MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **57** (2007) 111-134

ISSN 0340 - 6253

Quantitative Structure Property Relations (QSPRs) for Predicting Standard Absolute Entropy, S^{o}_{298}, of Inorganic Compounds

Lailong Mu[*], *Changjun Feng*

Department of Chemistry, Xuzhou Normal University, Xuzhou 221116, P. R. China

Hongmei He

XuZhou College of Industrial Technology, Xuzhou, 221006, P. R. China

MULL@XZNU.EDU.CN

（Received May 22, 2006）

For predicting the standard entropy of inorganic compound, two novel connectivity indexes ${}^{m}Q$, ${}^{m}G$ and their converse indexes ${}^{m}Q'$, ${}^{m}G'$ based on adjacency matrix of molecular graphs are proposed as follows: ${}^{m}Q=\Sigma(q_i.q_j.q_k.\ldots)^{0.5}$, ${}^{m}G = \Sigma (g_i.g_j.g_k.\cdots)^{0.5}$, ${}^{m}Q'=\Sigma(q_i.q_j.q_k.\ldots)^{-0.5}$, ${}^{m}G' =\Sigma (g_i.g_j.g_k.\cdots)^{-0.5}$. The q_i and g_i of adjacency matrix are defined as $q_i=(1+Z_i)/(1+n_i)$, $g_i=(1+Z_i)/(1+r_i+r_i^{-1})$, where Z_i, n_i , r_i are the charge number, the outer electronic shell primary quantum number, and the radii of ionic i respectively. The excellent QSPR models for the standard entropies can be constructed from ${}^{0}Q$, ${}^{0}Q'$, ${}^{0}G$, ${}^{1}G$, and ${}^{1}G'$, by using multivariate linear regression (MLR) method and artificial neural network (NN) method. The correlation coefficient r, the standard error, and the average error of the MLR model and NN model are 0.990, 0.992, 8.88 $J.K^{-1}.mol^{-1}$, 7.83 $J.K^{-1}.mol^{-1}$, 7.10 % and 6.36%, respectively, for 590 inorganic compounds. The cross-validation by using the leave-one-out method demonstrates that the MLR model is

[*] Tel:+86-516-83403163;Fax: +86-516-83403164

E-mail address: mull@xznu.edu.cn

highly reliable from the point of view of statistics. The results show that the current method is more effective than literature methods for estimating the standard entropy of inorganic compound. Both MLR and NN methods can provide acceptable models for the prediction of the standard entropies. The NN model for the standard entropy appears to be more reliable than the MLR model.

1. INTRODUCTION

The quantitative structure-property/activity relationship (QSPR/QSAR) studies of organic compounds have been a focus of great attention by the scientists for a long time[1-3]. Large numbers of QSPR/QSAR models have been developed by using various model parameters to describe and predict the physical properties and biological activities of organic compounds from their molecular structures. However, there are only a few paper[4-10] about the QSPR/ QSAR studies of inorganic compounds, due to the complexity of inorganic compound composition.

Absolute standard entropy, $S°_{298}$, represents thermodynamic data of special significance, forging the link between enthalpy and Gibbs energy, which is the true arbiter of chemical equilibrium and stability in processes whose outcome is determined by thermodynamic (as opposed to kinetic) considerations. While enthalpy data are widely published[11-16] or can be estimated[17-22] for many solid compounds, entropy values are often unavailable, when simple estimation procedures become particularly useful.

Latimer[23] reported an additive method for the estimation of the standard entropies of solids, monatomic aqueous ions, and nonpolar molecules, based on summation of elemental contributions obtained from the equation

$$S°_{298}/\mathrm{J\ K^{-1}mol^{-1}} = (3/2)R\ln M - 3.93 \qquad (1)$$

where R is the gas constant (=8.314 J K^{-1} mol^{-1}) and M is the atomic mass of the element in question. Contributions from anions are dependent on the charge residing on the cation. A more complex summation procedure was used for inorganic compound by Fyfe et al.,[24] who employed the entropy and volume of component oxides to derive an estimate for multiple oxide phases, effectively applying a “volume correction” to the individual oxide entropy contributions. Jenkins et al.[25] reported that formula unit volume, V_m, can be employed for the general estimation of standard entropy, $S°_{298}$, values for inorganic compounds (including minerals), through a simple linear correlation between entropy and molar volume. V_m can be obtained from a number of possible sources, or alternatively density, ρ, may be used as the source of data. The approach can also be extended to estimate entropies for hypothesized compounds.

In recent years, Mu L. L.[26], Feng C. J.[27] etc., by using various model parameters, have developed some QSPR/QSAR models to estimate the entropies of Alkali and Alkaline earth metal compounds. In this study, the ionic parameter g_i and q_i are defined based on the ionic radii, ionic outer electronic shell primary quantum number, ionic charge. Two new topological indexes and their converse indexes are proposed based on the Kier-Hall[1] index and g_i or q_i. These connectivity indexes have good correlations for standard entropies of inorganic solid compound.

2. MOLECULAR DESCRIPTORS

Inorganic solid compound are made up of positive and negative ions, their standard entropies is affected by the ionic radii, ionic charge, ionic outer electronic shell primary quantum number. The ionic parameter g_i and q_i is defined as:

$$q_i=(1+Z_i)/(1+n_i) \quad (2)$$

$$g_i=(1+Z_i)/(1+r_i+r_i^{-1}) \quad (3)$$

where Z_i, n_i , r_i is the charge number, the outer electronic shell primary quantum number, and the radii of ionic i respectively. The g_i and q_i of 155 ions are calculated and listed in Table 1.

Based on adjacency matrix of molecular graphs, the novel connectivity index ${}^mQ$, ${}^mG$ and their converse index ${}^mQ'$, ${}^mG'$ can be defined as follows:

$${}^mQ=\Sigma(q_i.q_j.q_k.\ldots)^{0.5} \quad (4)$$

$${}^mQ'=\Sigma(q_i.q_j.q_k.\ldots)^{-0.5} \quad (5)$$

$${}^mG=\Sigma(g_i.g_j.g_k.\ldots)^{0.5} \quad (6)$$

$${}^mG'=\Sigma(g_i.g_j.g_k.\ldots)^{-0.5} \quad (7)$$

where, m is the order of the molecular connectivity index. The ${}^0Q$, ${}^1Q$, ${}^0Q'$, ${}^1Q'$, ${}^0G$, ${}^1G$, ${}^0G'$, and ${}^1G'$ are defined as follows:

$${}^0Q=\Sigma(q_i)^{0.5} \quad (8)$$

$${}^1Q=\Sigma(q_i.q_j)^{0.5} \quad (9)$$

$${}^0Q'=\Sigma(q_i)^{-0.5} \quad (10)$$

$${}^1Q'=\Sigma(q_i.q_j)^{-0.5} \quad (11)$$

$${}^0G=\Sigma(g_i)^{0.5} \quad (12)$$

$${}^1G=\Sigma(g_i.g_j)^{0.5} \quad (13)$$

$${}^0G'=\Sigma(g_i)^{-0.5} \quad (14)$$

$${}^1G'=\Sigma(g_i.g_j)^{-0.5} \quad (15)$$

In expressions (8), (10), (12), and (14), the "Σ" is the sum of atomic of inorganic compound chemical formula. In expressions (9), (11), (13), and (15), the "Σ" is the sum of chemical single

bonds of chemical formula. For example, the ${}^0Q$, ${}^1Q$, ${}^0Q'$, ${}^1Q'$, ${}^0G$, ${}^1G$, ${}^0G'$, and ${}^1G'$ of $Fe_3Al_2Si_3O_{12}$ are calculated as follows:

For $Fe_3Al_2Si_3O_{12}$, it can be treated as consisting of three Fe^{2+}, two Al^{3+}, three Si^{4+} and twelve O^{2-}, it contains six Fe-O single bonds, six Al-O single bonds and twelve Si-O single bonds, so:

${}^0Q=3\times(0.7500)^{0.5}+2\times(1.3333)^{0.5}+3\times(1.6667)^{0.5}+12\times(1.0000)^{0.5}=20.7805$

${}^1Q=6\times(0.7500\times1.0000)^{0.5}+6\times(1.3333\times1.0000)^{0.5}+12\times(1.6667\times1.0000)^{0.5}=27.6163$

${}^0Q'=3\times(0.7500)^{-0.5}+2\times(1.3333)^{-0.5}+3\times(1.6667)^{-0.5}+12\times(1.0000)^{-0.5}=19.5199$

${}^1Q'=6\times(0.7500\times1.0000)^{-0.5}+6\times(1.3333\times1.0000)^{-0.5}+12\times(1.6667\times1.0000)^{-0.5}=21.4195$

${}^0G=3\times(0.9233)^{0.5}+2\times(1.1793)^{0.5}+3\times(1.2821)^{0.5}+12\times(0.9633)^{0.5}=20.2291$

${}^1G=6\times(0.9233\times0.9633)^{0.5}+6\times(1.1793\times0.9633)^{0.5}+12\times(1.2821\times0.9366)^{0.5}=25.3892$

${}^0G'=3\times(0.9233)^{-0.5}+2\times(1.1793)^{-0.5}+3\times(1.2821)^{-0.5}+12\times(0.9633)^{-0.5}=19.8398$

${}^1G'=6\times(0.9233\times0.9633)^{-0.5}+6\times(1.1793\times0.9633)^{-0.5}+12\times(1.2821\times0.9366)^{-0.5}=22.7896$

the ${}^0Q$, ${}^1Q$, ${}^0Q'$, ${}^1Q'$, ${}^0G$, ${}^1G$, ${}^0G'$, and ${}^1G'$ of 590 inorganic compounds are calculated, and listed in Table 2.

