Corrected Values for Boiling Points and Enthalpies of Vaporization of Elements in Handbooks

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The scientific community relies upon the veracity of the scientific data in handbooks and databases. In a previous work, the authors developed a systematic, intelligent, and potentially automatic method to detect errors in such resources based on artificial neural networks (ANNs). This method revealed variations from (10 to 900) % in tables of property data for elements in the periodic table and pointed out the ones that are most probably correct. In this paper, we focus on the details of employing this method for analyzing the data of boiling points and enthalpies of vaporization recorded in different handbooks. The method points out the values that are likely to be correct. To verify the method employed, a detailed discussion of the data with reference to the original literature sources is given as well as factors that may affect the accuracy of the prediction.

Introduction

It is well-known that both the boiling point and the enthalpy of vaporization are important thermodynamic properties that are required in product design and processes involving liquid and vapor phase transitions such as distillation, vaporization, and drying[1−3] and that, as a result, the quality and veracity of these data in handbooks are important for the academic and industrial scientific community.[4] However, it is accepted that errors in handbooks and databases are inescapable and are anticipated at rates of (1 to 5) %.[5−7]

This work challenges the inevitability of such high error rates. The values of boiling point and enthalpy of vaporization of the elements were recorded for testing, because these data are expected to be very reliable; only the elements with short half-lives were excluded. Tables 1 and 2 show the boiling point and enthalpy of vaporization values of elements in the periodic table taken from five different handbooks. Considerable variation in the values can be noticed, so it can be concluded that inconsistencies are extant within these handbooks, and these inconsistencies have persisted undetected into the 21st century.

In the authors' related work,[8] we developed a systematic and intelligent method based on artificial neural networks (ANNs) to detect wide levels of inconsistencies in handbooks and so stop their transmission to future researches and documents. In this paper, we are going to show the details of application of this method in the case of correcting values of the boiling point and enthalpy of vaporization for the elements.

Experimental Details

Data Collection and Neural Network Construction. The data are recorded from five different handbooks, including the *Chemistry Data Book* (CDB),[9] *The Lange's Handbook of Chemistry* (LAG),[10] *The Elements* (ELE),[11] *Table of Physical and Chemical Constants* (TPC),[12] and *CRC Handbook of Chemistry and Physics* (CRC).[13] The neural networks are constructed, trained, and simulated by employing MATLAB 7.4.0.287 (R2007a) software. A two-hidden layer network with tan-sigmoid transfer function in the first hidden layer and a linear transfer function in the second hidden layer was established. A loop program was applied to redistribute the database to make the training set cover the problem domain.[14,15] The detailed process of data collection and neural network construction has been described in the authors' related works.[8] The ANN finds indirect relationships between data sets and then identifies values which disobey the relationship.

Stages of Error Correction. This includes four different stages.

Stage 1. During the exploration of the indirect relationship between boiling point and enthalpy of vaporization using data from CDB (shown in Table 3) by an ANN, best linear fit equations with a regression coefficient of $R = 0.973$ and 0.972 were found (as shown in Figure 1). This result prompts us to raise the correlation hypothesis that the correlation applies to all of the elements.

Stage 2. In this stage, a conformity criterion is selected. On the basis of the inconsistency within different handbooks,

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Table 1. List of Boiling Points Divided by Kelvin from Five Handbooks[a]

element	CDB	LAG[b]	ELE	TPC	CRC	(max/min − 1)·100 %
Ag[c]	2483	2483	2485	2433	2435	2.14 %
Al[c]	2743	2743	2740	2793	2792	1.93 %
Ar	87.15	87.15	87.29	87.29	87.3	0.17 %
As (gray)[d]	886.2	886.2	889	883.2	876.2	1.46 %
Au	3243	3243	3080	3123	3129	5.29 %
Ba[e]	1913	1913	1910	2173	2170	13.80 %
Be[e]	2750	2750	3243[f]	2743	2744	18.20 %
B[c]	4203	4203	3931	4273	4273	8.70 %
Bi[c]	1833	1833	1883	1833	1837	2.73 %
Br	331.7	332	331.9	332.1	332	0.12 %
C (graphite)[e]	5103	5103	5100[d]	-	4098[d]	24.50 %
Ca	1760	1760	1757	1757	1757	0.17 %
Cd	1038	1038	1038	1043	1040	0.48 %
Ce[c]	3743	3743	3699	3693	3716	1.35 %
Cl	238.5	238.5	239.2	239.2	239.1	0.29 %
Co	3173	3173	3143	3203	3200	1.91 %
Cr	2755	2755	2945	2943	2944	6.90 %
Cs	963.2	963.2	951.6	943.2	944.2	2.12 %
Cu	2868	2868	2840	2833	2835	1.24 %
Dy	2873	2873	2835	2833	2840	1.41 %
Er	3173	3173	3136	3133	3141	1.28 %
Eu	1713	1713	1870	1873	1802	9.34 %
F	85.15	85.15	85.01	85.05	85.03	0.16 %
Fe	3273	3273	3023	3133	3134	8.27 %
Ga	2673	2673	2676	2473	2477	8.21 %
Gd	3273	3273	3539	3533	3546	8.34 %
Ge	3103	3103	3103	3103	3106	0.10 %
H	21.15	21.15	20.28	20.28	20.28	4.29 %
He	4.15	4.15	4.216	4.37	4.22	5.30 %
Hf[g]	5673	5673	5470	4873	4876	16.40 %
Hg	630.2	630.2	629.7	629.8	629.9	0.08 %
Ho[c]	2873	2873	2968	2973	2973	3.48 %
I (I_2)[c]	457.2	457.2	457.5	457.2	457.6	0.09 %
In	2273	2273	2353	2343	2345	3.52 %
Ir[g]	5573	5573	4403	4703	4701	26.60 %
K	1047	1047	1047	1033	1032	1.45 %
Kr[c]	121.2	121.2	120.9	120	119.9	1.08 %
La	3743	3743	3730	3733	3737	0.35 %
Li	1603	1603	1620	1613	1615	1.06 %
Lu	3603	3603	3668	3663	3675	2.00 %
Mg	1383	1383	1363	1363	1363	1.47 %
Mn	2373	2373	2235	2333	2334	6.17 %
Mo[g]	5833	5833	4885	4913	4912	19.40 %
N	77.15	77.15	77.4	77.35	77.36	0.32 %
Na[c]	1163	1163	1156	1153	1156	0.87 %
Nb[e]	3573	3573	5015	4973	5017	40.40 %
Nd	3303	3303	3341	3343	3347	1.33 %
Ne	27.15	27.15	27.1	27.07	27.07	0.30 %
Ni[b]	3003	3003	3005	3263	3186	8.66 %
O	90.15	90.15	90.19	90.19	90.2	0.06 %
Os[c]	5273	5273	5300	5273	5285	0.51 %
P (white)[c]	553.2	553.2	553	550.2	553.7	0.64 %
Pb	2017	2017	2013	2023	2022	0.50 %
Pd[e]	4253	4253	3413	3233	3236	31.60 %
Pr[e]	3403	3403	3785	3783	3793	11.50 %
Pt[b,h]	4803	4803	4100	4093	4098	17.40 %
Rb	961.2	961.2	961	963.2	961.2	0.23 %
Re[c]	5903	5903	5900	5873	5869	0.58 %
Rh[e]	4773	4773	4000	3973	3968	20.30 %
Ru[h]	5173	5173	4173	4423	4423	24.00 %
S (monoclinic)[c]	718.2	718.2	717.8	717.8	717.8	0.06 %
Sb[g]	1653	1653	1908	1860	1860	15.40 %
Sc	3003	3003	3104	3103	3109	3.53 %
Se[c]	958.2	958.2	958.1	958.2	958.2	0.01 %
Si[g]	2633	2633	2628	3533	3538	34.60 %
Sm[c]	2173	2173	2064	2063	2067	5.33 %
Sn[e]	2543	2543	2543	2893	2875	13.80 %
Sr	1653	1653	1657	1653	1655	0.24 %
Ta	5693	5693	5698	5833	5731	2.46 %
Tb[g]	3073	3073	3396	3493	3503	14.00 %
Te[c]	1263	1263	1263	1263	1261	0.16 %
Ti	3533	3533	3560	3563	3560	0.85 %
Tl	1733	1733	1730	1743	1746	0.92 %
Tm[e]	2003	2003	2220	2223	2223	11.00 %
V[e]	3273	3273	3650	3673	3680	12.40 %
W	6203	6203	5930	5823	5828	6.53 %

