The Thermodynamics
of Liquid Dilute Iron Alloys

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Data in the literature on the thermodynamic behaviour of solute elements in liquid dilute iron as the solvent have been collected and collated. The results have been expressed in terms of the first- and second-order free-energy interaction coefficients. Those based on composition in wt.-%, $e_i{}^j$ and $r_i{}^j$ are tabulated and the source materials are referenced. The thermodynamic properties of many alloying elements at infinite dilution in liquid iron are also tabulated.

NOTE:
Tables of interaction coefficients based on mole fraction as a composition co-ordinate have been compiled, but are not included herein. Tables of $\varepsilon_i{}^j$, and $\rho_i{}^j$, corresponding to Tables I–III of the paper, may be obtained from the Managing Editor, The Metals Society, 1 Carlton House Terrace, London SW1Y 5DB.

This paper is the latest in a series of publications[1-3] summarizing the available thermodynamics data on liquid iron alloys. The thermodynamics of binary liquid iron-based alloys has been reviewed, and the standard Gibbs free energy of solution has been tabulated for 24 elements. In addition, the free-energy interaction coefficients as first utilized by Wagner[4] and by Chipman,[1] and subsequently extended by Lupis and Elliott,[5-9] are compiled in this study for liquid iron. The interaction coefficients result from the Taylor series expansion of the partial excess Gibbs free energy of mixing, $G_i{}^E$, of dilute component i in the solvent (iron)

$$G_i{}^E = RT \ln \gamma_i \Big|_{T, P, X_1, X_2, \ldots X_n} \qquad \ldots (1)$$

where γ_i is the activity coefficient of component i. The expansion of equation (1) about the infinitely dilute solution as reference state is

$$RT \ln \gamma_i = RT \ln \gamma_i{}^0 \Big|_{T,P,X_1 \to 1} + \sum_{j=2}^{n} RT \frac{\delta \ln \gamma_i}{\delta X_j} \Big|_{T,P,X_1 \to 1} \cdot X_j$$

$$+ \sum_{j=2}^{n} \tfrac{1}{2} RT \frac{\delta^2 \ln \gamma_i}{\delta X_i{}^2} \Big|_{T,P,X_1 \to 1} \cdot X_j{}^2 + \sum_{j=2}^{n} \sum_{\substack{k=2 \\ j < k}}^{n}$$

$$\times \ RT \frac{\delta^2 \ln \gamma_4}{\delta X_j \delta X_k} \Big|_{T,P,X_1 \to 1} \cdot X_j X_k + O(X^3) \qquad \ldots (2)$$

Liquid iron, the solvent, is designated component 1 in our n-component system. The third-order terms are not considered, since the accuracy of the data available rarely allows their calculation. Using the notation of Lupis and Elliott,[5] equation (2) becomes

$$\ln \gamma_i = \ln \gamma_i{}^0 + \sum_{j=2}^{n} \varepsilon_i{}^j \cdot X_j + \sum_{j=2}^{n} \rho_i{}^j \cdot X_j{}^2$$

$$+ \sum_{j=2}^{n} \sum_{\substack{k=2 \\ j < k}}^{n} \rho_i{}^{j,k} \cdot X_j X_k + O(X^3) \qquad \ldots (3)$$

and describes the thermodynamic properties of the ith element in the n-component system. By convention, γ_i is the activity coefficient based on atom fraction as the composition co-ordinate, and $\gamma_i{}^0$ is the value at infinite dilution.

In many instances it is convenient to use a weight percent. composition co-ordinate. In this case the series expansion corresponding to equation (3) is

$$\log f_i = \sum_{j=2}^{n} e_i{}^j \cdot (\%j) + \sum_{j=2}^{n} r_i{}^j \cdot (\%j)^2$$

$$+ \sum_{j=2}^{n} \sum_{\substack{k=2 \\ j < k}}^{n} r_i{}^{j,k} \cdot (\%j)(\%k) + O \cdot (\%^3) \qquad \ldots (4)$$

Here the activity coefficient is f_i and the zeroeth-order term disappears in the transformation, since the activity coefficient at infinite dilution, $f_i{}^0$, is assigned the value one.

The transformation of interaction coefficients from one

composition co-ordinate (*X*) to the other (wt.-%) is accomplished by the equations given by Lupis and Elliott.[5] Some of the more useful relationships found in this paper are given below.

$$\varepsilon_i^j = \varepsilon_j^i \qquad \ldots (5)$$

$$\varepsilon_i^j = 230 \frac{M_j}{M_i} e_i^j + \frac{M_1 - M_j}{M_1} \qquad \ldots (6)$$

$$\rho_i^j = \frac{230}{(M_1)^2}\left[100M_j^2 r_i^j + M_j(M_1 - M_j)e_i^j\right] + \frac{1}{2}\left(\frac{M_1 - M_j}{M_1}\right)^2 \qquad \ldots (7)$$

$$\rho_i^{j,k} = \frac{230}{(M_1)^2}\left[100M_jM_k r_i^{j,k} + M_j(M_1 - M_k)e_i^j\right.$$
$$\left. + M_k(M_1 - M_j)e_i^k\right] + \frac{(M_1 - M_k)(M_1 - M_j)}{(M_1)^2} \qquad \ldots (8)$$

$$\rho_i^{i,j} + \varepsilon_i^j = 2\rho_j^i + \varepsilon_i^i \qquad \ldots (9)$$

$$\rho_i^{j,k} + \varepsilon_j^k = \rho_j^{i,k} + \varepsilon_k^i = \rho_k^{i,j} + \varepsilon_i^j \qquad \ldots (10)$$

The absence of second-order terms in one composition co-ordinate does not ensure the absence of second-order terms in the other when a transformation is made. Examination of equations (7) and (8) shows that second-order terms r_i^j and $r_i^{j,k}$ may appear during the transformation of interaction coefficients from atom fraction to weight percent, even though the values of ρ_i^j and $\rho_i^{j,k}$ are zero. This should be emphasized, since an appreciable error may be involved in some instances when second-order terms are omitted. The cross-product second-order terms ($\rho_i^{j,k}$ and $r_i^{j,k}$) should be calculated by equations (8)–(10) when the required accuracy of the thermodynamic calculations justifies their use. The cross-product interaction coefficients are not tabulated here, since very few are known with sufficient accuracy for them to be used generally. In the interest of brevity, therefore, these terms have been omitted in this compilation.