Table 1. Ionic parameters g_i and q_i

No	ionic	g_i	q_i	No	ionic	g_i	q_i	No	ionic	g_i	q_i
1	Ag^{+}	0.6623	0.4000	53	I^{-}	0.5473	0.3333	105	Re^{5+}	1.8159	1.0000
2	Al^{3+}	1.1793	1.3333	54	I^{5+}	1.9982	1.0000	106	Re^{6+}	2.0783	1.1667
3	Am^{3+}	1.3332	0.5714	55	In^{+}	0.6422	0.3333	107	Re^{7+}	2.3414	1.3333
4	Am^{4+}	1.6521	0.7143	56	In^{3+}	1.3115	0.8000	108	Rh^{2+}	0.9925	0.6000
5	As^{3-}	1.0898	0.8000	57	Ir^{2+}	0.9955	0.5000	109	Rh^{3+}	1.2648	0.8000
6	As^{3+}	1.2106	0.8000	58	Ir^{4+}	1.5541	0.8333	110	S^{2-}	0.8867	0.7500
7	As^{5+}	1.6511	1.5000	59	K^{+}	0.6442	0.5000	111	S^{4+}	1.2277	1.2500
8	Au^{+}	0.6452	0.3333	60	La^{2+}	0.9869	0.5000	112	S^{6+}	1.5108	2.3333
9	Au^{3+}	1.3217	0.6667	61	La^{3+}	1.3329	0.6667	113	Sb^{3-}	1.0368	0.6667
10	B^{3+}	0.8042	2.0000	62	Li^{+}	0.6502	1.0000	114	Sb^{3+}	1.3005	0.6667
11	Ba^{2+}	0.9706	0.5000	63	Lu^{3+}	1.3233	0.6667	115	Sb^{5+}	1.8367	1.2000
12	Be^{2+}	0.8169	1.5000	64	Mg^{2+}	0.9650	1.0000	116	Sc^{3+}	1.2973	1.0000
13	Bi^{3-}	1.1113	0.5714	65	Mn^{2+}	0.9885	0.7500	117	Se^{2-}	0.8608	0.6000
14	Bi^{3+}	1.3329	0.5714	66	Mn^{3+}	1.2106	1.0000	118	Si^{4-}	1.4347	1.2500
15	Br^{-}	0.5763	0.4000	67	Mn^{4+}	1.4634	1.2500	119	Si^{4+}	1.2821	1.6667
16	Br^{5+}	1.6678	1.2000	68	Mo^{3+}	1.2742	0.8000	120	Sm^{2+}	0.9812	0.5000
17	C^{4-}	1.2548	1.6667	69	Mo^{4+}	1.5682	1.0000	121	Sm^{3+}	1.3326	0.6667
18	C^{4+}	0.8065	2.5000	70	Mo^{5+}	1.8465	1.2000	122	Sn^{2+}	0.9999	0.5000
19	Ca^{2+}	1.0000	0.7500	71	Mo^{6+}	2.1310	1.4000	123	Sn^{4-}	1.3831	0.8333
20	Cd^{2+}	0.9991	0.6000	72	N^{3-}	1.2140	1.3333	124	Sn^{4+}	1.5927	1.0000
21	Ce^{3+}	1.3333	0.6667	73	N^{3+}	0.5398	1.3333	125	Sr^{2+}	0.9909	0.6000
22	Ce^{4+}	1.6559	0.8333	74	N^{5+}	0.6801	3.0000	126	Ta^{3+}	1.2866	0.6667
23	Cl^{-}	0.5948	0.5000	75	Na^{+}	0.6666	0.6667	127	Ta^{4+}	1.5870	0.8333
24	Cl^{5+}	1.4015	1.5000	76	Nb^{3+}	1.2866	0.8000	128	Ta^{5+}	1.8735	1.0000

25	Co^{2+}	0.9409	0.7500	77	Nb^{4+}	1.5870	1.0000	129	Te^{2-}	0.8191	0.5000
26	Co^{3+}	1.1876	1.0000	78	Nb^{5+}	1.8735	1.2000	130	Te^{4+}	1.6662	0.8333
27	Cr^{2+}	0.9678	0.7500	79	Ni^{2+}	0.9556	0.6000	131	Th^{3+}	1.3307	0.5714
28	Cr^{3+}	1.2373	1.0000	80	Ni^{3+}	1.1956	1.0000	132	Th^{4+}	1.6645	0.7143
29	Cr^{4+}	1.4845	1.2500	81	Np^{3+}	1.3333	0.5714	133	Ti^{2+}	0.9925	0.7500
30	Cr^{6+}	1.8854	1.7500	82	Np^{4+}	1.6559	0.7143	134	Ti^{3+}	1.2648	1.0000
31	Cs^{+}	0.6118	0.3333	83	Np^{5+}	1.9459	0.8571	135	Ti^{4+}	1.5388	1.2500
32	Cu^{+}	0.6517	0.5000	84	O^{2-}	0.9633	1.0000	136	Tl^{+}	0.6316	0.2857
33	Cu^{2+}	0.9678	0.7500	85	Os^{2+}	0.9955	0.5000	137	Tl^{3+}	1.3273	0.6667
34	Dy^{3+}	1.3294	0.6667	86	Os^{3+}	1.3138	0.6667	138	Tm^{3+}	1.3261	0.6667
35	Er^{3+}	1.3273	0.6667	87	Os^{6+}	2.0783	1.1667	139	U^{3+}	1.3329	0.5714
36	Eu^{2+}	0.9955	0.5000	88	P^{3-}	1.1137	1.0000	140	U^{4+}	1.6591	0.7143
37	Eu^{3+}	1.3322	0.6667	89	P^{5+}	1.4957	2.0000	141	U^{5+}	1.9507	0.8571
38	F^{-}	0.6490	0.6667	90	Pa^{3+}	1.3326	0.5714	142	U^{6+}	2.2582	1.0000
39	Fe^{2+}	0.9233	0.7500	91	Pa^{4+}	1.6605	0.7143	143	V^{2+}	0.9817	0.7500
40	Fe^{3+}	1.1876	1.0000	92	Pa^{5+}	1.9595	0.8571	144	V^{3+}	1.2490	1.0000
41	Fr^{+}	0.5960	0.2857	93	Pb^{2+}	0.9900	0.4286	145	V^{4+}	1.5133	1.2500
42	Ga^{2+}	0.9890	0.6000	94	Pb^{4-}	1.3831	0.7143	146	V^{5+}	1.7689	1.5000
43	Ga^{3+}	1.2373	1.0000	95	Pb^{4+}	1.6329	0.8333	147	W^{4+}	1.5747	0.8333
44	Gd^{3+}	1.3316	0.6667	96	Re^{4+}	1.5541	0.8333	148	W^{5+}	1.8559	1.0000
45	Ge^{2+}	0.9678	0.6000	97	Pd^{2+}	0.9925	0.6000	149	W^{6+}	2.1429	1.1667
46	Ge^{4-}	1.2232	1.0000	98	Pd^{4+}	1.5466	1.0000	150	W^{6+}	2.1429	1.1667
47	Ge^{4+}	1.4634	1.2500	99	Po^{4+}	1.6662	0.7143	151	Y^{3+}	1.3284	0.8000
48	H^{-}	0.6422	1.0000	100	Pt^{2+}	0.9836	0.5000	152	Yb^{2+}	0.9950	0.5000
49	Hf^{4+}	1.6034	0.8333	101	Pt^{4+}	1.5541	0.8333	153	Yb^{3+}	1.3248	0.6667
50	Hg^{+}	0.6600	0.2857	102	Pu^{3+}	1.3333	0.5714	154	Zn^{2+}	0.9704	0.7500
51	Hg^{2+}	0.9999	0.5000	103	Pu^{4+}	1.6541	0.7143	155	Zr^{4+}	1.6083	1.0000
52	Ho^{3+}	1.3285	0.6667	104	Rb^{+}	0.6293	0.4000				

3. DATA SET

The QSPR treatment started with the assembly of the data set. The experimental standard entropies, $S°_{298}$, data were compiled from Ref.11, Ref.12, Ref.16, Ref.25, and Ref.26. A total of 590 inorganic compounds with extensive structural diversity were selected as the data set (see Table 2). The quality and robustness of the predictive power of a QSPR model depends heavily on the diversity of data set. To select significant descriptors for the QSPR model that captures all the underlying interaction mechanisms, it is advisable to have as many as possible structural features represented in the data set. The working data set included ionic salts, oxide, and mineral. The structures include 81 elements and 155 ions.

4. MULTILINEAR REGRESSION MODELS

Linear QSPR models can be developed with several statistical techniques, such as multivariate linear regression, partial least-squares regression, and principal components

regression. In this study, we applied stepwise multivariate regression analysis to select significant descriptors for linear QSPR models.

Linear regression analysis is carried by SPSS. The best subsets regression of standard entropies, $S°_{298}$, versus ${}^0Q$, ${}^1Q$, ${}^0Q'$, ${}^1Q'$, ${}^0G$, ${}^1G$, ${}^0G'$, and ${}^1G'$ resulted in a five-parameter model with the correlation coefficient r of 0.990. The model is shown as follows:

$$S°_{298}=-1.164-42.532\,{}^0Q+44.665\,{}^0Q'-11.876\,{}^0G+7.111\,{}^1G+18.511\,{}^1G' \qquad (16)$$

n=590, r=0.990, r^2=0.979, s=8.88 J.K^{-1}.mol^{-1}, F=5476.26

The results of t-test show that these variables in these models are significant. The model (16) explains more than 97.9% of the variance in the experimental values of standard entropies, $S°_{298}$ for these inorganic compounds. The calculated results from Eq. (16) for 590 inorganic compounds are shown in Table 2 (Cal.1). The average absolute deviation is 6.87 J. K^{-1}.mol^{-1}. The calculated standard entropies versus experimental data is shown in Figure 1.

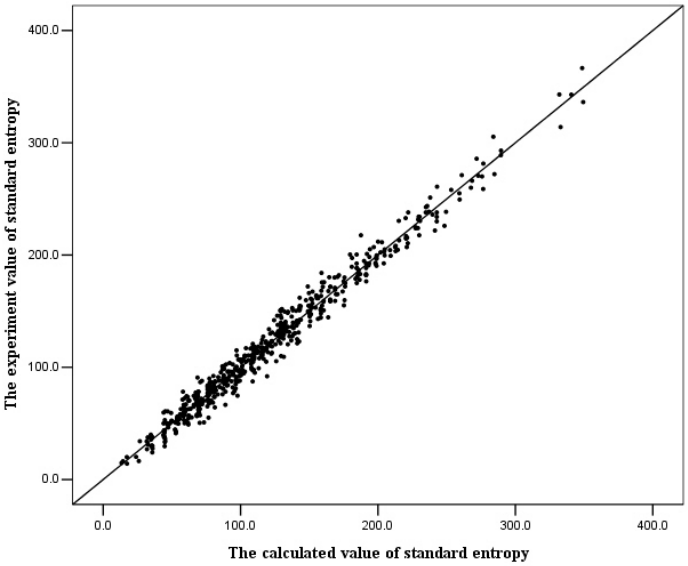

Figure 1. Plot of calculated vs experimental values of standard entropy, multilinear regression model

Finally, the model above generated for 690 inorganic compounds is verified by the cross-validation using leave-one-out method, and the correlation coefficients r_{cv} and standard deviations s_{cv} together with the normal r and s are 0.989(0.990), 8.96(8.85) J. K^{-1}.mol^{-1}, respectively. These data reveal that the results of the cross-validations for each model are very

close to the normal results of the models, which means that the model constructed in this work is stable.

5. ARTIFICIAL NEURAL NETWORK MODELS

Artificial neural networks (NN) are novel and powerful technique to build models that can effectively solve complex real world problems. These techniques are loosely inspired by the way the densely interconnected, parallel structure of the brain processes information. Neural networks are constructed from a number of highly interconnected nonlinear processing units (also called neurons) that are joined together with weighted connections in several ways to form various types of networks. Probably the most widely used type is a feed-forward multilayer neural network. This network has the capacity to learn, memorize, and find relationships among the data. The most common tasks approached by the use of neural networks are modeling and classification problems. Numerous application areas in chemistry[28,29] include QSAR/QSPR studies, spectroscopy (IR, NMR, and UV spectras), protein folding, process control in chemical industry, etc.