Table 1. Continued

element	CDB	LAG[b]	ELE	TPC	CRC	(max/min − 1)·100 %
Xe	165.2	165.2	166.1	165.1	165	0.67 %
Yb[e]	1703	1703	1466	1473	1469	16.20 %
Y[e]	3203	3203	3611	3613	3618	13.00 %
Zn	1180	1180	1180	1183	1180	0.25 %
Zr[g]	3853	3853	4650	4673	4682	21.50 %

[a] Acronyms as in text. This table does not have exclusions based on judgement. The elements are in alphabetical order. [b] The boiling point is different in different tables of LAG. For example, nickel (Ni) is 2884 °C in page 1.43 (Table 1.3) and 2730 °C in page 1.125 (Table 1.19). We selected most of the boiling points from the later table. [c] Category I: the data of the boiling point for these elements are consistent in different handbooks, but those of the enthalpy of vaporization are not. [d] Sublimation. [e] Category II: the data of the enthalpy of vaporization for these elements are consistent in different handbooks, but those of the boiling point are not. [f] Under pressure. [g] Category III: the data of neither the boiling point nor the enthalpy of vaporization for these elements are consistent in different handbooks. [h] The variation of boiling points of Pt and Ru are greater than 10 %, but here due to shortage of data in range of (3603.15 to 5693.15) K in category IV, they were classified into category IV by identifying the closest value from the literature to reduce the uncertainty in that range.[30,31]

elements were then classified into four different categories based on a 10 % variation between minimum and maximum values:

I. Boiling points of the elements are consistent, but enthalpies of vaporization are inconsistent (shown in Table 4).

II. Enthalpies of vaporization are consistent, but boiling points are inconsistent (shown in Table 5).

III. Both boiling points and enthalpies of vaporization are inconsistent (shown in Table 6).

IV. Both boiling points and enthalpies of vaporization are consistent (shown in Table 7).

Stage 3. We then use the data belonging to category IV to train a second set of ANNs: ANN1 and ANN2. ANN1 is used to predict enthalpies of vaporization from boiling points, while ANN2 is used to predict boiling points from enthalpies of vaporization. Here, ANN1 and ANN2 discover and capture an indirect correlation between just two properties from category IV data set, but this method can be applied in any situation when the correlations between several properties can be captured by ANNs.[8] We now suppose these two ANNs to have been trained on "consistent" data providing a robust correlation against which the consistency of other data can be judged. The details of construction for these two ANNs can be found in the authors' related work.[8]

Stage 4. Consistent values are now used to identify inconsistent data. At first, the ANN1 was used to predict enthalpies of vaporization of elements in category I using the consistent boiling points; then the outputs are compared with the handbook data to isolate suspect data for the enthalpy of vaporization. For example, Al has consistent boiling point values from (2740 to 2793) K (1.9 % difference) in all of the handbooks consulted, but enthalpies of vaporization vary from (29 to 294) $\mathrm{kJ \cdot mol^{-1}}$ (910 % difference). The ANN-predicted enthalpy of vaporization is 281 $\mathrm{kJ \cdot mol^{-1}}$, which is close to one handbook value, 284 $\mathrm{kJ \cdot mol^{-1}}$ (CDB). The difference between the predicted and the closest literature value is now 1.2 %.

The second part of stage 4 is to use the consistent enthalpies of vaporization as input values in ANN2 to predict boiling points of elements in category II for isolating suspect boiling point data.

In the third part of stage 4, for the data in category III, a method to calculate a comprehensive minimum of difference was constructed.[8]

Results and Discussion

In the first part of stage 4, the ANN1 is able to point out the correct enthalpies of vaporization from the inconsistent values from different handbooks. Most of the differences (11 out of 16, including Na, Al, B, Os, Kr, Ag, Te, Bi, Re, Ce, and Sm) between the predicted and the closest recorded values of enthalpy of vaporization are now less than 10 %. The results of this stage are listed in Table 8. The average error for enthalpy of vaporization in category I decreased from 231 % (Table 4) to 8.8 % (Table 8). Inconsistencies for another five elements (I, P (white), Se, Ho, S) have decreased dramatically as well but are still slightly greater than 10 %. That could be because none of the data in the handbooks was correct but that the ANN gave a correct estimate. Those five elements will be discussed later.