The use of second-order interaction coefficients is the logical outcome of several developments. First, recent thermodynamic data are sufficiently accurate so that the use of the first-order coefficients often does not describe adequately the thermodynamic behaviour of many solute elements. Secondly, work with intermediate and high-alloy steels requires knowledge of activity coefficients at compositions well away from the infinitely dilute reference state. As a consequence, the use of only the first-order term in either equation (3) or equation (4) is not sufficient for many elements. Thirdly, the increased mathematical difficulty resulting from the use of second-order terms is largely offset by the availability of computers and programmable calculators.

It is often necessary to convert from one standard state to another, especially when changing composition co-ordinates. A common change is the conversion from the pure substance as the standard state to the infinitely dilute (*i.d.*) solution as the reference state, with the standard state being at $X_i = 1$. The reaction and equation are

$$i \text{ (pure substance)} = \underline{i}\,(X, i.d.); \quad \Delta G^\circ(x) = RT\ln\gamma_i^0 \ldots (11)$$

For the transformation from mole to weight percent with the infinitely dilute solution as the reference state, and with iron as the solvent, the following applies

$$\underline{i}\,(x, i.d.) = \underline{i}\,(\%, i.d.); \quad \Delta G^\circ = RT\ln 0.5585/M_i \qquad \ldots (12)$$

where M_i is the atomic weight of *i*.
Summing equations (11) and (12) gives
$$i \text{ (pure substance)} = \underline{i}\,(\%, i.d.); \quad \Delta G^\circ(\%) =$$

$$RT\ln\left[\frac{\gamma_i^0 \cdot 0.5585}{M_i}\right] \qquad \ldots (13)$$

It is to be noted that (%, *i.d.*) signifies that the standard state is a hypothetical 1 wt.-% solution.

Scope of this Study

Five tables have been used to present the available thermodynamic data on iron alloy systems. Table I shows the first-order interaction coefficients in liquid iron at 1600° C. Table II shows the temperature-dependence of some of the first-order coefficients. In general, most of the thermodynamic measurements have been made at a single temperature, or the available data are not accurate enough to determine the temperature-dependence of the interaction coefficients. In these cases, the interaction coefficients may be assumed to be independent of temperature for most of the temperatures commonly found in steelmaking. When the temperature under concern is far different from 1600° C, however, it may be desirable to assume a temperature-dependent interaction coefficient based on the regular solution or the quasi-chemical models.[5] Table III lists the second-order coefficients at 1600° C. The above considerations on temperature-dependence also apply to the second-order terms. An asterisk appears next to values in Tables I and III when the temperature-dependence of that coefficient is known. Those values in Tables I–III, which have been determined and reported in the literature directly as *e* and *r*, are italicized. Values appearing in parenthesis are estimates and all others have been derived from information on e_i^j (or other forms) as reported by the original authors from their experimental data. Equations (5)–(8), and related equations where needed, have been used to make the necessary transformation.[10] It should be noted that most of the non-zero second-order coefficients result from a change of composition co-ordinate from the one used by the investigator to the one used in the table.

Table IV shows the references consulted for this compilation. The data in the italicized references have been used for the values appearing in Tables I–III. Reference numbers with asterisks indicate that the authors have determined (or recalculated) interaction coefficients from the data given in those studies. A complete listing of the references consulted is given to aid the reader in evaluating the data given in this paper. Compilations of this sort involves a good deal of personal judgment as to which experimental work is the most accurate. Should the reader wish to re-evaluate the data presented, it would be a simple matter to consult the references cited. Also, the values chosen for this paper are necessarily from studies where the experimental work is most accurate in relatively dilute solutions. If one is making thermodynamic calculations in composition ranges where second-order effects are very large, it would be wise to consult the original studies cited to determine how accurately the calculations reflect the

measured thermodynamic properties of the alloy. Many of the references not italicized contain experimental results in composition ranges that are not suitable for the calculation of interaction coefficients in iron-rich solutions, but do give reliable data at high solute concentrations.

Table V lists the standard free energy of solution of solute elements in liquid iron, as well as the activity coefficient at infinite dilution, γ_i^0, at 1600° C. Explanatory notes regarding the calculation of the values given in Table V are recorded in the table.

Concluding Remarks

An examination of the tables in this paper shows that much useful experimental work still remains to be done. In view of the potential value of calcium and magnesium as desulphurizing agents, their thermodynamic properties in multicomponent systems are two glaring examples of an urgent need. Also, very little is known about the elements at the end of the alphabet: Ti, U, V, W, and Zr. On the other hand, it is clear that considerable research effort has been spent studying systems that were already reasonably well known, which is unfortunate.