Neural network toolbox of MATLAB 7.0.1 was used to calculate NN models. Before the neural network treatment started, both the experimental property and descriptor values were normalized to have zero means and unity standard deviation. Feed-forward multilayer neural network models with a sigmoid activation function for hidden neurons and a linear transfer function for output neurons were chosen for the prediction of standard entropies. All networks had one input layer, one hidden layer, and one output layer, and they were trained with Levenberg-Marquardt training function. The input neurons are ${}^{0}Q$, ${}^{0}Q'$, ${}^{0}G$, ${}^{1}G$, and ${}^{1}G'$. The data set was divided into three data sets: training, test, and validation. The training, test, and validation sets represented 60% (354data points), 20% (118data points), and 20%(118data points), respectively, of the data. The neural network weights were initialized with random values. According to the training set error, the neural network weights were then adjusted with back-propagation algorithm to minimize the prediction error. The validation set error was monitored by the training algorithm to perform automatic early stopping in order to avoid over-training of the neural network. Also, early stopping significantly reduces time that is spent to train the network.

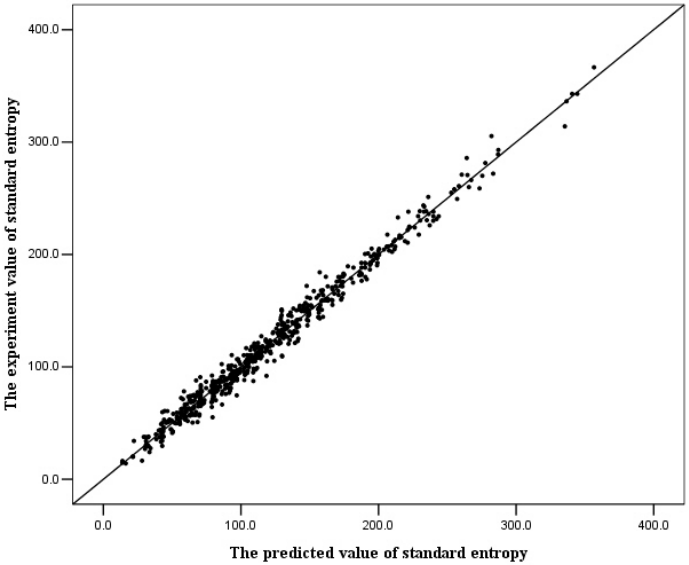

Figure 2. Plot of predicted vs experimental values of standard entropy, artificial neural network model

To find the optimal number of hidden neurons, neural network training with a 5:h:1 architecture was carried out. After examining neural nets with various numbers of hidden nodes, we found that 6 offered the most accurate results, and we therefore employ a 5:6:1 network architecture. The statistical fit of this NN model (see Figure 2) obtained is better than the MLR model. The training, validation and prediction sets had RMS errors 7.75 J. K^{-1}.mol^{-1}, 7.45 J. K^{-1}.$mol^{-1}$and 8.51 J. K^{-1}.mol^{-1}, respectively. The predicted values for 590 inorganic compounds are shown in Table 2 (Cal.2). The R^2 and average absolute deviation between predicted and experimental values for the training set are 0.992 and 6.87 J. K^{-1}.mol^{-1}.

6. RESULTS AND DISCUSSION

The q_i defined in this paper is various for different ions due to various the charge number and the outer electronic shell primary quantum number. However, for the different ions having the same charge number and outer electronic shell primary quantum number, the q_i is equal. For example, the q_i of Ag^+ and Rb^+ both are 0.4000. Whenas, the g_i defined in this paper is various for different ions due to various radii and charge. For Ag^+ and Rb^+, the g_i are 0.6623 and 0.6293, respectively, in other words, the g_i is different. So, the q_i together with the g_i can reflect the characteristic of different ion.

The theoretical prediction of the standard entropy for inorganic compound is a complicated task that requires information both from the electron, atom, and molecule level. Obviously, the limiting factor here is not in the use of particular QSPR method but rather the molecular descriptors that fail to account for all the details of the underlying system. The results of multivariate regression analysis have shown that the linear model (16) is excellent, and the correlation coefficient *r* is 0.990. The estimated standard entropies of 590 inorganic compounds are listed in Table 2 (Cal.1). As shown in Table 2 (Cal.1), our calculated values agree well with the available experimental values. The average error of 590 crystals is 7.10 % (10.23% for S<100 $J.K^{-1}.mol^{-1}$, 5.00% for 200>S>100 $J.K^{-1}.mol^{-1}$, 3.67% for S>200 $J.K^{-1}.mol^{-1}$). The NN model developed for the prediction of standard entropies performed better than the MLR model and the correlation coefficient *r* and the RMS errors are 0.992 and 7.83 $J.K^{-1}.mol^{-1}$. The predicted standard entropies of 590 inorganic compounds from the NN model are listed in Table 2 (Cal.2). The average prediction errors of 590 compounds is 6.36%(9.52% for S<100 $J.K^{-1}.mol^{-1}$, 4.35% for 200>S>100 $J.K^{-1}.mol^{-1}$, 2.58% for S>200 $J.K^{-1}.mol^{-1}$).The results show that the current method is more effective than literature methods[25,26] for inorganic compounds .

It is useful to be able to estimate standard entropy data. First, there is a paucity of standard entropy data for inorganic compounds in standard thermochemical tables.[11-13] Second, experimental determination of absolute entropy, $S°_{298}$, by calorimetry is both a lengthy and nontrivial procedure; such measurements are no longer fashionable science and, for this reason, increasing reliance has to be placed on estimation techniques for thermochemical data. Standard entropy estimation involves only simple arithmetic, easily performed even on a pocket calculator. The procedure can be applied for new (or even hypothetical) salts, as well as for already synthesized, existing, inorganic compounds. The approach's ultimate importance is in its use to estimate changes in Gibbs energy for reactions. In the estimation of Gibbs energy data via the $T\Delta S$ contribution to the ΔG term (in kJ mol^{-1}) at 298 K, the value of ΔS/J K^{-1} mol^{-1}, derived as the absolute standard entropy differences of products and reactants, is multiplied by the factor T/(K J kJ^{-1})=0.298. Effectively, a consequence of this factor is that a larger error can be tolerated in the standard entropies. This significant point renders the correlation reported here of enhanced value. Furthermore, the $T\Delta S$ term in ΔG is generally quite small relative to ΔH at or near room temperature, where much of chemistry is studied, so that rule-of-thumb procedures are likely to prove suitable even when the entropy may be somewhat in error.

7. CONCLUSION

Two novel connectivity index ${}^{m}Q$, ${}^{m}G$ and their converse index ${}^{m}Q'$, ${}^{m}G'$ are proposed from the ionic parameters q_i and g_i, for predicting the standard entropy of inorganic compound. The excellent QSPR models for the standard entropies can be constructed from ${}^{0}Q$, ${}^{0}Q'$, ${}^{0}G$, ${}^{1}G$, and ${}^{1}G'$, by using MLR method and NN method. The correlation coefficient r, standard error, and average error of the MLR model and NN model are 0.990, 0.992, 8.88 $J.K^{-1}.mol^{-1}$, 7.83 $J.K^{-1}.mol^{-1}$, 7.10 % and 6.36%, respectively, for the 690 inorganic compounds. The cross-validation by using the leave-one-out method demonstrates that the MLR model is highly reliable from the point of view of statistics. The results show that the current method is more effective than literature methods for estimating the standard entropy of inorganic compound. Both MLR and NN methods can provide acceptable models for the prediction of the standard entropies. The NN model for the standard entropy appears to be more reliable than the MLR model.

8. ACKNOWLEDGEMENT

This work is supported by the university natural science foundation of Jiangsu Province in china (contract grant number:04KJD150195). The authors express our gratitude to the referees for their value comments.

Table2. The calculated and experimental standard entropies of 590 inorganic compounds ($J\ K^{-1}\ mol^{-1}$)

No	Compound	${}^{0}Q$	${}^{0}Q'$	${}^{0}G$	${}^{1}G$	${}^{1}G'$	S^{o}_{298}				
							Exp.	Cal.1	Er.1	Cal.2	Er.2
1	AgBr	1.2649	3.1623	1.5730	0.6178	1.6185	107.1	102.0	-5.1	104.7	-2.4
2	AgCl	1.3396	2.9954	1.5851	0.6277	1.5932	96.3	90.8	-5.5	93.9	-2.4
3	AgF	1.4490	2.8059	1.6194	0.6556	1.5253	83.7	76.2	-7.5	78.9	-4.8
4	AgI	1.2098	3.3132	1.5536	0.6021	1.6610	115.5	111.9	-3.6	114.4	-1.1
5	Ag_2O	2.2649	4.1623	2.6092	1.5975	2.5038	121.3	115.1	-6.2	112.6	-8.7
6	Ag_2S	2.1309	4.3170	2.5693	1.5327	2.6098	144.0	129.7	-14.3	129.3	-14.7
7	Ag_2Se	2.0395	4.4533	2.5555	1.5102	2.6487	150.3	140.4	-9.9	140.6	-9.7
8	Ag_2Te	1.9720	4.5765	2.5327	1.4731	2.7153	154.8	150.0	-4.8	151.1	-3.7
9	$AlBr_3$	3.0521	5.6094	3.3635	2.4733	3.6389	180.2	164.6	-15.6	161.9	-18.3
10	Al_4C_3	8.4918	5.7879	7.7044	14.5977	9.8646	89.0	91.1	2.1	96.3	7.3
11	$AlCl_3$	3.2760	5.1087	3.3996	2.5126	3.5820	109.3	131.5	22.2	130.1	20.8
12	AlF_3	3.6042	4.5403	3.5027	2.6245	3.4293	66.5	88.9	22.4	86.3	19.8
13	AlH_3	4.1547	3.8660	3.4901	2.6108	3.4473	30.0	35.7	5.7	30.9	0.9
14	AlN	2.3094	1.7321	2.1878	3.5896	2.5072	20.2	23.9	3.7	21.3	1.1
15	Al_2O_3	5.3094	4.7321	5.1163	6.3951	5.6294	50.9	73.3	22.4	68.5	17.6
16	Al_2S_3	4.9075	5.1962	4.9968	6.1354	5.8676	116.9	115.1	-1.8	112.9	-4.0
17	Am_2O_3	4.5119	5.6458	5.2537	6.7994	5.2946	154.7	143.1	-11.6	145.7	-9.0