In the second part of stage 4, in a similar way, ANN2 is able to point out the correct boiling point from inconsistent values. Predicted and closest recorded values of boiling points for most of the samples now differ by less than 10 % (10 out of 12 elements, including Pd, Nb, Yb, Rh, Y, C (graphite), Be, Sn, V, Pr), as shown in Table 9. The average error of the boiling point in category II decreased from 18.9 % (Table 5) to 6.4 % (Table 9). Deviations of another two elements (Ba, Tm) have decreased as well but are still higher than 10 %, and these will be discussed later.

In the last part of stage 4, both ANN1 and ANN2 are used to point out the correct enthalpies of vaporization and boiling point of those elements (Tb, Hf, Ir, Mo, Sb, Si, and Zr). The predicted and closest recorded values for both boiling point and enthalpies of vaporization for category III now differ by less than 10 % (Table 10).

Finally, after the correction made for data in category I, category II, and category III, two new ANNs were trained with the "corrected" values inserted (shown in Table 11), and the results are shown in Figure 2. For forward and backward predictions, respectively, statistics are given in the third and fourth rows of Table 12. To make the comparison, the statistical analysis for Figure 1 is shown in the first and second row of Table 12. After correction, the moduli have decreased dramatically.

In this method, all that is required is a sufficient correlation, which can itself be established by the ANNs that are then employed to discriminate between the majority of well-correlated data points and an outlying minority. Further, more than two properties can be correlated, and the details of the procedures for doing so have been discussed.[8] It also needs to be pointed out that the "consistent" data in all handbooks does not necessarily mean they are "correct". However, the ANN could detect them if they do not follow the trend. It is arguable that the term "outlier" should not be used to justify a predictive replacement, for it is often the case that unusual results are indicators of new knowledge.[16]

It needs to be pointed out that the boiling point and enthalpy of vaporization are *indirectly* related based on the Clausius−Clapeyron equation $(\mathrm{d}P_{\mathrm{vap}}/\mathrm{d}T) = (\Delta_{\mathrm{vap}}H_{\mathrm{m}})/(T\Delta V_{\mathrm{vap}}) = (\Delta_{\mathrm{vap}}H_{\mathrm{m}})/((RT^2/P_{\mathrm{vap}})\Delta Z_{\mathrm{vap}})$, which in its integrated form gives $P_{\mathrm{vap}} = i$

Table 2. List of Enthalpies of Vaporization Divided by kJ·mol^{-1} from Five Handbooks[a]

element	CDB	LAG	ELE	TPC	CRC	(max/min − 1)·100 %
Ag[b]	254	258	255	25.5	-	912 %
Al[b]	284	294	294	29.1	294	910 %
Ar	6.53	6.43	6.53	6.52	6.43	1.56 %
As (gray)	32.4	-	31.9	-	-	1.57 %
Au	342	324	324	324	324	5.56 %
Ba[c]	149	140	151	140	140	7.86 %
Be[c]	309	297	309	298	-	4.04 %
B[b]	540	480	539	508	480	12.50 %
Bi[b]	179	151	179	187	151	23.80 %
Br	30	30	30	29.6	30	1.35 %
C (graphite)[c]	715	-	711	-	-	0.56 %
Ca	153	155	150	155	-	3.33 %
Cd	100	99.9	99.9	99.9	99.9	0.10 %
Ce[b]	-	398	314	314	-	26.80 %
Cl	20.4	20.4	20.4	20.4	20.4	0.00 %
Co	390	377	382	373	-	4.56 %
Cr	347	340	349	340	-	2.65 %
Cs	66.1	63.9	65.9	67.8	-	6.10 %
Cu	305	300	305	301	-	1.67 %
Dy	-	280	293	-	-	4.64 %
Er	-	280	293	293	-	4.64 %
Eu	-	176	176	176	-	0.00 %
F	6.32	6.62	6.55	6.54	6.62	4.75 %
Fe	354	340	351	350	-	4.12 %
Ga	256	254	256	256	254	0.79 %
Gd	-	301.3	311.7	311.7	-	3.45 %
Ge	330	334	334	334	334	1.21 %
H	0.9	-	0.92	0.9	0.9	2.22 %
He	0.084	0.083	0.082	0.08	0.08	5.00 %
Hf[d]	648	571	661	661	-	15.80 %
Hg	58.2	59.1	59.2	59.1	59.1	1.72 %
Ho[b]	-	71	251	251	-	254 %
I (I_2)[b]	22	41.6	41.7	41.9	41.6	90.50 %
In	225	232	226	226	-	3.11 %
Ir[d]	636	232	564	564	-	174 %
K	79.1	76.9	77.5	76.9	-	2.86 %
Kr[b]	10	9.08	9.05	9.03	9.08	10.70 %
La	400	402	400	400	-	0.50 %
Li	136	147	135	147	-	8.89 %
Lu	-	414	428	-	-	3.38 %
Mg	132	128	129	128	-	3.13 %
Mn	225	221	220	220	-	2.27 %
Mo[d]	536	617	594	590	-	15.10 %
N	5.58	5.57	5.58	5.59	5.57	0.36 %
Na[b]	101	97.4	89	97.4	-	13.50 %
Nb[c]	694	690	697	690	-	1.01 %
Nd	-	289	284	284	-	1.76 %
Ne	1.8	1.71	1.74	1.77	1.71	5.26 %
Ni	379	378	372	378	-	1.88 %
O	6.82	6.82	6.82	6.82	6.82	0.00 %
Os[b]	678	738	628	628	-	17.50 %
P (white)[b]	12.4	12.4	51.9	-	12.4	319 %
Pb	177	180	179	178	180	1.69 %
Pd[c]	380	362	393	393	-	8.56 %
Pr[c]	-	331	333	333	-	0.60 %
Pt	510	469	511	511	-	8.96 %
Rb	69	75.8	69.2	69.2	-	9.86 %
Re[b]	636	704	707	707	-	11.20 %
Rh[c]	531	494	495	495	-	7.49 %
Ru	619	592	568	568	-	8.98 %
S (monoclinic)[b]	10	45	9.62	-	45	368 %
Sb[d]	195	193	67.9	67.9	-	187 %
Sc	310	333	305	305	-	9.18 %
Se[b]	14	95.5	26.3	26.3	95.5	582 %
Si[d]	300	359	383	359	-	27.70 %
Sm[b]	-	165	192	192	-	16.40 %
Sn[c]	290	296	290	290	-	2.07 %
Sr	141	137	139	137	-	2.92 %
Ta	753	733	753	737	-	2.73 %
Tb[d]	-	293	391	-	-	33.50 %
Te[b]	49.8	114	50.6	50.6	114	129 %
Ti	427	425	429	425	-	0.94 %
Tl	162	165	162	162	-	1.85 %
Tm[c]	-	247	247	-	-	0.00 %
V[c]	444	459	459	447	-	3.38 %
W	774	807	799	806	-	4.26 %