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TABLE I
First Order Interaction Coefficients, e_i^j, in Liquid Iron

i j→	Ag	Al	As	Au	B	C	Ca	Ce
Ag	(−0.04)	−0.08	—	—	—	0.22	—	—
Al	−0.017	0.045*	—	—	—	0.091	−0.047	—
As	—	—	—	—	—	0.25	—	—
Au	—	—	—	—	—	—	—	—
B	—	—	—	—	0.038	0.22	—	—
C	0.028	0.043	0.043	—	0.24	0.14*	−0.097	—
Ca	—	−0.072	—	—	—	−0.34	(−0.002)	—
Ce	—	—	—	—	—	—	—	—
Co	—	—	—	—	—	0.021	—	—
Cr	(−0.002)	—	—	—	—	−0.12	—	—
Cu	—	—	—	—	—	0.066	—	—
Ge	—	—	—	—	—	(0.03)	—	—
H	—	0.013	—	—	0.05	0.06	—	0.0
La	—	—	—	—	—	—	—	—
Mg	—	—	—	—	—	(0.15)	—	—
Mn	—	—	—	—	—	−0.07	—	—
Mo	—	—	—	—	—	−0.097	—	—
N	—	−0.028*	0.018	—	0.094*	0.13	—	—
Nb	—	—	—	—	—	−0.49	—	—
Nd	—	—	—	—	—	—	—	—
Ni	—	—	—	—	—	0.042	−0.067	—
O	—	−3.9*	—	−0.005	−2.6	−0.45	—	(−3.)
P	—	—	—	—	—	0.13	—	—
Pb	—	0.021	—	—	—	0.066	—	—
Pd	—	—	—	—	—	—	—	—
Pt	—	—	—	—	—	—	—	—
Rh	—	—	—	—	—	—	—	—
S	—	0.035	0.0041	0.0042	0.13	0.11	—	—
Sb	—	—	—	—	—	—	—	—
Se	—	—	—	—	—	—	—	—
Si	—	0.058	—	—	0.20	0.18*	−0.067	—
Sn	—	—	—	—	—	0.37	—	—
Ta	—	—	—	—	—	−0.37	—	—
Te	—	—	—	—	—	—	—	—
Ti	—	—	—	—	—	—	—	—
U	—	0.059	—	—	—	—	—	—
V	—	—	—	—	—	−0.34	—	—
W	—	—	—	—	—	−0.15	—	—
Zr	—	—	—	—	—	—	—	—

i j→	Co	Cr	Cu	Ge	H	La	Mg	Mn
Ag	—	(−0.01)	—	—	—	—	—	—
Al	—	—	—	—	0.24	—	—	—
As	—	—	—	—	—	—	—	—
Au	—	—	—	—	—	—	—	—
B	—	—	—	—	0.49	—	—	—
C	0.0076	−0.024	0.016	(0.008)	0.67	—	(0.07)	−0.012
Ca	—	—	—	—	—	—	—	—
Ce	—	—	—	—	−0.60	—	—	—
Co	0.0022	−0.022	—	—	−0.14	—	—	—
Cr	−0.019	−0.0003	0.016	—	−0.33	—	—	—
Cu	—	0.018	0.023	—	−0.24	—	—	—
Ge	—	—	—	(0.007)	0.41	—	—	—
H	0.0018	−0.0022	0.0005	0.01	0.0	−0.027	—	−0.0014
La	—	—	—	—	−4.3	—	—	—
Mg	—	—	—	—	—	—	—	—
Mn	—	—	—	—	−0.31	—	—	0.0
Mo	—	−0.0003	—	—	−0.20	—	—	—
N	0.011	−0.047	0.009	—	—	—	—	−0.02
Nb	—	—	—	—	−0.61	—	—	—
Nd	—	—	—	—	−6.0	—	—	—

TABLE I cont.

First-Order Interaction Coefficients, e_i^j, in Liquid Iron

i j→	Co	Cr	Cu	Ge	H	La	Mg	Mn
Ni	—	−0·0003	—	—	−0·25	—	—	—
O	0·008	−0·04	−0·013	—	−3·1	(−5·)	—	−0·021
P	—	−0·03	0·024	—	0·21	—	—	0·0
Pb	0·0	0·02	−0·028	—	—	—	—	−0·023
Pd	—	—	—	—	0·20	—	—	—
Pt	—	—	—	—	—	—	—	—
Rh	—	—	—	—	0·37	—	—	—
S	0·0026	−0·011*	−0·0084	0·014	0·12	—	—	−0·026
Sb	—	—	—	—	—	—	—	—
Se	—	—	—	—	—	—	—	—
Si	—	−0·0003	0·014	—	0·64	—	—	0·002
Sn	—	0·015	—	—	0·12	—	—	—
Ta	—	—	—	—	−4·4	—	—	—
Te	—	—	—	—	—	—	—	—
Ti	—	0·055	—	—	−1·1	—	—	—
U	—	—	—	—	—	—	—	—
V	—	—	—	—	−0·59	—	—	—
W	—	—	—	—	0·088	—	—	—
Zr	—	—	—	—	—	—	—	—