18	AmO_2	2.8452	3.1832	3.2483	5.0461	3.1707	83.7	76.0	-7.7	71.0	-12.7
19	AsI_3	2.6265	6.3142	3.3196	2.4419	3.6857	213.1	215.3	2.2	212.4	-0.7
20	As_2O_3	4.7889	5.2361	5.1450	6.4794	5.5561	107.5	116.8	9.3	114.4	6.9
21	As_2S_3	4.3869	5.7002	5.0254	6.2163	5.7912	163.6	158.6	-5.0	160.0	-3.6
22	As_2Se_3	4.1126	6.1091	4.9840	6.1250	5.8775	194.7	189.9	-4.8	196.3	1.6
23	As_2O_5	7.4495	6.6330	7.4773	12.6116	7.9292	105.4	125.9	20.5	124.4	19.0
24	AuBr	1.2098	3.3132	1.5624	0.6098	1.6399	113.0	111.5	-1.5	113.6	0.6
25	AuCl	1.2845	3.1463	1.5745	0.6195	1.6143	92.9	100.3	7.4	103.0	10.1
26	AuI	1.1547	3.4641	1.5430	0.5942	1.6829	119.3	121.5	2.2	123.1	3.8
27	$AuCl_3$	2.9378	5.4674	3.4633	2.6599	3.3836	148.1	158.5	10.4	156.8	8.7
28	AuF_3	3.2660	4.8990	3.5664	2.7784	3.2393	114.3	116.1	1.8	114.4	0.1
29	Au_2O_3	4.6330	5.4495	5.2437	6.7701	5.3175	130.4	129.5	-0.9	130.0	-0.4
30	BN	2.5689	1.5731	1.9986	2.9643	3.0361	14.8	13.4	-1.4	13.8	-1.0
31	B_2O_3	5.8284	4.4142	4.7380	5.2811	6.8168	54.0	55.6	1.6	58.9	4.9
32	$BaBr_2$	1.9720	4.5765	2.5035	1.4959	2.6740	148.5	149.8	1.3	149.5	1.0
33	$BaCl_2$	2.1213	4.2426	2.5277	1.5197	2.6322	123.7	127.6	3.9	128.3	4.6
34	BaF_2	2.3401	3.8637	2.5964	1.5873	2.5200	96.4	99.0	2.6	98.3	1.9
35	BaH_2	2.7071	3.4142	2.5880	1.5790	2.5332	63.0	63.6	0.6	62.1	-0.9
36	BaI_2	1.8618	4.8783	2.4648	1.4577	2.7441	165.1	169.4	4.3	168.1	3.0
37	BaO	1.7071	2.4142	1.9667	1.9339	2.0683	70.4	62.7	-7.7	63.5	-6.9
38	BaS	1.5731	2.5689	1.9268	1.8554	2.1559	78.2	76.9	-1.3	79.8	1.6
39	BaSe	1.4817	2.7052	1.9130	1.8282	2.1880	90.8	87.4	-3.4	92.0	1.2
40	BaTe	1.4142	2.8284	1.8903	1.7833	2.2430	99.6	96.8	-2.8	103.0	3.4
41	$BeBr_2$	2.4897	3.9788	2.4222	1.3723	2.9147	106.3	105.6	-0.7	108.3	2.0
42	Be_2C	3.7405	2.4076	2.9279	4.0499	3.9507	16.3	14.4	-1.9	13.9	-2.4
43	$BeCl_2$	2.6390	3.6449	2.4463	1.3942	2.8691	75.8	83.4	7.6	86.1	10.3
44	BeF_2	2.8577	3.2660	2.5150	1.4562	2.7468	53.4	54.5	1.1	55.3	1.9
45	BeI_2	2.3794	4.2806	2.3834	1.3373	2.9911	120.5	125.4	4.9	127.8	7.3
46	Be_3N_2	5.9836	4.1815	4.9152	5.9753	6.0248	34.1	26.8	-7.3	22.3	-11.8
47	BeO	2.2247	1.8165	1.8853	1.7742	2.2545	14.1	17.3	3.2	16.3	2.2
48	BeS	2.0908	1.9712	1.8455	1.7022	2.3499	34.0	31.6	-2.4	31.0	-3.0
49	$BiCl_3$	2.8772	5.5655	3.4682	2.6712	3.3692	171.7	165.2	-6.5	163.3	-8.4
50	BiF_3	3.2054	4.9971	3.5713	2.7902	3.2256	122.7	122.8	0.1	121.3	-1.4
51	BiI_3	2.4880	6.5190	3.3739	2.5623	3.5125	224.8	227.4	2.6	222.6	-2.2
52	Bi_2O_3	4.5119	5.6458	5.2535	6.7989	5.2950	151.5	143.1	-8.4	145.7	-5.8
53	Bi_2S_3	4.1099	6.1099	5.1339	6.5228	5.5191	200.4	184.5	-15.9	190.5	-9.9
54	Bi_2Te_3	3.6332	6.8884	5.0242	6.2695	5.7421	260.9	243.2	-17.7	258.7	-2.2
55	Ca_3Bi_2	4.1099	6.1099	5.1083	6.3250	5.6917	177.9	186.6	8.7	191.6	13.7
56	$CaBr_2$	2.1309	4.3170	2.5183	1.5183	2.6345	130.0	130.7	0.7	130.3	0.3
57	Ca_2C	3.0230	3.0840	3.1202	4.4808	3.5708	70.0	68.9	-1.1	66.3	-3.7
58	$CaCl_2$	2.2802	3.9831	2.5425	1.5425	2.5933	104.6	108.5	3.9	108.7	4.1
59	CaF_2	2.4990	3.6042	2.6112	1.6112	2.4827	68.5	79.9	11.4	78.6	10.1
60	CaH_2	2.8660	3.1547	2.6027	1.6027	2.4957	41.4	44.5	3.1	42.5	1.1
61	CaI_2	2.0207	4.6188	2.4795	1.4795	2.7035	145.3	150.3	5.0	148.9	3.6
62	Ca_3N_2	4.9075	5.1962	5.2037	6.6110	5.4455	105.0	108.2	3.2	106.5	1.5
63	CaO	1.8660	2.1547	1.9815	1.9630	2.0377	39.7	43.9	4.2	42.7	3.0
64	Ca_3P_2	4.5981	5.4641	5.1106	6.3319	5.6855	123.9	136.9	13.0	135.6	11.7

65	Ca_2Pb	2.5772	3.4926	3.1760	4.7042	3.4012	105.0	103.9	-1.1	103.6	-1.4
66	CaS	1.7321	2.3094	1.9416	1.8833	2.1240	56.5	58.0	1.5	58.4	1.9
67	CaSe	1.6406	2.4457	1.9278	1.8556	2.1556	67.0	68.5	1.5	70.3	3.3
68	Ca_2Si	2.8501	3.2038	3.1978	4.7912	3.3395	81.2	78.6	-2.6	74.8	-6.4
69	Ca_2Sn	2.6449	3.4048	3.1760	4.7042	3.4012	100.5	97.1	-3.4	95.9	-4.6
70	CaTe	1.5731	2.5689	1.9050	1.8101	2.2098	79.5	77.8	-1.7	81.1	1.6
71	$CdBr_2$	2.0395	4.4533	2.5179	1.5177	2.6356	137.2	140.7	3.5	140.1	2.9
72	$CdCl_2$	2.1888	4.1194	2.5420	1.5418	2.5944	115.3	118.5	3.2	118.8	3.5
73	CdF_2	2.4076	3.7405	2.6107	1.6104	2.4838	83.7	89.9	6.2	88.8	5.1
74	CdI_2	1.9293	4.7551	2.4791	1.4789	2.7047	158.4	160.3	1.9	158.7	0.3
75	CdO	1.7746	2.2910	1.9810	1.9621	2.0386	54.8	53.8	-1.0	53.5	-1.3
76	CdS	1.6406	2.4457	1.9412	1.8824	2.1249	69.1	68.0	-1.1	69.6	0.5
77	CdSe	1.5492	2.5820	1.9274	1.8548	2.1566	83.3	78.5	-4.8	81.6	-1.7
78	CdTe	1.4817	2.7052	1.9046	1.8093	2.2108	92.9	87.8	-5.1	92.5	-0.4
79	$CeBr_3$	2.7139	5.9682	3.4322	2.6298	3.4223	182.1	191.3	9.2	187.7	5.6
80	$CeCl_3$	2.9378	5.4674	3.4684	2.6716	3.3688	151.0	158.3	7.3	156.4	5.4
81	CeF_3	3.2660	4.8990	3.5714	2.7906	3.2252	115.1	115.9	0.8	114.2	-0.9
82	CeI_3	2.5485	6.4209	3.3740	2.5626	3.5121	214.8	220.4	5.6	215.5	0.7
83	CeN	1.9712	2.0908	2.2565	3.8168	2.3580	44.4	52.4	8.0	49.2	4.8
84	Ce_2O_3	4.6330	5.4495	5.2538	6.7998	5.2943	150.6	129.1	-21.5	129.8	-20.8
85	Ce_2S_3	4.2311	5.9136	5.1342	6.5237	5.5184	180.5	170.6	-9.9	174.4	-6.1
86	CeO_2	2.9129	3.0954	3.2498	5.0520	3.1671	62.3	69.2	6.9	63.3	1.0
87	$CoBr_2$	2.1309	4.3170	2.4883	1.4728	2.7160	134.0	132.2	-1.8	133.3	-0.7
88	$CoCl_2$	2.2802	3.9831	2.5125	1.4962	2.6735	109.2	110.0	0.8	111.6	2.4
89	CoF_2	2.4990	3.6042	2.5812	1.5628	2.5595	82.0	81.4	-0.6	81.1	-0.9
90	CoI_2	2.0207	4.6188	2.4495	1.4352	2.7872	153.2	151.9	-1.3	152.1	-1.1
91	CoO	1.8660	2.1547	1.9515	1.9041	2.1008	53.0	45.0	-8.0	44.2	-8.8
92	CoS	1.7321	2.3094	1.9116	1.8267	2.1897	62.4	59.1	-3.3	60.0	-2.4
93	CoF_3	3.4495	4.6742	3.5065	2.6337	3.4173	95.0	101.2	6.2	99.5	4.5
94	$CrBr_2$	2.1309	4.3170	2.5021	1.4937	2.6780	134.8	131.5	-3.3	131.9	-2.9
95	$CrCl_2$	2.2802	3.9831	2.5262	1.5174	2.6361	115.3	109.3	-6.0	110.3	-5.0
96	CrF_2	2.4990	3.6042	2.5949	1.5850	2.5237	83.7	80.7	-3.0	79.9	-3.8
97	CrS	1.7321	2.3094	1.9254	1.8527	2.1590	64.1	58.6	-5.5	59.3	-4.8
98	$CrBr_3$	2.8974	5.7434	3.3898	2.5333	3.5526	159.8	175.7	15.9	173.0	13.2
99	$CrCl_3$	3.1213	5.2426	3.4260	2.5736	3.4971	123.0	142.6	19.6	141.3	18.3
100	CrF_3	3.4495	4.6742	3.5291	2.6882	3.3480	93.9	100.1	6.2	98.0	4.1
101	CrI_3	2.7321	6.1962	3.3316	2.4686	3.6458	199.7	204.9	5.2	200.7	1.0
102	CrN	2.1547	1.8660	2.2142	3.6768	2.4478	38.0	35.7	-2.3	32.8	-5.2
103	Cr_2O_3	5.0000	5.0000	5.1691	6.5504	5.4959	81.2	96.4	15.2	92.8	11.6
104	CrO_2	3.1180	2.8944	3.1814	4.7833	3.3450	51.1	53.7	2.6	47.6	-3.5
105	CrO_3	4.3229	3.7559	4.3175	8.0860	4.4521	72.0	71.4	-0.6	70.4	-1.6
106	CsBr	1.2098	3.3132	1.5414	0.5938	1.6840	113.1	112.5	-0.6	115.2	2.1
107	CsCl	1.2845	3.1463	1.5534	0.6033	1.6577	101.2	101.3	0.1	104.5	3.3
108	CsF	1.3938	2.9568	1.5878	0.6301	1.5870	88.3	86.6	-1.7	89.5	1.2
109	CsI	1.1547	3.4641	1.5220	0.5787	1.7281	123.1	122.5	-0.6	124.8	1.7
110	Cs_2O	2.1547	4.4641	2.5459	1.5354	2.6051	127.6	135.5	7.9	132.4	4.8
111	CuBr	1.3396	2.9954	1.5665	0.6129	1.6316	96.1	91.6	-4.5	95.2	-0.9