Table 2. Continued

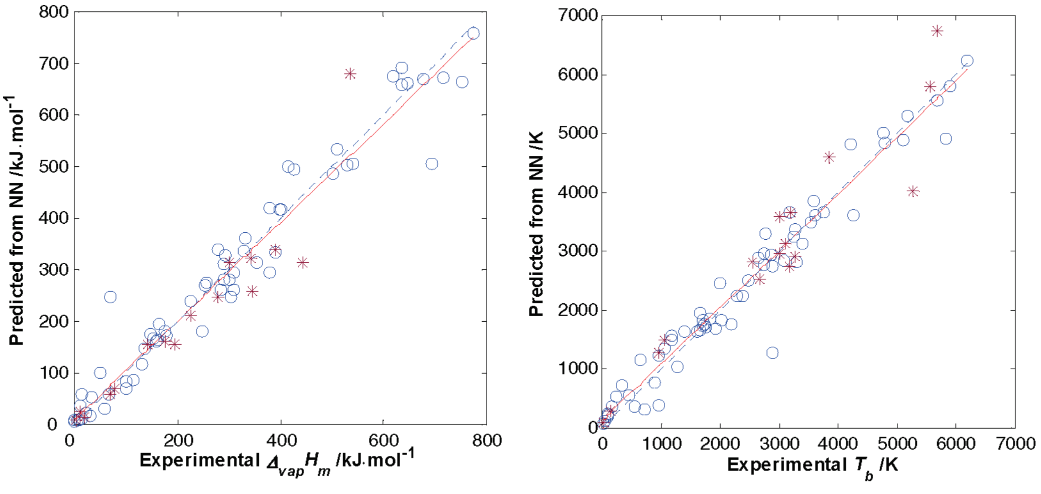
element	CDB	LAG	ELE	TPC	CRC	(max/min − 1)·100 %
Xe	12.6	12.6	12.7	12.6	12.6	0.79 %
Yb[c]	-	159	159	-	-	0.00 %
Y[c]	390	365	393	393	-	7.67 %
Zn	115	124	115	115	-	7.83 %
Zr[d]	502	573	582	591	-	17.70 %

[a] Acronyms as in text. This table does not have exclusions based on judgement. The elements are sorted in alphabetical order. [b] Category I: the data for the boiling point for these elements are consistent in different handbooks, but those for the enthalpy of vaporization are not. [c] Category II: the data for the enthalpy of vaporization for these elements are consistent in different handbooks, but those of the boiling point are not. [d] Category III: the data for neither the boiling point nor the enthalpy of vaporization for these elements are consistent in different handbooks.

Table 3. Data Set First Used to Train the ANNs Shown in Figure 1[a]

element	T_b K	$\Delta_{vap}H_m$ kJ·mol^{-1}	element	T_b K	$\Delta_{vap}H_m$ kJ·mol^{-1}	element	T_b K	$\Delta_{vap}H_m$ kJ·mol^{-1}
Ag	2483	254	H	21.15	0.90	Pr	3403	331
Al	2743	284	He	4.150	0.08	Pt	4803	510
Ar	87.20	6.53	Hf	5673	648	Rb	961.2	69.0
As (gray)	886.2	32.4	Hg	630.2	59.1	Re	5903	636
Au	3243	342	Ho	2873	71.0	Rh	4773	531
B	4203	540	I (I_2)	457.2	22.0	Ru	5173	619
Ba	1913	149	In	2273	225	S (mono.)	718.2	10.0
Be	2750	309	Ir	5573	636	Sb	1653	195
Bi	1833	179	K	1047	79.1	Sc	3003	310
Br	331.7	30.0	Kr	121.2	9.04	Se	958.2	14.0
C (graphite)	5103	715	La	3743	400	Si	2633	300
Ca	1760	153	Li	1603	136	Sm	2173	165
Cd	1038	100	Lu	3603	414	Sn	2543	290
Ce	3743	398	Mg	1383	132	Sr	1653	141
Cl	238.5	20.4	Mn	2373	225	Ta	5693	753
Co	3173	390	Mo	5833	536	Tb	3073	293
Cr	2755	347	N	77.15	5.58	Te	1263	49.8
Cs	963.2	66.1	Na	1163	101	Ti	3533	427
Cu	2868	305	Nb	3573	694	Tl	1733	162
Dy	2873	280	Nd	3303	289	Tm	2003	247
Er	3173	280	Ne	27.15	1.80	V	3273	444
Eu	1713	176	Ni	3003	379	W	6203	774
F	85.15	6.32	O	90.15	6.82	Xe	165.2	12.6
Fe	3273	354	Os	5273	678	Y	3203	390
Ga	2673	256	P (white)	553.2	12.4	Yb	1703	159
Gd	3273	301	Pb	2017	177	Zn	1180	115
Ge	3103	330	Pd	4253	380	Zr	3853	502

[a] The majority were taken from the Chemistry Data Book (CDB) without judgement. A few data unavailable in CDB were taken from LAG and ELE. (T_b: boiling point; $\Delta_{vap}H_m$: enthalpy of vaporization).



(a) (b)

Figure 1. Prediction of (a) enthalpy of vaporization ($\Delta_{vap}H_m$) from boiling point (T_b), $R = 0.973$; (b) boiling point (T_b) from enthalpy of vaporization ($\Delta_{vap}H_m$), $R = 0.972$; using data from CDB, LAG, and ELE. ○, training data points; ∗, test data points; —, best linear fit; ----, exp. = prediction.

exp[($\Delta_{vap}H_m$)/(RT)], and the boiling point is the temperature at which P_{vap} reaches ambient (i is a constant of integration).[17] The pre-exponential coefficient is not directly related. The ANN can find clusters of properties that are indirectly related in this way to identify suspect data.