i j→	Mo	N	Nb	Nd	Ni	O	P	Pb
Ag	—	—	—	—	—	—	—	—
Al	—	−0·058*	—	—.	—	−6·6*	—	0·0065
As	—	0·077	—	—	—	—	—	—
Au	—	—	—	—	—	−0·11	—	—
B	—	0·074*	—	—	—	−1·8	—	—
C	−0·0083	0·11	−0·06	—	0·012	−0·34	0·051	0·0079
Ca	—	—	—	—	−0·044	—	—	—
Ce	—	—	—	—	—	—	—	—
Co	—	0·032	—	—	—	0·018	—	0·003
Cr	0·0018	−0·19	—	—	0·0002	−0·14	−0·053	0·0083
Cu	—	0·026	—	—	—	−0·065	0·044	−0·0056
Ge	—	—	—	—	—	—	—	—
H	0·0022	—	−0·0023	−0·038	0·0	−0·19	0·011	—
La	—	—	—	—	—	—	—	—
Mg	—	—	—	—	—	—	—	—
Mn	—	−0·091	—	—	—	−0·083	−0·0035	−0·0029
Mo	—	−0·10	—	—	—	−0·0007	—	0·0023
N	−0·011	0·0	−0·06*	—	0·01	0·05	0·045	—
Nb	—	−0·42*	(0)	—	—	−0·83	—	—
Nd	—	—	—	—	—	—	—	—
Ni	—	0·028	—	—	0·0009	0·01	−0·0035	−0·0023
O	0·0035	0·057	−0·14	—	0·006	−0·20*	0·07	—
P	—	0·094	—	—	0·0002	0·13	0·062	0·011
Pb	0·0	—	—	—	−0·019	—	0·048	—
Pd	—	—	—	—	—	−0·084	—	—
Pt	—	—	—	—	—	0·0063	—	—
Rh	—	—	—	—	—	0·11	—	—
S	0·0027	0·01	−0·013	—	0·0	−0·27	0·29	−0·046
Sb	—	0·043	—	—	—	−0·20	—	—
Se	—	0·014	—	—	—	—	—	—
Si	—	0·09	—	—	0·005	−0·23	0·11	0·01
Sn	—	0·027	—	—	—	−0·11	0·036	0·035
Ta	—	−0·47*	—	—	—	—	—	—
Te	—	0·60	—	—	—	—	—	—
Ti	—	−1·8*	—	—	—	−1·8	—	—
U	—	—	—	—	—	—	—	—

TABLE I cont.

First-Order Interaction Coefficients e_i^j, in Liquid Iron

i $j\to$	Mo	N	Nb	Nd	Ni	O	P	Pb
V	—	−0·35*	—	—	—	−0·97	—	—
W	—	−0·072	—	—	—	−0·052	—	0·0005
Zr	—	−4·1	—	—	—	—	—	—

i $j\to$	Pd	Pt	Rh	S	Sb	Se	Si	Sn
Ag	—	—	—	—	—	—	—	—
Al	—	—	—	0·030	—	—	0·0056	—
As	—	—	—	0·0037	—	—	—	—
Au	—	—	—	0·0037	—	—	—	—
B	—	—	—	0·048	—	—	0·078	—
C	—	—	—	0·046	—	—	0·08*	0·041
Ca	—	—	—	—	—	—	−0·097	—
Ce	—	—	—	—	—	—	—	—
Co	—	—	—	0·0011	—	—	—	—
Cr	—	—	—	−0·020*	—	—	−0·0043	0·009
Cu	—	—	—	−0·021	—	—	0·027	—
Ge	—	—	—	0·027	—	—	—	—
H	0·0062	—	0·0063	0·008	—	—	0·027	0·0053
La	—	—	—	—	—	—	—	—
Mg	—	—	—	—	—	—	—	—
Mn	—	—	—	−0·048	—	—	0	—
Mo	—	—	—	−0·0005	—	—	—	—
N	—	—	—	0·007	0·0088	0·006	0·047	0·007
Nb	—	—	—	−0·047	—	—	—	—
Nd	—	—	—	—	—	—	—	—
Ni	—	—	—	−0·0037	—	—	0·0057	—
O	−0·009	0·0045	0·014	−0·133	−0·023	—	−0·131	−0·0111
P	—	—	—	0·028	—	—	0·12	0·013
Pb	—	—	—	−0·32	—	—	0·048	0·057
Pd	(0·002)	—	—	—	—	—	—	—
Pt	—	—	—	0·032	—	—	—	—
Rh	—	—	—	—	—	—	—	—
S	—	0·0089	—	−0·028*	0·0037	—	0·063	−0·0044
Sb	—	—	—	0·0019	—	—	—	—
Se	—	—	—	—	—	—	—	—
Si	—	—	—	0·056	—	—	0·11*	0·017
Sn	—	—	—	−0·028	—	—	0·057	0·0016
Ta	—	—	—	−0·021	—	—	—	—
Te	—	—	—	—	—	—	—	—
Ti	—	—	—	−0·11	—	—	—	—
U	—	—	—	—	—	—	—	—
V	—	—	—	−0·028	—	—	0·042	—
W	—	—	—	0·035	—	—	—	—
Zr	—	—	—	−0·16	—	—	—	—

i $j\to$	Ta	Te	Ti	U	V	W	Zr
Ag	—	—	—	0·011	—	—	—
Al	—	—	—	—	—	—	—
As	—	—	—	—	—	—	—
Au	—	—	—	—	—	—	—
B	—	—	—	—	—	—	—
C	−0·021	—	—	—	−0·077	−0·0056	—
Ca	—	—	—	—	—	—	—
Ce	—	—	—	—	—	—	—
Co	—	—	—	—	—	—	—
Cr	—	—	0·059	—	—	—	—
Cu	—	—	—	—	—	—	—
Ge	—	—	—	—	—	—	—

TABLE I cont.

