
76 Os	4	6.505	92.67	11.3901	1.35	0.67	5.2	48.97
77 Ir	4	5.8414	9.1	11.3901	1.35	0.66	5.2	-17.1
78 Pt	2	5.2907	27.563	6.8667	1.38	0.52	0.4	1.563
79 Au	1	3.3627	9.225	3.9728	1.44	1.37	0	0
80 Hg	2	0.6131	29.193	5.812	1.5	1.12	0.4	0.319
81 Tl	3	1.68	56.366	5.7255	1.71	1.06	2.2	25.124
82 Pb	2	1.8596	22.448	4.27	1.75	1.32	0.4	-0.384
83 Bi	3	1.0862	49.539	5.1732	1.82	1.2	2.2	19.141
90 Th	4	5.637	67.2	0.000	1.80	1.10	5.2	40.00
92 U	4	4.3799	67.2	0.000	1.38	1.05	5.2	40.00