112	CuCl	1.4142	2.8284	1.5785	0.6226	1.6061	86.2	80.4	-5.8	84.1	-2.1
113	CuF	1.5236	2.6390	1.6129	0.6503	1.5376	64.9	65.8	0.9	69.0	4.1
114	CuI	1.2845	3.1463	1.5471	0.5972	1.6744	96.7	101.6	4.9	105.1	8.4
115	Cu_2O	2.4142	3.8284	2.5961	1.5847	2.5241	93.1	94.3	1.2	93.1	0.0
116	Cu_2S	2.2802	3.9831	2.5562	1.5204	2.6310	120.9	108.9	-12.0	109.9	-11.0
117	Cu_2Te	2.1213	4.2426	2.5197	1.4613	2.7373	134.8	129.2	-5.6	132.0	-2.8
118	$CuBr_2$	2.1309	4.3170	2.5021	1.4937	2.6780	129.0	131.5	2.5	131.9	2.9
119	$CuCl_2$	2.2802	3.9831	2.5262	1.5174	2.6361	108.1	109.3	1.2	110.3	2.2
120	CuF_2	2.4990	3.6042	2.5949	1.5850	2.5237	77.5	80.7	3.3	79.9	2.5
121	CuO	1.8660	2.1547	1.9652	1.9311	2.0714	42.6	44.4	1.8	43.5	0.9
122	CuS	1.7321	2.3094	1.9254	1.8527	2.1590	66.5	58.6	-7.9	59.3	-7.2
123	CuSe	1.6406	2.4457	1.9116	1.8255	2.1912	78.3	69.1	-9.2	71.2	-7.1
124	CuTe	1.5731	2.5689	1.8888	1.7807	2.2463	86.7	78.5	-8.2	82.0	-4.7
125	Dy_2O_3	4.6330	5.4495	5.2504	6.7898	5.3020	149.8	129.3	-20.5	129.8	-20.0
126	ErF_3	3.2660	4.8990	3.5688	2.7843	3.2324	117.6	116.0	-1.6	114.3	-3.3
127	$EuCl_2$	2.1213	4.2426	2.5402	1.5390	2.5991	137.7	127.0	-10.7	127.1	-10.6
128	EuI_2	1.8618	4.8783	2.4773	1.4762	2.7097	169.1	168.8	-0.3	166.7	-2.4
129	EuO	1.7071	2.4142	1.9792	1.9585	2.0424	62.8	62.3	-0.5	62.8	0.0
130	$EuBr_3$	2.7139	5.9682	3.4317	2.6287	3.4238	183.0	191.3	8.3	187.7	4.7
131	$EuCl_3$	2.9378	5.4674	3.4679	2.6705	3.3702	144.1	158.3	14.2	156.5	12.4
132	Eu_2O_3	4.6330	5.4495	5.2528	6.7969	5.2965	146.0	129.2	-16.8	129.8	-16.2
133	$FeBr_2$	2.1309	4.3170	2.4792	1.4589	2.7418	140.6	132.7	-7.9	134.3	-6.3
134	$FeCl_2$	2.2802	3.9831	2.5033	1.4821	2.6989	118.0	110.5	-7.5	112.5	-5.5
135	FeF_2	2.4990	3.6042	2.5720	1.5481	2.5838	87.0	81.8	-5.2	81.9	-5.1
136	FeI_2	2.0207	4.6188	2.4404	1.4216	2.8136	167.4	152.4	-15.0	153.2	-14.2
137	FeO	1.8660	2.1547	1.9423	1.8861	2.1207	60.8	45.3	-15.5	44.7	-16.1
138	FeS	1.7321	2.3094	1.9025	1.8096	2.2105	60.3	59.5	-0.8	60.5	0.2
139	$FeCl_3$	3.1213	5.2426	3.4035	2.5214	3.5695	142.3	143.8	1.5	143.2	0.9
140	FeF_3	3.4495	4.6742	3.5065	2.6337	3.4173	98.0	101.2	3.2	99.5	1.5
141	Fe_2O_3	5.0000	5.0000	5.1240	6.4175	5.6097	87.4	98.1	10.7	94.0	6.6
142	FrCl	1.2416	3.2850	1.5433	0.5954	1.6795	113.0	109.7	-3.3	112.4	-0.6
143	Fr_2O	2.0690	4.7417	2.5255	1.5155	2.6395	156.9	152.3	-4.6	147.0	-9.9
144	GaS	1.6406	2.4457	1.9361	1.8729	2.1358	57.8	68.2	10.4	69.8	12.0
145	GaSe	1.5492	2.5820	1.9223	1.8454	2.1676	70.3	78.7	8.4	81.9	11.6
146	GaTe	1.4817	2.7052	1.8995	1.8001	2.2221	85.4	88.0	2.6	92.8	7.4
147	GaAS	1.8944	2.1180	2.1563	3.4836	2.5836	62.9	59.9	-3.0	60.2	-2.7
148	$GaBr_3$	2.8974	5.7434	3.3898	2.5333	3.5526	180.0	175.7	-4.3	173.0	-7.0
149	$GaCl_3$	3.1213	5.2426	3.4260	2.5736	3.4971	142.0	142.6	0.6	141.3	-0.7
150	GaF_3	3.4495	4.6742	3.5291	2.6882	3.3480	106.8	100.1	-6.7	98.0	-8.8
151	GaI_3	2.7321	6.1962	3.3316	2.4686	3.6458	205.0	204.9	-0.1	200.7	-4.3
152	GaN	2.1547	1.8660	2.2142	3.6768	2.4478	29.7	35.7	6.0	32.8	3.1
153	Ga_2O_3	5.0000	5.0000	5.1691	6.5504	5.4959	85.0	96.4	11.4	92.8	7.8
154	GaP	2.0000	2.0000	2.1676	3.5216	2.5557	52.3	49.7	-2.6	49.0	-3.3
155	Ga_2S_3	4.5981	5.4641	5.0495	6.2844	5.7285	139.8	138.1	-1.7	137.5	-2.3
156	GaSb	1.8165	2.2247	2.1305	3.3978	2.6488	76.1	68.8	-7.3	70.7	-5.4
157	$GdBr_3$	2.7139	5.9682	3.4315	2.6282	3.4245	192.6	191.3	-1.3	187.8	-4.8
158	$GdCl_3$	2.9378	5.4674	3.4677	2.6699	3.3709	151.4	158.3	6.9	156.5	5.1

159	GdI_3	2.5485	6.4209	3.3733	2.5610	3.5142	216.9	220.4	3.5	215.5	-1.4
160	Gd_2O_3	4.6330	5.4495	5.2524	6.7956	5.2976	150.6	129.2	-21.4	129.8	-20.8
161	GeF_2	2.4076	3.7405	2.5949	1.5850	2.5237	84.2	90.7	6.5	90.1	5.9
162	GeO	1.7746	2.2910	1.9652	1.9311	2.0714	50.0	54.4	4.4	54.4	4.4
163	GeS	1.6406	2.4457	1.9254	1.8527	2.1590	66.0	68.6	2.6	70.4	4.4
164	GeSe	1.5492	2.5820	1.9116	1.8255	2.1912	78.3	79.1	0.8	82.5	4.2
165	GeTe	1.4817	2.7052	1.8888	1.7807	2.2463	90.0	88.5	-1.5	93.4	3.4
166	GeI_4	3.4274	7.8226	4.1688	3.5796	4.4698	271.1	261.1	-10.0	260.9	-10.2
167	GeS_2	2.8501	3.2038	3.0929	4.5563	3.5116	87.5	81.4	-6.1	79.8	-7.7
168	$HfBr_4$	3.4427	7.4200	4.3029	3.8451	4.1611	238.6	237.1	-1.5	234.9	-3.7
169	HfC	2.2039	1.8700	2.3864	5.6737	2.8200	41.2	52.8	11.6	50.1	8.9
170	$HfCl_4$	3.7413	6.7523	4.3512	3.9063	4.0960	190.8	193.2	2.4	194.0	3.2
171	HfF_4	4.1789	5.9944	4.4885	4.0802	3.9214	136.1	137.1	1.0	142.4	6.3
172	HfI_4	3.2223	8.0236	4.2253	3.7469	4.2702	270.0	275.7	5.7	275.6	5.6
173	HfO_2	2.9129	3.0954	3.2292	4.9712	3.2186	59.3	69.8	10.5	64.3	5.0
174	HgCl	1.2416	3.2850	1.5836	0.6265	1.5960	98.4	107.9	9.5	109.3	10.9
175	HgF	1.3510	3.0956	1.6180	0.6545	1.5280	87.5	93.4	5.9	94.7	7.2
176	HgI	1.1119	3.6029	1.5522	0.6010	1.6639	121.4	129.1	7.7	129.0	7.6
177	$HgBr_2$	1.9720	4.5765	2.5183	1.5182	2.6346	172.0	149.0	-23.0	148.0	-24.0
178	HgI_2	1.8618	4.8783	2.4795	1.4794	2.7037	170.8	168.7	-2.1	166.4	-4.4
179	HgO	1.7071	2.4142	1.9814	1.9628	2.0379	70.3	62.2	-8.1	62.7	-7.6
180	HgS	1.5731	2.5689	1.9416	1.8831	2.1241	82.4	76.3	-6.1	79.0	-3.4
181	HgSe	1.4817	2.7052	1.9277	1.8555	2.1558	100.9	86.9	-14.0	91.1	-9.8
182	$HoBr_3$	2.7139	5.9682	3.4301	2.6251	3.4285	188.4	191.4	3.0	187.9	-0.5
183	HoF_3	3.2660	4.8990	3.5693	2.7856	3.2310	111.0	116.0	5.0	114.3	3.3
184	InBr	1.2098	3.3132	1.5605	0.6084	1.6437	113.0	111.6	-1.4	113.8	0.8
185	InCl	1.2845	3.1463	1.5726	0.6180	1.6180	95.0	100.4	5.4	103.1	8.1
186	InI	1.1547	3.4641	1.5411	0.5928	1.6868	130.0	121.6	-8.4	123.3	-6.7
187	InAs	1.7889	2.2361	2.1891	3.5865	2.5094	75.7	68.6	-7.1	69.1	-6.6
188	$InBr_3$	2.7918	5.8615	3.4227	2.6082	3.4507	178.8	183.7	4.9	180.4	1.6
189	$InCl_3$	3.0157	5.3607	3.4589	2.6496	3.3967	141.1	150.6	9.5	149.0	7.9
190	InF_3	3.3439	4.7923	3.5619	2.7676	3.2519	110.1	108.2	-1.9	106.3	-3.8
191	InI_3	2.6265	6.3142	3.3645	2.5416	3.5411	203.5	212.8	9.3	207.9	4.4
192	InN	2.0491	1.9841	2.2470	3.7854	2.3775	43.5	44.5	1.0	41.2	-2.3
193	In_2O_3	4.7889	5.2361	5.2348	6.7439	5.3381	108.0	113.6	5.6	112.2	4.2
194	InP	1.8944	2.1180	2.2005	3.6256	2.4823	59.8	58.5	-1.3	57.7	-2.1
195	In_2S_3	4.3869	5.7002	5.1153	6.4701	5.5641	163.6	155.1	-8.5	156.8	-6.8
196	InSb	1.7109	2.3428	2.1634	3.4982	2.5728	86.2	77.5	-8.7	79.7	-6.5
197	$IrCl_2$	2.1213	4.2426	2.5402	1.5390	2.5991	129.8	127.0	-2.8	127.1	-2.7
198	IrI_2	1.8618	4.8783	2.4773	1.4762	2.7097	159.1	168.8	9.7	166.7	7.6
199	IrO_2	2.9129	3.0954	3.2096	4.8942	3.2692	57.3	70.4	13.1	65.2	7.9
200	KBr	1.3396	2.9954	1.5618	0.6093	1.6412	95.9	91.8	-4.1	95.5	-0.4
201	KCl	1.4142	2.8284	1.5739	0.6190	1.6155	82.6	80.6	-2.0	84.4	1.8
202	KF	1.5236	2.6390	1.6082	0.6466	1.5466	66.6	66.0	-0.6	69.3	2.7
203	KH	1.7071	2.4142	1.6040	0.6432	1.5547	50.2	48.4	-1.8	51.9	1.7
204	KI	1.2845	3.1463	1.5424	0.5938	1.6842	106.3	101.8	-4.5	105.4	-0.9
205	K_2O	2.4142	3.8284	2.5867	1.5755	2.5389	94.1	94.6	0.5	93.6	-0.5