First-Order Interaction Coefficients e_i^j, in Liquid Iron

i $j\rightarrow$	Ta	Te	Ti	U	V	W	Zr
H	−0·02	—	−0·019	—	−0·0074	0·0048	—
La	—	—	—	—	—	—	—
Mg	—	—	—	—	—	—	—
Mn	—	—	—	—	—	—	—
Mo	—	—	—	—	—	—	—
N	−0·032*	0·07	−0·53*	—	−0·093*	−0·0015	−0·63
Nb	—	—	—	—	—	—	—
Nd	—	—	—	—	—	—	—
Ni	—	—	—	—	—	—	—
O	—	—	−0·6	—	−0·3	−0·0085	(−3·)
P	—	—	—	—	—	—	—
Pb	—	—	—	—	—	0·0	—
Pd	—	—	—	—	—	—	—
Pt	—	—	—	—	—	—	—
Rh	—	—	—	—	—	—	—
S	−0·0002	—	−0·072	—	−0·016	0·0097	−0·052
Sb	—	—	—	—	—	—	—
Se	—	—	—	—	—	—	—
Si	—	—	—	—	0·025	—	—
Sn	—	—	—	—	—	—	—
Ta	—	—	—	—	—	—	—
Te	—	—	—	—	—	—	—
Ti	—	—	0·013	—	—	—	—
U	—	—	—	0·013	—	—	—
V	—	—	—	—	0·015	—	—
W	—	—	—	—	—	—	—
Zr	—	—	—	—	—	—	—

* See Table II for additional information.

TABLE II

First-Order Interaction Coefficients, e_i^j, in Liquid Iron as a Function of Temperature

i $j\rightarrow$	Al	B	C	Cr	N	Nb
Al	63/T +0·011	—	—	—	1650/T −0·94	—
B	—	—	—	—	714/T −0·307	—
C	—	—	158/T+ 0·0581	—	—	—
Cr	—	—	—	—	—	—
N	859/T −0·487	975/T −0·4	—	—	—	−260/T +0·0796
Nb	—	—	—	—	−1720/T +0·503	—
O	−20600/T +7·15	—	—	—	—	—
S	—	—	—	−94·2/T +0·0396	—	—
Si	—	—	380/T −0·023	—	—	—
Ta	—	—	—	—	−1960/T +0·581	—
Ti	—	—	—	—	−13900/T +5·61	—
V	—	—	—	—	−1270/T +0·33	—

i $j\rightarrow$	O	S	Si	Ta	Ti	V
Al	−34740/T +11·95	—	—	—	—	—

TABLE II cont.

First-Order Interaction Coefficients, e_i^j in Liquid Iron as a Function of Temperature

i j→	O	S	Si	Ta	Ti	V
B	—	—	—	—	—	—
C	—	—	162/T −0·008	—	—	—
Cr	—	−153/T +0·062	—	—	—	—
N	—	—	—	−152/T +0·049	−4070/T +1·643	−350/T +0·094
Nb	—	—	—	—	—	—
O	−1750/T +0·734	—	—	—	—	—
S	—	233/T −0·153	—	—	—	—
Si	—	—	34·5/T +0·089	—	—	—
Ta	—	—	—	—	—	—
Ti	—	—	—	—	—	—
V	—	—	—	—	—	—

TABLE III

Second-Order Interaction Coefficients, r_i^j, in Liquid Iron

i j→	Al	As	Au	B	C	Ce	Co	Cr	Cu
Ag	0·0008	—	—	—	−0·008	—	—	—	—
Al	−0·001*	—	—	—	−0·004	—	—	—	—
B	—	—	—	0	0	—	—	—	—
C	−0·0007	−0·0001	—	—	0·0074*	—	—	0	0
Ca	0·0007	—	—	—	0·012	—	—	—	—
Co	—	—	—	—	—	—	0	—	—
Cr	—	—	—	—	—	—	0	0	—
Cu	—	—	—	—	—	—	—	—	0·0001
H	0	—	—	0	0	0	0	0	0
Mn	—	—	—	—	—	—	—	—	—
N	0	0	—	0	0	—	0	−0·0004	0
Ni	—	—	—	—	—	—	—	—	—
O	1·7	—	0	0	0	(0)	0	0	0
P	—	—	—	—	—	—	—	0·0008	0
Pb	0	—	—	—	0	—	0	0	0
S	0·0009	0	0	0·0074	0·0058	—	0	0	0
Si	—	—	—	—	—	—	—	—	—
Sn	—	—	—	—	—	—	—	—	—
Ti	—	—	—	—	—	—	—	0	—
U	—	—	—	—	—	—	—	—	—
V	—	—	—	—	—	—	—	—	—

* Note that $r_{Al}^{Al} = 0.17/T − 0.0011$ $r_C^C = 8.94T + 0.0026$ $r_C^{Si} = 1.94T − 0.0003$ $r_{Si}^{Si} = 6.5T − 0.0055$

i j→	Ge	H	La	Mn	Mo	N	Nb	Nd	Ni	O	P	Pd
Ag	—	—	—	—	—	—	—	—	—	—	—	—
Al	—	—	—	—	—	—	—	—	—	—	—	—
B	—	—	—	—	—	—	—	—	—	—	—	—
C	—	—	—	0	0	—	0	—	0	—	0·0041	—
Ca	—	—	—	—	—	—	—	—	0	—	—	—
Co	—	—	—	—	—	—	—	—	—	—	—	—
Cr	—	—	—	0	—	—	—	—	0	—	0·0025	—
Cu	—	—	—	—	—	—	—	—	—	—	—	—

TABLE III cont.