Verification of the Method by Referring to Original Sources. To verify the method, original sources were consulted where possible to (1) check whether the refined values were sensible, (2) to reveal and analyze the origin of the differences between handbook data, and (3) to find whether the neural

Table 4. List of Category I Elements: Boiling Points of the Elements Are Consistent, but Enthalpies of Vaporization Are Inconsistent

	T_b	$\Delta_{vap}H_m/kJ\cdot mol^{-1}$					
element	K	CDB	LAG	ELE	TPC	CRC	(max/min − 1)·100 %
Ag	2483	254	258	255	25.5	-	912 %
Al	2743	284	294	294	29.1	294	910 %
B	4203	540	480	539	508	480	12.5 %
Bi	1833	179	151	179	187	151	23.8 %
Ce	3743	-	398	314	314	-	26.8 %
Ho	2873	-	71	251	251	-	254 %
I (I_2)	457.2	22	41.6	41.7	41.9	41.6	90.5 %
Kr	121.2	10	9.08	9.05	9.03	9.08	10.7 %
Na	1163	101	97.4	89	97.4	-	13.5 %
Os	5273	678	738	628	628	-	17.5 %
P (white)	553.2	12.4	12.4	51.9	-	12.4	319 %
Re	5903	636	704	707	707	-	11.2 %
S	718.2	10	45	9.62	-	45	368 %
Se	958.2	14	95.5	26.3	26.3	95.5	582 %
Sm	2173	-	165	192	192	-	16.4 %
Te	1263	49.8	114	50.6	50.6	114	129 %
average							231 %

Table 5. List of Category II Elements: Enthalpies of Vaporization Are Consistent, but Boiling Points Are Inconsistent

	$\Delta_{vap}H_m$	T_b/K					
element	$kJ\cdot mol^{-1}$	CDB	LAG	ELE	TPC	CRC	(max/min − 1)·100 %
Ba	149	1913	1913	1910	2173	2170	13.8 %
Be	309	2750	2750	3243	2743	2744	18.2 %
C (graphite)	715	5103	5103	5100	-	4098	24.5 %
Nb	694	3573	3573	5015	4973	5017	40.4 %
Pd	380	4253	4253	3413	3233	3236	31.6 %
Pr	331	3403	3403	3785	3783	3793	11.5 %
Rh	531	4773	4773	4000	3973	3968	20.3 %
Sn	290	2543	2543	2543	2893	2875	13.8 %
Tm	247	2003	2003	2220	2223	2223	11.0 %
V	444	3273	3273	3650	3673	3680	12.4 %
Y	390	3203	3203	3611	3613	3618	13.0 %
Yb	159	1703	1703	1466	1473	1469	16.2 %
average							18.9 %

Table 6. List of Category III Elements: Both Boiling Points and Enthalpies of Vaporization Are Inconsistent

	T_b/K					$\Delta_{vap}H_m/kJ\cdot mol^{-1}$				
element	CDB	LAG	ELE	TPC	CRC	CDB	LAG	ELE	TPC	CRC
Tb	3073	3073	3396	3493	3503	-	293	391	-	-
Hf	5673	5673	5470	4873	4876	648	571	661	661	-
Ir	5573	5573	4403	4703	4701	636	232	564	564	-
Mo	5833	5833	4885	4913	4912	536	617	594	590	-
Sb	1653	1653	1908	1860	1860	195	193	67.9	67.9	-
Si	2633	2633	2628	3533	3538	300	359	383	359	-
Zr	3853	3853	4650	4673	4682	502	573	582	591	-

network can give values closer to the original literature. Some errors are quickly attributable to incorrect unit conversions or to misplaced decimal points, but some arise from different reference conditions, and representative examples are shown below.

Table 8 indicates that predicted and closest recorded values of enthalpy of vaporization for most elements differ by less than 10 % after removal of incorrect data. The exceptions are I (15.6 %), P (17.2 %), Se (17.9 %), Ho (19.1 %), and S (26.7 %). Data for elements I, P, and S depend on the polyatomic nature of these molecules; this accounts for the differences shown in Table 2, but handbooks do not always state how the value is normalized. Because I, P, and S exist in polyatomic molecular forms, the values for polyatomic forms should be clarified. From Table 8, it is seen that the neural networks have a capability to locate values which are in the right magnitude, although the difference is still greater than 10 %. However, the values for Ho and Se need more detailed investigation.

Ho. The predicted enthalpy of vaporization of holmium by ANN is 299 $kJ\cdot mol^{-1}$, and the values in handbooks are 71 $kJ\cdot mol^{-1}$ (LAG), 251 $kJ\cdot mol^{-1}$ (ELE), and 251 $kJ\cdot mol^{-1}$ (TPC) (no record in CDB and CRC for Ho). If we select 251 $kJ\cdot mol^{-1}$ as a correct value, this gives a 19.1 % deviation between ANN prediction and the handbook value. From the following analysis and search of original papers, we believe the ANN prediction is more accurate than the handbook.

There are two sources of discrepancy. The first is the unit of the values. Original research papers offer the values for $\Delta_{vap}H_{m,st}$: 301 $kJ\cdot mol^{-1}$ (71910 $cal\cdot mol^{-1}$),[18] 291 k $J\cdot mol^{-1}$ (69500 $cal\cdot mol^{-1}$),[19] 314 $kJ\cdot mol^{-1}$ (75040 $cal\cdot mol^{-1}$),[20] 339 $kJ\cdot mol^{-1}$ (81150 $cal\cdot mol^{-1}$),[18] and 295 $kJ\cdot mol^{-1}$ (70600 $cal\cdot mol^{-1}$).[21] Clearly these results indicate that the enthalpy of vaporization of holmium is around 297 $kJ\cdot mol^{-1}$ (which is very close to 299 $kJ\cdot mol^{-1}$ predicted by ANN), rather than the 71 $kJ\cdot mol^{-1}$ (the number in LAG but the unit is different) recorded in LAG, and the source of error is the transcription of units. Indeed, in the earlier 12th edition of *Lange's Handbook Chemistry*,[22] the value was 251 $kJ\cdot mol^{-1}$ (60 $kcal\cdot mol^{-1}$), placing it in the correct range.