206	K_2S	2.2802	3.9831	2.5469	1.5115	2.6463	105.0	109.2	4.2	110.4	5.4
207	LaS	1.5731	2.5689	1.9351	1.8709	2.1380	71.2	76.6	5.4	79.3	8.1
208	LaSe	1.4817	2.7052	1.9213	1.8435	2.1698	81.2	87.1	5.9	91.5	10.3
209	LaTe	1.4142	2.8284	1.8985	1.7982	2.2244	88.3	96.4	8.1	102.5	14.2
210	$LaBr_3$	2.7139	5.9682	3.4320	2.6294	3.4228	182.1	191.3	9.2	187.7	5.6
211	$LaCl_3$	2.9378	5.4674	3.4682	2.6712	3.3692	144.4	158.3	13.9	156.4	12.0
212	LaF_3	3.2660	4.8990	3.5713	2.7902	3.2256	113.5	115.9	2.4	114.2	0.7
213	LaI_3	2.5485	6.4209	3.3739	2.5623	3.5125	214.8	220.4	5.6	215.5	0.7
214	LaN	1.9712	2.0908	2.2564	3.8163	2.3583	44.4	52.4	8.0	49.2	4.8
215	La_2O_3	4.6330	5.4495	5.2535	6.7989	5.2950	127.3	129.2	1.9	129.8	2.5
216	La_2S_3	4.2311	5.9136	5.1339	6.5228	5.5191	165.1	170.6	5.5	174.5	9.4
217	La_2Se_3	3.9568	6.3225	5.0925	6.4271	5.6013	202.3	201.9	-0.4	210.0	7.7
218	La_2Te_3	3.7543	6.6921	5.0242	6.2695	5.7421	231.6	229.3	-2.3	242.4	10.8
219	LiBr	1.6325	2.5811	1.5655	0.6122	1.6335	74.3	60.7	-13.6	64.7	-9.6
220	LiCl	1.7071	2.4142	1.5776	0.6219	1.6080	59.3	49.5	-9.8	53.5	-5.8
221	LiF	1.8165	2.2247	1.6120	0.6496	1.5394	35.7	34.9	-0.8	38.5	2.8
222	LiH	2.0000	2.0000	1.6077	0.6462	1.5475	20.0	17.2	-2.8	21.6	1.6
223	LiI	1.5774	2.7321	1.5461	0.5965	1.6764	86.8	70.7	-16.1	74.8	-12.0
224	Li_3N	4.1547	3.8660	3.5210	2.6655	3.3765	37.7	34.4	-3.3	29.4	-8.3
225	Li_2O	3.0000	3.0000	2.5942	1.5829	2.5270	37.6	32.5	-5.1	30.7	-6.9
226	Li_2S	2.8660	3.1547	2.5544	1.5186	2.6340	60.7	47.1	-13.6	46.7	-14.0
227	Li_2Se	2.7746	3.2910	2.5406	1.4963	2.6732	71.2	57.8	-13.4	58.0	-13.2
228	Li_2Te	2.7071	3.4142	2.5178	1.4596	2.7404	77.5	67.4	-10.1	68.6	-8.9
229	Lu_2O_3	4.6330	5.4495	5.2451	6.7742	5.3143	110.0	129.4	19.4	129.9	19.9
230	$MgBr_2$	2.2649	4.1623	2.5007	1.4915	2.6818	117.2	119.0	1.8	119.0	1.8
231	$MgCl_2$	2.4142	3.8284	2.5248	1.5152	2.6399	89.6	96.8	7.2	97.3	7.7
232	MgF_2	2.6330	3.4495	2.5935	1.5827	2.5273	57.2	68.2	11.0	67.0	9.8
233	Mg_2Ge	3.0000	3.0000	3.0706	4.3458	3.6817	73.0	67.8	-5.2	67.1	-5.9
234	MgH_2	3.0000	3.0000	2.5851	1.5744	2.5406	31.1	32.8	1.7	31.2	0.1
235	MgI_2	2.1547	4.4641	2.4619	1.4534	2.7522	129.7	138.6	8.9	137.8	8.1
236	Mg_3N_2	5.3094	4.7321	5.1507	6.4942	5.5434	87.9	72.0	-15.9	67.5	-20.4
237	MgO	2.0000	2.0000	1.9638	1.9283	2.0744	27.0	31.9	4.9	30.3	3.3
238	MgS	1.8660	2.1547	1.9240	1.8500	2.1622	50.3	46.0	-4.3	45.6	-4.7
239	Mg_3Sb_2	4.6330	5.4495	4.9834	6.0014	5.9987	130.4	139.7	9.3	138.9	8.5
240	MgSe	1.7746	2.2910	1.9101	1.8228	2.1944	62.8	56.6	-6.2	57.3	-5.5
241	MgTe	1.7071	2.4142	1.8874	1.7781	2.2496	74.5	65.9	-8.6	67.9	-6.6
242	$MnBr_2$	2.1309	4.3170	2.5126	1.5096	2.6497	138.1	131.0	-7.1	130.8	-7.3
243	$MnCl_2$	2.2802	3.9831	2.5367	1.5336	2.6083	118.2	108.8	-9.4	109.3	-8.9
244	MnF_2	2.4990	3.6042	2.6054	1.6019	2.4971	92.3	80.2	-12.1	79.0	-13.3
245	MnI_2	2.0207	4.6188	2.4738	1.4710	2.7192	150.6	150.6	0.0	149.5	-1.1
246	MnO	1.8660	2.1547	1.9757	1.9517	2.0495	59.7	44.1	-15.6	43.0	-16.7
247	MnS	1.7321	2.3094	1.9359	1.8724	2.1363	78.2	58.2	-20.0	58.7	-19.5
248	MnSe	1.6406	2.4457	1.9221	1.8449	2.1681	90.8	68.7	-22.1	70.6	-20.2
249	MnAs	1.8944	2.1180	2.1442	3.4458	2.6119	67.0	60.3	-6.7	60.9	-6.1
250	MnF_3	3.4495	4.6742	3.5170	2.6591	3.3846	104.7	100.7	-4.0	98.8	-5.9
251	Mn_2O_3	5.0000	5.0000	5.1450	6.4794	5.5561	110.5	97.3	-13.2	93.4	-17.1
252	MnP	2.0000	2.0000	2.1556	3.4834	2.5837	52.3	50.1	-2.2	49.7	-2.6

253	MnO_2	3.1180	2.8944	3.1727	4.7492	3.3690	53.1	54.0	0.9	48.2	-4.9
254	MnSi	2.2361	1.7889	2.4075	5.7958	2.7606	46.5	47.4	0.9	43.8	-2.7
255	$MoBr_3$	2.7918	5.8615	3.4063	2.5708	3.5008	175.0	184.5	9.5	181.7	6.7
256	MoC	2.2910	1.7746	2.3724	5.6111	2.8515	34.3	45.2	10.9	42.8	8.5
257	MoI_4	3.3094	7.9282	4.2114	3.7056	4.3178	266.2	268.5	2.3	267.7	1.5
258	$MoCl_5$	4.6310	7.9839	5.2150	5.2400	4.7710	238.0	222.1	-15.9	222.0	-16.0
259	$MoCl_6$	5.4259	9.3304	6.0872	6.7550	5.3294	255.0	259.2	4.2	253.2	-1.8
260	MoO_3	4.1832	3.8452	4.4042	8.5965	4.1878	77.7	79.0	1.3	81.0	3.3
261	NaBr	1.4490	2.8059	1.5756	0.6198	1.6134	86.8	78.1	-8.7	81.8	-5.0
262	NaCl	1.5236	2.6390	1.5877	0.6297	1.5881	72.1	66.9	-5.2	70.6	-1.5
263	NaF	1.6330	2.4495	1.6220	0.6577	1.5204	51.1	52.3	1.2	55.5	4.4
264	NaH	1.8165	2.2247	1.6178	0.6543	1.5284	40.0	34.7	-5.3	38.2	-1.8
265	NaI	1.3938	2.9568	1.5562	0.6040	1.6557	98.5	88.1	-10.4	91.8	-6.7
266	Na_2O	2.6330	3.4495	2.6144	1.6026	2.4959	75.1	67.5	-7.6	65.8	-9.3
267	Na_2S	2.4990	3.6042	2.5745	1.5376	2.6015	79.5	82.0	2.5	82.4	2.9
268	Na_2Te	2.3401	3.8637	2.5379	1.4778	2.7066	94.6	102.3	7.7	104.6	10.0
269	$NbCl_3$	3.0157	5.3607	3.4480	2.6244	3.4293	147.4	151.2	3.8	149.8	2.4
270	NbN	2.0491	1.9841	2.2361	3.7494	2.4004	44.0	44.8	0.8	41.8	-2.2
271	NbC	2.2910	1.7746	2.3800	5.6447	2.8345	36.4	45.0	8.6	42.3	5.9
272	$NbCl_4$	3.8284	6.6569	4.3447	3.8863	4.1170	184.2	185.6	1.4	186.6	2.4
273	NbO_2	3.0000	3.0000	3.2227	4.9457	3.2351	54.5	62.0	7.5	55.8	1.3
274	$NbBr_5$	4.2577	8.8186	5.1646	5.1956	4.8117	258.8	276.3	17.5	273.5	14.7
275	$NbCl_5$	4.6310	7.9839	5.2249	5.2782	4.7365	210.5	221.6	11.1	221.4	10.9
276	NbF_5	5.1779	7.0366	5.3967	5.5133	4.5345	160.3	152.0	-8.3	161.9	1.6
277	Nb_2O_5	7.1909	6.8257	7.6449	13.4342	7.4437	137.3	140.4	3.1	141.9	4.6
278	$NiBr_2$	2.1309	4.3170	2.4959	1.4843	2.6949	136.1	131.8	-4.3	132.5	-3.6
279	$NiCl_2$	2.2802	3.9831	2.5200	1.5079	2.6528	97.7	109.7	12.0	110.8	13.1
280	NiF_2	2.4990	3.6042	2.5887	1.5750	2.5397	73.6	81.0	7.4	80.4	6.8
281	NiI_2	2.0207	4.6188	2.4571	1.4464	2.7656	154.1	151.5	-2.6	151.3	-2.8
282	NiO	1.8660	2.1547	1.9590	1.9189	2.0845	38.0	44.7	6.7	43.8	5.8
283	NiS	1.7321	2.3094	1.9192	1.8410	2.1727	53.0	58.8	5.8	59.6	6.6
284	NiAs	1.8944	2.1180	2.1373	3.4243	2.6282	51.9	60.5	8.6	61.3	9.4
285	NiSb	1.8165	2.2247	2.1116	3.3400	2.6946	78.3	69.5	-8.8	71.7	-6.6
286	$NpCl_3$	2.8772	5.5655	3.4684	2.6716	3.3688	160.4	165.2	4.8	163.3	2.9
287	NpF_3	3.2054	4.9971	3.5714	2.7906	3.2252	118.5	122.8	4.3	121.3	2.8
288	$NpCl_4$	3.6736	6.8401	4.3718	3.9698	4.0304	199.7	199.0	-0.7	199.3	-0.4
289	NpF_4	4.1111	6.0822	4.5091	4.1466	3.8586	152.8	143.0	-9.8	148.2	-4.6
290	NpO_2	2.8452	3.1832	3.2498	5.0520	3.1671	80.3	76.0	-4.3	70.9	-9.4
291	NpF_5	5.0083	7.2038	5.4229	5.6188	4.4494	171.7	165.5	-6.2	173.9	2.2
292	Np_2O_5	6.8516	7.1602	7.6973	13.6914	7.3039	180.0	168.4	-11.6	171.1	-8.9
293	$OsCl_2$	2.1213	4.2426	2.5402	1.5390	2.5991	129.8	127.0	-2.8	127.1	-2.7
294	OsF_2	2.3401	3.8637	2.6089	1.6075	2.4883	106.8	98.4	-8.4	97.2	-9.6
295	OsF_3	3.2660	4.8990	3.5629	2.7701	3.2490	117.2	116.3	-0.9	114.6	-2.6
296	OsP_2	3.0801	2.9258	3.5522	9.1281	3.9438	82.1	94.2	12.1	90.5	8.4
297	$PaCl_3$	2.8772	5.5655	3.4681	2.6709	3.3696	159.1	165.2	6.1	163.3	4.2
298	$PaBr_4$	3.3750	7.5078	4.3253	3.9131	4.0888	234.0	242.8	8.8	240.1	6.1
299	$PaCl_4$	3.6736	6.8401	4.3735	3.9753	4.0249	196.8	198.9	2.1	199.2	2.4