Second-Order Interaction Coefficients, r_i^j, in Liquid Iron

i \ $j\rightarrow$	Ge	H	La	Mn	Mo	N	Nb	Nd	Ni	O	P	Pd
H	*0*	*0*	*0*	*0*	*0*	—	*0*	*0*	*0*	*0*	*0*	0
Mn	—	—	—	0	—	—	—	—	—	—	—	—
N	—	—	—	0	0	0	0	—	0	0	0	—
Ni	—	—	—	—	—	—	—	—	0	—	—	—
O	—	—	*(0)*	0	0	—	*0*	—	0	0	*0*	*0*
P	—	—	—	0	—	—	—	—	0	—	−0·001	—
Pb	—	—	—	0	0	—	—	—	0	—	*0*	—
S	0·0002	—	—	0	0	—	−0·0001	—	0	—	0·0006	—
Si	—	—	—	—	—	—	—	—	0	—	—	—
Sn	—	—	—	—	—	—	—	—	—	—	—	—
Ti	—	—	—	—	—	—	—	—	—	—	—	—
U	—	—	—	—	—	—	—	—	—	—	—	—
V	—	—	—	—	—	—	—	—	—	—	—	—

i \ $j\rightarrow$	Pt	Rh	S	Sb	Se	Si	Sn	Ta
Ag	—	—	—	—	—	—	—	—
Al	—	—	—	—	—	−0·0006	—	—
B	—	—	—	—	—	0	—	—
C	—	—	—	—	—	0·0007*	0·0002	−0·0002
Ca	—	—	—	—	—	0·0009	—	—
Co	—	—	—	—	—	—	—	—
Cr	—	—	—	—	—	0	0	—
Cu	—	—	—	—	—	−0·0003	—	—
H	—	0	*0*	—	—	*0*	*0*	*0*
Mn	—	—	—	—	—	*0*	—	—
N	—	—	*0*	*0*	*0*	*0*	*0*	*0*
Ni	—	—	—	—	—	—	—	—
O	*0*	0	*0*	*0*	—	0	0	—
P	—	—	—	—	—	−0·001	0·0001	—
Pb	—	—	*0*	—	—	0	0	—
S	0·0001	—	−0·0009	0	—	0·0017	0	0
Si	—	—	—	—	—	−0·0021*	—	—
Sn	—	—	—	—	—	0	0	—
Ti	—	—	—	—	—	—	—	—
U	—	—	—	—	—	—	—	—
V	—	—	—	—	—	−0·0006	—	—

i \ $j\rightarrow$	Te	Ti	U	V	W	Zr
Ag	—	—	—	—	—	—
Al	—	—	0·0001	—	—	—
B	—	—	—	—	—	—
C	—	—	—	0·0001	0	—
Ca	—	—	—	—	—	—
Co	—	—	—	—	—	—
Cr	—	—	—	—	—	—
Cu	—	—	—	—	—	—
H	—	*0*	—	*0*	*0*	—
Mn	—	—	—	—	—	—
N	*0*	*0*	—	*0*	*0*	*0*
Ni	—	—	—	—	—	—
O	—	*0·031*	—	0	0	*(0)*
P	—	—	—	—	—	—
Pb	—	—	—	—	0	—
S	—	0·0001	—	0	0·0001	−0·0002
Si	—	—	—	—	—	—
Sn	—	—	—	—	—	—
Ti	—	−0·001	—	—	—	—
U	—	—	0·0001	—	—	—
V	—	—	—	−0·0001	—	—