The second source of discrepancy is the reference temperature. The values from the research papers listed above are corrected to standard temperature. However, the category IV

Table 7. List of Category IV Elements: Both Boiling Points and Enthalpies of Vaporization Are Consistent

element	T_b K	$\Delta_{vap}H_m$ kJ·mol^{-1}	element	T_b K	$\Delta_{vap}H_m$ kJ·mol^{-1}
Ar	87.15	6.53	K	1047	79.1
As	886.2	32.4	La	3743	400
Au	3243	342	Li	1603	136
Br	331.7	30.0	Lu	3603	414
Ca	1760	153	Mg	1383	132
Cd	1038	100	Mn	2373	225
Cl	238.5	20.4	N	77.15	5.58
Co	3173	390	Nd	3303	289
Cr	2755	347	Ne	27.15	1.90
Cs	963.2	66.1	Ni	3003	379
Cu	2868	305	O	90.15	6.82
Dy	2873	280	Pb	2017	177
Er	3173	280	Pt	4100	510
Eu	1713	176	Rb	961.2	69.0
F	85.15	6.32	Ru	4423	619
Fe	3273	354	Sc	3003	310
Ga	2673	256	Sr	1653	141
Gd	3273	301	Ta	5693	753
Ge	3103	330	Ti	3533	427
H	21.15	0.90	Tl	1733	162
He	4.15	0.0840	W	6203	774
Hg	630.2	58.2	Xe	165.2	12.6
In	2273	225	Zn	1180	115

Table 8. List of Category I Elements with Predicted and Selected Correct Values of Enthalpy of Vaporization and Difference Percentage

element	T_b K	predicted enthalpy of vaporization kJ·mol^{-1}	selected enthalpy of vaporization kJ·mol^{-1}	difference percentage
Na	1163	97.6	97.4	0.21 %
Al	2743	281	284	1.06 %
B	4203	499	508	1.77 %
Os	5273	664	678	2.06 %
Kr	121.2	8.8	9.03	2.55 %
Ag	2483	246	254	3.15 %
Te	1263	107	114	6.14 %
Bi	1833	168	179	6.15 %
Re	5903	752	707	6.36 %
Ce	3743	427	398	7.29 %
Sm	2173	207	192	7.81 %
I_2	457.2	35.1	41.6	15.6 %
P (white)	553.2	43	51.9	17.2 %
Se	958.2	78.4	95.5	17.9 %
Ho	2873	299	251	19.1 %
S	718.2	57	45	26.7 %
average				8.81 %

Table 9. List of Category II Elements with Predicted and Selected Correct Values of the Boiling Point and Difference Percentage

element	$\Delta_{vap}H_m$ kJ·mol^{-1}	predicted boiling point K	selected boiling point K	difference percentage
Pd	380	3221	3233	0.37 %
Nb	694	5078	5017	1.22 %
Yb	159	1671	1703	1.88 %
Rh	531	4137	4000	3.43 %
Y	390	3317	3203	3.56 %
C (graphite)	715	5326	5103	4.37 %
Be	309	3100	3243	4.41 %
Sn	290	3060	2893	5.77 %
V	444	3939	3680	7.04 %
Pr	331	3081	3403	9.46 %
Ba	149	1600	1910	16.2 %
Tm	247	2655	2223	19.4 %
average				6.43 %

values used for training ANNs 1 and 2 are all referenced to the boiling point (with the exception of four elements). Values for the enthalpy of vaporization of Ho at the boiling point are available:[21,23] 280 kJ·mol^{-1} (67 kcal·mol^{-1}) and 270 kJ·mol^{-1} (64.7 kcal·mol^{-1}). These values are close to the value predicted by the ANN (which is 299 kJ·mol^{-1}), and this demonstrates the remarkable discernment of the ANN in detection of inconsistency and identification of true values.

Se. The handbook values are (14, 26.3, and 95.5) kJ·mol^{-1}, and the ANN predicts 78.4 kJ·mol^{-1} from the well-established boiling point of 958 K. The source of 95.5 kJ·mol^{-1} can be found[24] and is supported by Hultgren et al.[18] who gives a value at 625 K where, of the eight chemical allotropes for gaseous Se, Se_6 predominates.[25] The value of 13.8 kJ·mol^{-1} for atomic Se corresponds to 82.8 kJ·mol^{-1} for Se_6.[18] This may explain the handbook value of 14 kJ·mol^{-1} if that value is for atomic Se. The inconsistent handbook value of 26.3 kJ·mol^{-1} looks like a transcription of units error of Se_6 by 4.18 J·cal^{-1} (i.e., should be 26.3 kcal·mol^{-1} or 82.8 kJ·mol^{-1}). The selected value of 95.5 kJ·mol^{-1} still deviates by more than 10 % from the ANN predicted value 78.4 kJ·mol^{-1}. A possible reason for this, as discussed by Bagnall[25] and Reid et al.,[26] is associated with constants in the Clapeyron equation and is described in the following section.

Factors that Affect the Accuracy in the Prediction. In this section, the factors that affect the accuracy of prediction of boiling points and enthalpies of vaporization in this case can be identified as follows.

1. Determination of the Constant after Clausius−Clapeyron Integration. As mentioned in Reid et al.,[26] it is not easy to trace the origin of many experimental enthalpies of vaporization. A few were determined from calorimetric measurements, but in a large number of cases the values were obtained directly from Clausius−Clapeyron equation $(\mathrm{d}\ln P_{vap})/(\mathrm{d}(1/T)) = -(\Delta H_{vap})/(R\Delta Z_{vap})$, in which the ΔZ_{vap} were determined separately, and $(\mathrm{d}\ln P_{vap})/\mathrm{d}T$ was found by numerical differentiation of experimental vapor pressure data or by differentiating some $P_{vap}-T$ correlation analytically. The constants in one equation may be optimized for correlating vapor pressures, but it does not necessarily follow that these same constants give the best fit for computing slopes. For this reason, the uncertainty is present in using any analytical vapor pressure−temperature equation to obtain accurate values of slopes $(\mathrm{d}\ln P_{vap})/\mathrm{d}T$.