300	PaF_4	4.1111	6.0822	4.5109	4.1523	3.8533	150.7	142.9	-7.8	148.2	-2.5
301	PaO_2	2.8452	3.1832	3.2516	5.0590	3.1627	74.5	75.9	1.4	70.8	-3.7
302	$PaBr_5$	4.0881	8.9858	5.1956	5.3135	4.7050	289.0	289.5	0.5	287.2	-1.8
303	$PaCl_5$	4.4614	8.1512	5.2560	5.3979	4.6314	238.0	234.9	-3.1	233.3	-4.7
304	$PbBr_2$	1.9196	4.6898	2.5133	1.5107	2.6478	161.5	156.6	-4.9	155.2	-6.3
305	$PbCl_2$	2.0689	4.3560	2.5374	1.5347	2.6063	136.0	134.4	-1.6	134.2	-1.8
306	PbF_2	2.2876	3.9770	2.6061	1.6031	2.4952	110.5	105.8	-4.7	104.6	-5.9
307	PbI_2	1.8094	4.9916	2.4745	1.4721	2.7172	174.9	176.2	1.3	173.6	-1.3
308	PbO	1.6547	2.5275	1.9765	1.9531	2.0480	66.5	69.7	3.2	71.1	4.6
309	PbS	1.5207	2.6822	1.9366	1.8738	2.1347	91.2	83.8	-7.4	87.5	-3.7
310	PbSe	1.4293	2.8185	1.9228	1.8463	2.1665	102.5	94.3	-8.2	99.7	-2.8
311	PbTe	1.3618	2.9417	1.9000	1.8010	2.2210	110.0	103.7	-6.3	110.7	0.7
312	PbO_2	2.9129	3.0954	3.2408	5.0167	3.1893	68.6	69.4	0.8	63.7	-4.9
313	$PdCl_2$	2.1888	4.1194	2.5387	1.5366	2.6031	105.0	118.7	13.7	119.1	14.1
314	PdF_2	2.4076	3.7405	2.6074	1.6051	2.4921	88.8	90.1	1.3	89.0	0.2
315	PdI_2	1.9293	4.7551	2.4758	1.4740	2.7138	150.7	160.5	9.8	159.0	8.3
316	PdO	1.7746	2.2910	1.9777	1.9555	2.0455	56.1	54.0	-2.1	53.7	-2.4
317	PdS	1.6406	2.4457	1.9379	1.8761	2.1320	56.5	68.1	11.6	69.7	13.2
318	PdTe	1.4817	2.7052	1.9013	1.8033	2.2182	89.7	87.9	-1.8	92.7	3.0
319	PdS_2	2.7321	3.3094	3.1269	4.6841	3.4158	87.9	89.9	2.0	88.2	0.3
320	$PdTe_2$	2.4142	3.8284	3.0537	4.5022	3.5538	126.7	128.7	2.0	134.0	7.3
321	$PoCl_4$	3.6736	6.8401	4.3757	3.9820	4.0181	196.8	198.8	2.0	199.1	2.3
322	PoO_2	2.8452	3.1832	3.2538	5.0676	3.1573	71.0	75.8	4.8	70.7	-0.3
323	$PtBr_2$	1.9720	4.5765	2.5101	1.5058	2.6563	154.9	149.4	-5.5	148.9	-6.0
324	$PtCl_2$	2.1213	4.2426	2.5342	1.5298	2.6148	129.8	127.3	-2.5	127.7	-2.1
325	PtO	1.7071	2.4142	1.9732	1.9468	2.0547	56.5	62.5	6.0	63.2	6.7
326	PtS	1.5731	2.5689	1.9334	1.8678	2.1416	55.1	76.6	21.5	79.4	24.3
327	$PtBr_4$	3.4427	7.4200	4.2833	3.7856	4.2265	251.2	238.1	-13.1	236.6	-14.6
328	$PtCl_4$	3.7413	6.7523	4.3316	3.8458	4.1604	205.2	194.2	-11.0	195.2	-10.0
329	PtI_4	3.2223	8.0236	4.2057	3.6889	4.3373	281.4	276.7	-4.7	278.0	-3.4
330	PtO_2	2.9129	3.0954	3.2096	4.8942	3.2692	69.1	70.4	1.3	65.2	-3.9
331	PtS_2	2.6449	3.4048	3.1299	4.6955	3.4075	74.7	97.7	23.0	97.0	22.3
332	$PuBr_3$	2.6533	6.0663	3.4322	2.6298	3.4223	192.9	198.2	5.3	194.5	1.6
333	$PuCl_3$	2.8772	5.5655	3.4684	2.6716	3.3687	159.0	165.2	6.2	163.3	4.3
334	PuF_3	3.2054	4.9971	3.5714	2.7906	3.2251	113.0	122.8	9.8	121.3	8.3
335	PuH_3	3.7559	4.3229	3.5588	2.7760	3.2420	64.9	69.7	4.8	66.0	1.1
336	PuI_3	2.4880	6.5190	3.3740	2.5626	3.5120	224.0	227.4	3.4	222.6	-1.4
337	PuN	1.9106	2.1889	2.2565	3.8169	2.3580	72.4	59.3	-13.1	56.6	-15.8
338	Pu_2O_3	4.5119	5.6458	5.2538	6.7999	5.2942	152.3	143.1	-9.2	145.7	-6.6
339	Pu_2s_3	4.1099	6.1099	5.1343	6.5238	5.5183	192.5	184.5	-8.0	190.5	-2.0
340	PuF_4	4.1111	6.0822	4.5084	4.1443	3.8608	161.9	143.0	-18.9	148.3	-13.6
341	PuO_2	2.8452	3.1832	3.2491	5.0492	3.1688	82.4	76.0	-6.4	70.9	-11.5
342	RbBr	1.2649	3.1623	1.5525	0.6023	1.6604	110.0	102.9	-7.1	106.2	-3.8
343	RbCl	1.3396	2.9954	1.5645	0.6118	1.6344	91.7	91.7	0.0	95.3	3.6
344	RbF	1.4490	2.8059	1.5989	0.6391	1.5648	75.3	77.1	1.8	80.2	4.9
345	RbI	1.2098	3.3132	1.5331	0.5869	1.7039	118.4	112.9	-5.5	115.9	-2.5
346	Rb_2O	2.2649	4.1623	2.5681	1.5572	2.5686	114.6	116.5	1.9	114.9	0.3