TABLE IV

Reference Numbers for Interaction Coefficients Used in this
Study

System	References	System	References
Fe–Ag	11	Fe–H–Si	41, 99, 100*, *101*, 102, 103, *105*, *110*, 120, *121*, 122, 123
Fe–Ag–Al	12*	Fe–H–Sn	95, 111
Fe–Ag–Cr	11	Fe–H–Ta	95, *115*
Fe–Al	12, 13, 14, *15*, *16*, *17**, 18, 19*	Fe–H–Ti	99, *105*, *110*, 111, 115*
Fe–Al–Ca	20	Fe–H–V	99, 100*, 105, 110, 111, *112*, *113*, *114*, *119*
Fe–Al–Pb	21, 22	Fe–H–W	*105*, *108*, 111, 112, 114, *124**
Fe–Al–Si	12, 13, 23	Fe–Mg	27
Fe–Al–U	24	Fe–Mn	125, *126**
Fe–B	25, 26, 27, 28, *29*	Fe–Mn–Pb	21, 22
Fe–B–Si	26	Fe–Mn–Si	127, *128**
Fe–C	11, *30**, *31**, *32*, *33**, *34*, 35, 36, *37*, *38**, 39, 40, 41, *42**	Fe–Mo–Pb	21, 22
Fe–C–Ag	12*	Fe–N	*129*, *130*, *131*, *132*, *133*, *134*, *135*, 136, *137*, 138
Fe–C–Al	12, 13	Fe–N–Al	135, 139, *140**, *141**, *142**, 143
Fe–C–As	27, 43	Fe–N–As	*144*
Fe–C–B	26, 27	Fe–N–B	25, 29*, 145
Fe–C–Ca	20	Fe–N–C	*129**, 135, *141**, *144**, 146, *147**, *148*, 149
Fe–C–Co	34, 43, 44, *45*, 46	Fe–N–Co	107, *135*, 144, 150
Fe–C–Cr	11, *34*, 45, *47*, *48*, 49*, 50, *51*, 52	Fe–N–Cr	41, *129**, *134*, 135, 144, 146, 150, *151**, 152*, *153**, *154*
Fe–C–Cu	34, 43, *53*, 54, 55	Fe–N–Cu	*135*, 144
Fe–C–Ge	56	Fe–N–Mn	133, *135*, *144*, 146, *148*, *152**, 153*, *155*, 156
Fe–C–Mg	27	Fe–N–Mo	*130**, *133*, *135*, 144, *150*, 154
Fe–C–Mn	37, 57*, 58*, 59	Fe–N–Nb	*135*, *154*, 157*, 158
Fe–C–Mo	34, 43, *44*, *45*, 46, 55	Fe–N–Ni	*130**, *134*, *135*, *144*, 146, 150, 152*, *153**, *154*
Fe–C–Nb	34, 46	Fe–N–O	*132*, *135*, 139*, 143, 144, 159*, 160
Fe–C–Ni	34, 43, 44, 45, 47, 48, 60	Fe–N–P	*129**, *144*
Fe–C–O	32, *36**, 37, 40, *41*, 61, 62, 63, 64, *65*, 66	Fe–N–S	144, *160*
Fe–C–P	*11*, 37, 50, 60, 67, 68	Fe–N–Sb	*144*
Fe–C–Pb	21, 22, 69	Fe–N–Se	132, *160*
Fe–C–S	34, 37, *41*, 60, *70**, *71**, *72*, 73	Fe–N–Si	41, *132*, 133, *135*, 144, 147, *148*, *154*, 159*, 161*, 162*
Fe–C–Si	23, *41*, 48, *73*, 74, 75, *76**, 77, *78**, 79, 80	Fe–N–Sn	*135*, 144
Fe–C–Sn	34, *43**, 54, *60**	Fe–N–Ta	*135*, 157*
Fe–C–Ta	46	Fe–N–Te	*160*
Fe–C–V	34, 44, *45*, 46	Fe–N–Ti	139, 142*, 143, *157**, 163
Fe–C–W	34, 43, 44, *46*, 55	Fe–N–V	*41*, *130**, *135*, *137**, 142, *144*, 150, 151*, *157**
Fe–Ca	20, *81*	Fe–N–W	*135**
Fe–Ca–Ni	20, *81*	Fe–N–Zr	*157*
Fe–Ca–Si	20	Fe–Nb	*158**
Fe–Co	*82**	Fe–Ni	82*, 88, 89*, *164**, *165**
Fe–Co–Cr	83	Fe–Ni–Pb	21, 22, 69
Fe–Co–Pb	21, 22	Fe–Ni–Si	*166** *167*
Fe–Cr	*11**, 50, 84*, *85**, 86, 87*, 88, 89*	Fe–O	*168*, *169*, *170**, 171, 172, 173
Fe–Cr–Cu	54, 83	Fe–O–Al	2, *14*, *19**, 41, 174, 175, 176, 177*
Fe–Cr–Mo	83	Fe–O–Au	*168*, 178
Fe–Cr–Ni	83, *88*, 89	Fe–O–B	28
Fe–Cr–Pb	21, 22	Fe–O–Ce	249
Fe–Cr–Si	83*, 90, *91**	Fe–O–Co	46, *168*, 171, *179*, 180, *181*, 182*, *247*
Fe–Cr–Sn	54	Fe–O–Cr	14, 48, 52, 85, *171*, 174, 177, 179, *183**, 184, *185*, *186*, 187, 188, 246
Fe–Cr–Ti	90	Fe–O–Cu	168, *181*, 189
Fe–Cu	16, 53, 92, 93*, 94*	Fe–O–La	249
Fe–Cu–Pb	21, 22	Fe–O–Mn	37, 41, 173, *187*
Fe–Cu–Si	53, *54*	Fe–O–Mo	46, *168*, 171, 190
Fe–Ge	*56**	Fe–O–Nb	46, *191*
Fe–H	95, 96	Fe–O–Ni	47, *171*, *179*, 180, *181*, 182*, *185*, *192**, 193*, *194*, 247
Fe–H–Al	95, 97, 98, 99	Fe–O–P	37, 41, 64, 67, 195, 196, *197*, 198, 199*
Fe–H–B	95, 100	Fe–O–Pd	200
Fe–H–C	95, 99, 101 102, *103*, *104* 105	Fe–O–Pt	*168*, 201
Fe–H–Ce	106*	Fe–O–Rh	200
Fe–H–Co	95, 98, 99, 102, 105, 107, 108, 109, 110, 111	Fe–O–S	37, 64, 202*, 203*, 204
Fe–H–Cr	95, *97*, 99, 102, 105, 108, *110*, 111, *112*, 113, 114	Fe–O–Sb	186
Fe–H–Cu	95, *98*, 105, 111	Fe–O–Si	48, 65, 205, 206, 207, 208, 209*
Fe–H–Ge	95, 111	Fe–O–Sn	*171*, 186
Fe–H–La	106*	Fe–O–Ti	19*, 90, 210, 211, 212, 213
Fe–H–Mn	95, 98, 99, 111	Fe–O–V	28, 46, 174, *179*, 186, *187*, 214, 215, 216
Fe–H–Mo	97, 99, *102*, 105, 108, 110, 111, *112*, *114*	Fe–O–W	46, *168*, 171, *186*, 190
Fe–H–Nb	95, *105*, 110, 111, *115**	Fe–O–Zr	249
Fe–H–Nd	106*	Fe–P	*11*, 50, 217, 218, 219, 220, 221
Fe–H–Ni	95, 96, 98, 99, *101*, 102, *105*, *107*, *109*, 110, 111, 113, *116*, *117*	Fe–P–Cr	*11*, 50, 83, *222*
Fe–H–O	99, 118	Fe–P–Cu	*54*
Fe–H–P	95, *101*, *105*, 110	Fe–P–Mn	*222*
Fe–H–Pd	111, *119*	Fe–S–Mn	*70*, 72, 73, 236*
Fe–H–Rh	111, *119*		
Fe–H–S	95, 97		

TABLE IV cont.