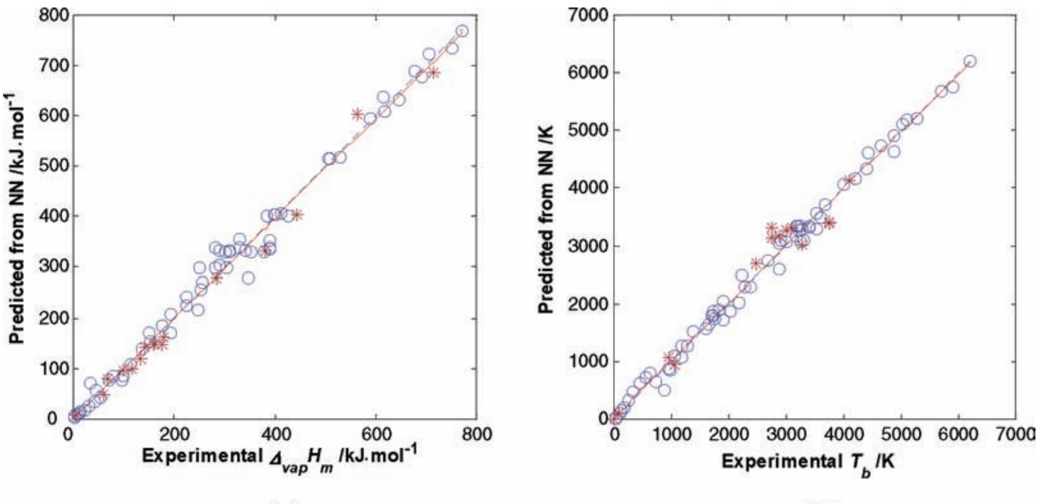
Table 10. List of Category III Elements with Predicted and Selected Correct Values and the Difference Percentage (Only the Corrected Pairs Are Shown)

element	predicted enthalpy of vaporization kJ·mol^{-1}	selected enthalpy of vaporization kJ·mol^{-1}	difference percentage	predicted boiling point K	selected boiling point K	difference percentage
Hf	604	648	6.79 %	4610	4876	5.46 %
Ir	530	564	6.03 %	4158	4403	5.56 %
Mo	605	617	1.94 %	4375	4885	10.4 %
Sb	176	193	8.81 %	1968	1908	3.14 %
Si	395	383	3.13 %	3250	3533	8.01 %
Tb	374	391	4.35 %	3328	3396	2.00 %
Zr	569	591	3.72 %	4236	4650	8.90 %

Table 11. List of "Corrected" Values (Including Data from Category IV and Corrected Category I, II, and III)

element	T_b K	$\Delta_{vap}H_m$ kJ·mol^{-1}	element	T_b K	$\Delta_{vap}H_m$ kJ·mol^{-1}	element	T_b K	$\Delta_{vap}H_m$ kJ·mol^{-1}
Ag	2483	254	H	21.15	0.9	Pr	3403	331
Al	2743	284	He	4.15	0.08	Pt	4100	510
Ar	87.15	6.53	Hf	4876	648	Rb	961.2	69
As	886.2	32.4	Hg	630.2	58.2	Re	5903	707
Au	3243	342	Ho	2873	251	Rh	4000	531
B	4203	508	I_2	457.2	41.6	Ru	4423	619
Ba	1910	149	In	2273	225	S	718.2	45
Be	3243	309	Ir	4403	564	Sb	1908	193
Bi	1833	179	K	1047	79.1	Sc	3003	310
Br	331.7	30	Kr	121.2	9.03	Se	958.2	95.5
C (graphite)	5103	715	La	3743	400	Si	3533	383
Ca	1760	153	Li	1603	136	Sm	2173	192
Cd	1038	100	Lu	3603	414	Sn	2893	290
Ce	3743	398	Mg	1383	132	Sr	1653	141
Cl	238.5	20.4	Mn	2373	225	Ta	5693	753
Co	3173	390	Mo	4885	617	Tb	3396	391
Cr	2755	347	N	77.15	5.58	Te	1263	114
Cs	963.2	66.1	Na	1163	97.4	Ti	3533	427
Cu	2868	305	Nb	5017	694	Tl	1733	162
Dy	2873	280	Nd	3303	289	Tm	2223	247
Er	3173	280	Ne	27.15	1.9	V	3680	444
Eu	1713	176	Ni	3003	379	W	6203	774
F	85.15	6.32	O	90.15	6.82	Xe	165.2	12.6
Fe	3273	354	Os	5273	678	Y	3203	390
Ga	2673	256	P (white)	553.2	51.9	Yb	1703	159
Gd	3273	301	Pb	2017	177	Zn	1180	115
Ge	3103	330	Pd	3233	380	Zr	4650	591

2. Enthalpy of Vaporization Varies with Temperature. $\Delta_{vap}H_m$ is always treated as a weak function of temperature, and an assumption is made that this value does not vary with temperature[26,27] during the integration of the Clausius–Clapeyron equation. However, it is not true for each element.[18] For some elements, the variation is narrow, such as Ga (from 258 kJ·mol^{-1} at normal boiling point to 272 kJ·mol^{-1} at room temperature, 5.2 % difference), Zr (from 58 kJ·mol^{-1} at normal boiling point to 61 kJ·mol^{-1} at room temperature, 5.0 % difference), W (from 823 kJ·mol^{-1} at normal boiling point to



(a) (b)

Figure 2. Prediction of (a) enthalpy of vaporization ($\Delta_{vap}H_m$) from the boiling point (T_b); (b) the boiling point (T_b) from the enthalpy of vaporization ($\Delta_{vap}H_m$); using "consistent" data. ○, training data points; $*$, test data points; —, best linear fit; ----, exp. = prediction. The general correlation performance has been increased, and the values of M (the slope of the linear regression line) and R are greater being $M = 0.99$, $R = 0.994$ and $M = 0.993$, $R = 0.995$ (for forward and backward predictions, respectively).

Table 12. Statistical Analysis for ANN Performance in Figures 1 and 2

	test set						whole set					
conditions	*M*	*R*	mean of error modulus	SD of error modulus	mean of percentage error modulus/%	SD of percentage error modulus/%	*M*	*R*	mean of error modulus	SD of error modulus	mean of percentage error modulus/%	SD of percentage error modulus/%
Figure 1a	0.991	0.943	38.1 $kJ\cdot mol^{-1}$	44.1 $kJ\cdot mol^{-1}$	35.4	57.2	0.96	0.973	32.4 $kJ\cdot mol^{-1}$	36.9 $kJ\cdot mol^{-1}$	114	720
Figure 1b	0.982	0.954	409 K	354 K	36.9	64.1	0.963	0.972	269 K	284 K	45.9	139
Figure 2a	0.986	0.995	18.1 $kJ\cdot mol^{-1}$	14.8 $kJ\cdot mol^{-1}$	10.1	6.38	0.99	0.994	16.7 $kJ\cdot mol^{-1}$	15.7 $kJ\cdot mol^{-1}$	48.5	308
Figure 2b	1	0.986	196 K	167 K	35.9	109	0.993	0.995	119 K	108 K	14.7	50.5

Table 13. List of Category II Elements with Predicted and Selected Correct Values of the Boiling Point and Difference Percentage (Record of Enthalpies of Vaporization under the Normal Boiling Point)

element	$\Delta_{vap}H_m$	predicted boiling point	selected boiling point	difference percentage
	$kJ\cdot mol^{-1}$	K	K	
Yb	129	1460	1466	0.41 %
Nb	682	4944	4973	0.58 %
Y	363	3111	3203	2.87 %
C (graphite)	709	5254	5103	2.96 %
Tm	191	1943	2003	3.00 %
Rh	493	4144	4000	3.60 %
Pd	358	3093	3233	4.33 %
Be	292	3068	3243	5.40 %
Sn	296	3081	2893	6.50 %
V	451	3995	3680	8.56 %
Pr	297	3084	3403	9.37 %
Ba	142	1551	1910	18.8 %
average				5.53 %

849 $kJ\cdot mol^{-1}$ at room temperature, 3.1 % difference) but for others, the variation is wide, and the value of $\Delta_{vap}H_m$ decreases with rising temperature, such as Ba (from 141 $kJ\cdot mol^{-1}$ at the normal boiling point to 182 $kJ\cdot mol^{-1}$ at room temperature, 28.7 %) and Tm (from 191 $kJ\cdot mol^{-1}$ at the normal boiling point to 232 $kJ\cdot mol^{-1}$ at room temperature, 21.7 %). The data for the enthalpy of vaporization are recorded in many handbooks in a mixed fashion without mention of the temperatures to which the values apply. This introduces uncertainties in finding the correlation and reduces the accuracy of predictions. After comparing the values in Category IV with the values recorded in *Selected Values of the Thermodynamic Properties of the Elements*,[18] which tabulates enthalpies of vaporization over a temperature range, it is found that all but four (Dy, Eu, Gd, and Lu) are recorded at the normal boiling points. Thus, Pb (Category IV), for example, has a value 175 $kJ\cdot mol^{-1}$ at the boiling point and 192 $kJ\cdot mol^{-1}$ at room temperature,[18] and we infer that 177 $kJ\cdot mol^{-1}$ is the enthalpy of vaporization at the boiling point. Thus, neural networks (ANN1 and ANN2) have found the correlation between normal boiling points and the enthalpy of vaporization under normal boiling points.

3. Clausius–Clapeyron Equation Is Not the Only Equation for Estimating Enthalpies of Vaporization. Other methods such as Pitzer's acentric factor correlation, Riedel's method, Chen's method, and Vetere's method are also used. More accurate estimates may be obtained when specific correlations are employed and demand recourse to original sources.

These factors mean that differences between predicted and corrected values cannot be avoided. The first and third factors account for small differences (< 10 %) since these just affect the accuracy of the enthalpies of vaporization. The large deviations (>10 %) may be attributed to the second factor. For Category I, the problems of the second factor do not attend the records of boiling point so the prediction of enthalpy of vaporization for these elements from the consistent boiling point can be treated as reliable. However, the second factor affects predictions for the elements in Category II; so enthalpies of vaporization used for these elements were rechecked with the values recorded in *Selected Values of the Thermodynamic Properties of the Elements*,[18] and another set of predictions based on the enthalpy of vaporization referenced to the normal boiling point was made. The results are shown in Table 13.

From the comparison of the results in Table 9 with Table 13, it can be seen that most of the boiling points are the same, except for Yb and Tm. As a result, it is interesting to analyze which prediction is more sensible.

For Yb, 159 $kJ\cdot mol^{-1}$ is the value corresponding to room temperature according to *Selected Values of the Thermodynamic Properties of the Elements* on page 564,[18] which gives 129 $kJ\cdot mol^{-1}$ at the normal boiling point and 152 $kJ\cdot mol^{-1}$ at room temperature. A higher value of enthalpy of vaporization at the normal boiling point corresponds to a higher value of the normal boiling point, so 159 $kJ\cdot mol^{-1}$ was used to predict the boiling point giving the higher value of boiling point for Yb. Two factors need to be considered: (1) For different elements, those having higher boiling points always have higher enthalpies of vaporization at the boiling point; (2) for a given element, the enthalpy of vaporization varies inversely with temperature. For Yb, the boiling point is higher than ambient, and so the enthalpy of vaporization at the boiling point is lower than the value at ambience. Previously, the enthalpy of vaporization at room temperature was used to predict the boiling point, and the first factor means the boiling point was overestimated. Now the enthalpy of vaporization at the boiling point is employed, and the boiling point prediction is correct. Using 129 $kJ\cdot mol^{-1}$, the corresponding boiling point is 1460 K, which is closer to 1466 K (within 0.40 %), and this value is confirmed by the work of Habermann and Daane.[28] In their work, the vapor pressures of the rare-earth metals were measured by the Knudsen effusion technique using a quartz-fiber microbalance, and then a combination of second and third law methods were used to calculate the normal boiling point for each rare-earth metal, and for Yb this value is 1466 (± 5) K.

For Tm, 247 $kJ\cdot mol^{-1}$ is the value corresponding to ambient temperature, according to *Selected Values of the Thermodynamic Properties of the Elements* on page 533,[18] which gives 191 $kJ\cdot mol^{-1}$ at the normal boiling point and 232 $kJ\cdot mol^{-1}$ at room temperature and is greater than the value recorded at the normal boiling point, which is about 191 $kJ\cdot mol^{-1}$. For similar reasons, 247 $kJ\cdot mol^{-1}$ was used to predict the boiling point producing a higher value. Using the value of 191 $kJ\cdot mol^{-1}$, it is found that the boiling point is 1943 K, which is closer to 2003 K (within 3.00 %) and is consistent with the value obtained by Spedding et al. after purifying this element at the Ames Laboratory of the U.S. Atomic Energy Commission,[29] which was 2000 K.

From this analysis, the prediction of boiling point in these cases is more justifiable than before. So it emerges that although there are several factors, especially the second, that may mislead the neural network method, when care is taken and critical surveys are employed, it turns out to be robust and reliable.

Conclusions

The data in handbooks were thought to be very reliable, especially the data for elements in the periodic table. The ANN is able to find out many inconsistencies by a systematic and automatic method and the development of this technique. Its wider application and, more interestingly, its integration into databases as an immune system suggest that it may no longer be necessary to accept error rates at 5 %. The boiling point and enthalpy of vaporization of most elements (except radioactive elements) have been corrected in this paper, and the errors have brought down from a maximum of 900 % to less than 10 %. Factors affecting the accuracy of the prediction have been discussed.

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