Reference Numbers for Interaction Coefficients Used in this Study

System	References	System	References
Fe–S–Mo	72	Fe–P–Ni	222
Fe–S–Nb	72	Fe–P–Pb	21, 22
Fe–S–Ni	72, 73, 229, 230	Fe–P–S	41, 70, 72, 73
..Fe–S–Pb	21, 22	Fe–P–Si	166*, 221
Fe–S–Pt	72	Fe–P–Sn	54
Fe–S–Sb	72	Fe–Pb–Si	21, 22
Fe–S–Si	70, 71, 72, 73, 227*	Fe–Pb–Sn	21, 22
Fe–S–Sn	54, 72	Fe–Pb–W	21, 22
Fe–S–Ta	72	Fe–Pd	224
Fe–S–Ti	72	Fe–S	27, 70*, 72, 225, 226*, 227, 228*, 229, 230*,
Fe–S–V	72		231, 232
Fe–S–W	72, 237	Fe–S–Al	70*, 72, 73
Fe–S–Zr	72	Fe–S–As	72
Fe–Si	16, 23, 41, 65, 75*, 76, 78, 79*, 92, 205, 206,	Fe–S–Au	72
	207, 209*, 238*, 239*, 240, 241*, 242, 243, 248	Fe–S–B	72
Fe–Si–Sn	54	Fe–S–Co	72, 230*
Fe–Si–V	215, 248	Fe–S–Cr	72, 223, 233*, 234
Fe–Sn	54, 244	Fe–S–Cu	41, 70*, 72, 73, 235
Fe–Ti	19, 213, 245	Fe–S–Ge	72
Fe–U	24		
Fe–V	28, 214		

Italicized numbers indicate principal references used in selecting data reported in Tables I–III.
* Present authors have calculated, or recalculated, interaction coefficients from data given.

TABLE V

Behaviour of Elements at Infinite Dilution in Liquid Iron

Element, i†	$\gamma_i{}^0(1873)$*	M (pure) = M($i.d.$, X, liq.) $\Delta G(x)$, cal/g atom	M (pure) = M($i.d.$, wt.-%, liq.) $\Delta G(\%)$, cal/g atom	Ref. and Notes
Ag (l)	200	19 700	19 700 − 10·46T	11, 2; from solubility data, regular solution is assumed.
Al (l)	0·029	−15 100 + 1·03T	−15 100 − 6·67T	19
B (s)	0·022	−15 600 + 0·71T	−15 600 − 5·15T	29: from solubility of BN, using values for nitrogen given below.
C (gr)	0·57	5 400 − 4·0T	5 400 − 10·1T	42, 2
Ca (v)	2240	− 9 430 + 20·3T	− 9 430 + 11·8T	20; from solubility data, regular solution is assumed.
Co (l)	1·07	240	240 − 9·26T	82, 2; regular solution is assumed.
Cr (l)	1·0	0	− 9·01T ⎫	87, 86, 88, 89; liquid Fe–Cr alloys ideal at
Cr (s)	1·14	4 600 − 2·19T	4 600 − 11·20T ⎬	low Cr concentration.
Cu (l)	8·6	8 000	8 000 − 9·41T	93, 2
1/2 H₂ (g)	—	—	8 720 + 7·28T	95, 96, 2; $\Delta G°$(ppm) = 8,720−11·02T
Mn (l)	1·3	976	976 − 9·12T	125, 126, 2
Mo (l)	1	0	− 10·23T	Ideal behaviour assumed.
Mo (s)	1·86	6 600 − 2·29T	6 600 − 12·52T	Ideal behaviour of liquid solution, transfer of standard state.
1/2 N₂ (g)	—	—	860 + 5·71T	135
Nb (l)	1·0	0	− 10·2 ⎫	See Mo above.
Nb (s)	1·4	5 500 − 2·3T	5 500 − 12·5 ⎬	
Ni (l)	0·66	− 5 000 + 1·80T	− 5 000 − 7·42T	164, 2
1/2 O₂ (g)	—	—	−28 000 − 0·69T	168
1/2 P₂ (g)	—	—	− 29 200 − 4·6T	218
Pb (l)	1400	50 800 − 12·7T	50 800 − 25·4T	21; calculated from data on solubility.
1/2 S₂ (g)	—	—	−32 280 + 5·6T	72
Si (l)	0·0013	−31 430 + 3·64T	−31 430 − 4·12T	16, 243
Sn (l)	2·8	3 820	3 820 − 10·62T	244; regular solution assumed.
Ti (l)	0·037	−11,100	−11 000 − 8·85T	19; regular solution assumed.
Ti (s)	0·038	− 7 440 − 1·90T	− 7 440 − 10·75T	19
U (l)	0·027	−13 400	−13 400 − 12·0T	24; regular solution assumed.
V (l)	0·08	−10 100 + 0·37T	−10 100 − 8·6T ⎫	28
V (s)	0·1	− 4 950 − 1·93T	− 4 950 − 10·9T ⎬	
W (l)	1	0	− 11·5T ⎫	Assumed ideal liquid solution.
W (s)	1·2	+ 7 500 − 3·65T	+ 7 500 − 15·2T ⎬	
Zr (l)	0·037	−12 200	−12 200 − 10·13T ⎫	$\gamma°_{Zr}$ assumed equal to $\gamma°_{Ti_{ij}}$,
Zr (s)	0·043	− 8 300 − 1·82T	− 8 300 − 11·95T ⎬	and regular solution assumed.

* $\gamma_i{}^0 = \dfrac{\lim}{X_i \to 0} a_i/X_i$

† The letters in parentheses indicate the standard states used. All are of one atmosphere pressure.

1 cal = 4·18 J