347	Rb_2S	2.1309	4.3170	2.5283	1.4940	2.6774	133.1	131.2	-1.9	131.8	-1.3
348	ReF_4	4.1789	5.9944	4.4689	4.0170	3.9830	150.7	138.1	-12.6	143.1	-7.6
349	ReO_2	2.9129	3.0954	3.2096	4.8942	3.2692	62.8	70.4	7.6	65.2	2.4
350	ReSi	2.0309	1.9899	2.4444	5.9728	2.6788	55.4	64.4	9.0	60.2	4.8
351	$ReCl_5$	4.5355	8.0711	5.2037	5.1964	4.8110	230.3	230.6	0.3	230.6	0.3
352	ReF_5	5.0825	7.1237	5.3754	5.4278	4.6059	175.8	160.9	-14.9	169.8	-6.0
353	ReO_3	4.0801	3.9258	4.3861	8.4895	4.2405	80.8	87.4	6.6	88.7	7.9
354	Re_2O_7	9.3094	8.7321	9.9307	21.0254	9.3220	207.1	197.0	-10.1	206.2	-0.9
355	$RhCl_2$	2.1888	4.1194	2.5387	1.5366	2.6031	121.4	118.7	-2.7	119.1	-2.3
356	RhO	1.7746	2.2910	1.9777	1.9555	2.0455	54.1	54.0	-0.1	53.7	-0.4
357	$RhBr_3$	2.7918	5.8615	3.4021	2.5614	3.5138	188.4	184.8	-3.6	182.0	-6.4
358	RhF_3	3.3439	4.7923	3.5414	2.7179	3.3113	108.9	109.2	0.3	107.5	-1.4
359	Rh_2O_3	4.7889	5.2361	5.1937	6.6228	5.4357	110.9	115.1	4.2	113.1	2.2
360	$SbCl_3$	2.9378	5.4674	3.4541	2.6385	3.4110	184.1	159.0	-25.1	157.4	-26.7
361	SbF_3	3.2660	4.8990	3.5571	2.7560	3.2656	127.3	116.5	-10.8	115.0	-12.3
362	SbI_3	2.5485	6.4209	3.3597	2.5309	3.5561	215.5	221.2	5.7	216.8	1.3
363	Sb_2O_3	4.6330	5.4495	5.2252	6.7156	5.3607	132.7	130.1	-2.6	130.4	-2.3
364	Sb_2S_3	4.2311	5.9136	5.1057	6.4429	5.5875	182.0	171.6	-10.4	175.4	-6.6
365	Sb_2Se_3	3.9568	6.3225	5.0642	6.3483	5.6708	211.4	202.9	-8.5	211.2	-0.2
366	Sb_2Te_3	3.7543	6.6921	4.9959	6.1926	5.8134	234.0	230.4	-3.6	243.9	9.9
367	Sb_2O_5	7.1909	6.8257	7.6179	13.3016	7.5179	125.1	141.1	16.0	141.9	16.8
368	$ScBr_3$	2.8974	5.7434	3.4165	2.5941	3.4695	167.5	174.2	6.7	170.8	3.3
369	$ScCl_3$	3.1213	5.2426	3.4527	2.6353	3.4152	121.3	141.2	19.9	139.4	18.1
370	ScF_3	3.4495	4.6742	3.5557	2.7526	3.2696	92.0	98.8	6.8	96.5	4.5
371	ScN	2.1547	1.8660	2.2408	3.7649	2.3905	29.7	34.9	5.2	31.3	1.6
372	Sc_2O_3	5.0000	5.0000	5.2224	6.7074	5.3672	77.0	94.5	17.5	91.5	14.5
373	SiC	2.5820	1.5492	2.2525	5.0735	3.1537	16.5	25.9	9.4	28.1	11.6
374	SiI_4	3.6004	7.7028	4.0914	3.3505	4.7754	258.1	253.4	-4.7	255.4	-2.7
375	Si_3N_4	8.4918	5.7879	7.8042	14.9710	9.6186	101.3	88.0	-13.3	93.3	-8.0
376	SiO_2	3.2910	2.7746	3.0952	4.4452	3.5994	43.4	44.3	0.9	40.3	-3.1
377	SiS_2	3.0230	3.0840	3.0155	4.2647	3.7517	67.0	72.0	5.0	72.2	5.2
378	$SmCl_2$	2.1213	4.2426	2.5330	1.5279	2.6179	127.7	127.4	-0.3	127.8	0.1
379	SmF_2	2.3401	3.8637	2.6017	1.5960	2.5063	96.3	98.7	2.4	97.9	1.6
380	SmF_3	3.2660	4.8990	3.5711	2.7898	3.2260	113.0	115.9	2.9	114.2	1.2
381	Sm_2O_3	4.6330	5.4495	5.2532	6.7980	5.2957	151.0	129.2	-21.8	129.8	-21.2
382	$SnBr_2$	1.9720	4.5765	2.5183	1.5182	2.6346	149.9	149.0	-0.9	148.0	-1.9
383	$SnCl_2$	2.1213	4.2426	2.5424	1.5424	2.5934	130.0	126.9	-3.1	126.9	-3.1
384	SnI_2	1.8618	4.8783	2.6111	1.6110	2.4829	167.9	163.9	-4.0	158.4	-9.5
385	SnO	1.7071	2.4142	1.9814	1.9628	2.0379	57.2	62.2	5.0	62.7	5.5
386	SnS	1.5731	2.5689	1.9416	1.8831	2.1241	77.0	76.3	-0.7	79.0	2.0
387	SnSe	1.4817	2.7052	1.9277	1.8555	2.1558	98.2	86.9	-11.3	91.1	-7.1
388	SnTe	1.4142	2.8284	1.9050	1.8100	2.2100	98.8	96.2	-2.6	102.1	3.3
389	SnO_2	3.0000	3.0000	3.2250	4.9546	3.2293	49.0	61.9	12.9	55.7	6.7
390	SnS_2	2.7321	3.3094	3.1453	4.7535	3.3660	87.0	89.2	2.2	87.0	0.0
391	$SnSe_2$	2.5492	3.5820	3.1176	4.6837	3.4161	118.1	109.9	-8.2	111.0	-7.1
392	$SrBr_2$	2.0395	4.4533	2.5138	1.5114	2.6465	141.5	140.9	-0.6	140.6	-0.9
393	$SrCl_2$	2.1888	4.1194	2.5379	1.5355	2.6051	117.2	118.7	1.5	119.2	2.0

394	SrF_2	2.4076	3.7405	2.6066	1.6038	2.4940	89.6	90.1	0.5	89.1	-0.5
395	SrH_2	2.7746	3.2910	2.5982	1.5955	2.5071	49.8	54.7	4.9	52.9	3.1
396	SrI_2	1.9293	4.7551	2.4750	1.4728	2.7159	159.1	160.5	1.4	159.1	0.0
397	Sr_3N_2	4.6332	5.6050	5.1900	6.5810	5.4703	134.8	138.5	3.7	140.7	5.9
398	SrO	1.7746	2.2910	1.9769	1.9540	2.0470	54.4	54.0	-0.4	53.7	-0.7
399	SrS	1.6406	2.4457	1.9371	1.8747	2.1337	68.2	68.1	-0.1	69.8	1.6
400	$TaCl_3$	2.9378	5.4674	3.4480	2.6244	3.4293	154.9	159.3	4.4	157.9	3.0
401	TaN	1.9712	2.0908	2.2361	3.7494	2.4004	42.7	52.9	10.2	50.4	7.7
402	TaC	2.2039	1.8700	2.3800	5.6447	2.8345	42.3	53.0	10.7	50.5	8.2
403	$TaCl_4$	3.7413	6.7523	4.3447	3.8863	4.1170	192.6	193.6	1.0	194.4	1.8
404	$TaBr_5$	4.1623	8.9057	5.1646	5.1956	4.8117	305.4	284.3	-21.1	282.8	-22.6
405	$TaCl_5$	4.5355	8.0711	5.2249	5.2782	4.7365	234.1	229.6	-4.5	229.0	-5.1
406	TaF_5	5.0825	7.1237	5.3967	5.5133	4.5345	171.7	159.9	-11.8	169.0	-2.7
407	TaI_5	3.8868	9.6603	5.0676	5.0629	4.9379	343.0	332.2	-10.8	344.8	1.8
408	Ta_2O_5	7.0000	7.0000	7.6449	13.4342	7.4437	143.1	156.3	13.2	157.5	14.4
409	$TeBr_4$	3.4427	7.4200	4.3275	3.9197	4.0819	243.7	235.9	-7.8	233.0	-10.7
410	$TeCl_4$	3.7413	6.7523	4.3757	3.9820	4.0181	201.0	192.0	-9.0	192.6	-8.4
411	TeO_2	2.9129	3.0954	3.2538	5.0676	3.1573	74.1	69.0	-5.1	63.2	-10.9
412	ThN	1.9106	2.1889	2.2554	3.8131	2.3603	57.4	59.4	2.0	56.7	-0.7
413	ThP	1.7559	2.3229	2.2089	3.6521	2.4643	70.3	73.3	3.0	73.6	3.3
414	Th_2S_3	4.1099	6.1099	5.1320	6.5173	5.5237	180.0	184.6	4.6	190.5	10.5
415	$ThBr_4$	3.3750	7.5078	4.3268	3.9178	4.0839	230.0	242.7	12.7	240.0	10.0
416	ThC	2.1361	1.9578	2.4104	5.7809	2.7677	50.2	59.1	8.9	55.6	5.4
417	$ThCl_4$	3.6736	6.8401	4.3751	3.9801	4.0200	190.4	198.9	8.5	199.1	8.7
418	ThF_4	4.1111	6.0822	4.5125	4.1573	3.8486	142.0	142.9	0.9	148.1	6.1
419	Th_3N_4	7.1543	7.0137	8.2778	17.0586	8.4415	183.0	187.1	4.1	174.7	-8.3
420	ThO_2	2.8452	3.1832	3.2531	5.0651	3.1589	65.2	75.9	10.7	70.8	5.6
421	Th_3P_4	6.5355	7.5496	8.0918	16.3384	8.8136	221.8	241.3	19.5	221.4	-0.4
422	ThS_2	2.5772	3.4926	3.1734	4.8594	3.2926	96.2	103.0	6.8	102.1	5.9
423	$TiCl_2$	2.2802	3.9831	2.5387	1.5366	2.6031	87.4	108.7	21.3	109.1	21.7
424	TiH_2	2.8660	3.1547	2.5990	1.5967	2.5052	29.7	44.7	15.0	42.8	13.1
425	TiO	1.8660	2.1547	1.9777	1.9555	2.0455	50.0	44.0	-6.0	42.9	-7.1
426	TiS	1.7321	2.3094	1.9379	1.8761	2.1320	56.5	58.1	1.6	58.6	2.1
427	$TiBr_3$	2.8974	5.7434	3.4021	2.5614	3.5138	176.6	175.0	-1.6	171.9	-4.7
428	$TiCl_3$	3.1213	5.2426	3.4383	2.6021	3.4588	139.7	141.9	2.2	140.4	0.7
429	TiF_3	3.4495	4.6742	3.5414	2.7179	3.3113	88.0	99.5	11.5	97.3	9.3
430	TiI_3	2.7321	6.1962	3.3440	2.4959	3.6059	192.6	204.2	11.6	199.5	6.9
431	TiN	2.1547	1.8660	2.2265	3.7175	2.4210	30.3	35.3	5.0	32.1	1.8
432	Ti_2O_3	5.0000	5.0000	5.1937	6.6228	5.4357	78.8	95.5	16.7	92.1	13.3
433	TiC	2.4090	1.6690	2.3607	5.5583	2.8786	24.2	35.7	11.5	33.6	9.4
434	TiF_4	4.3840	5.7934	4.4628	3.9972	4.0028	134.0	120.7	-13.3	125.9	-8.1
435	TiI_4	3.4274	7.8226	4.1996	3.6707	4.3589	249.4	259.4	10.0	257.3	7.9
436	TiO_2	3.1180	2.8944	3.2034	4.8700	3.2854	50.6	52.9	2.3	46.3	-4.3
437	TiS_2	2.8501	3.2038	3.1237	4.6722	3.4245	78.4	80.2	1.8	77.5	-0.9
438	TiSi	2.2361	1.7889	2.4383	5.9433	2.6921	49.0	46.8	-2.2	42.1	-6.9
439	TlBr	1.1670	3.4520	1.5539	0.6033	1.6575	120.5	119.9	-0.6	121.1	0.6
440	TlCl	1.2416	3.2850	1.5660	0.6129	1.6316	111.3	108.7	-2.6	110.6	-0.7

441	TlF	1.3510	3.0956	1.6003	0.6402	1.5620	95.8	94.1	-1.7	95.9	0.1
442	TlI	1.1119	3.6029	1.5345	0.5879	1.7009	127.6	129.9	2.3	130.5	2.9
443	Tl_2S	1.9351	4.8964	2.5311	1.4967	2.6726	159.1	165.3	6.2	161.1	2.0
444	Tl_2Se	1.8436	5.0327	2.5172	1.4747	2.7124	172.0	176.0	4.0	172.4	0.4
445	$TlBr_3$	2.7139	5.9682	3.4296	2.6239	3.4300	176.6	191.4	14.8	187.9	11.3
446	$TlCl_3$	2.9378	5.4674	3.4658	2.6656	3.3764	152.4	158.4	6.0	156.6	4.2
447	Tl_2O_3	4.6330	5.4495	5.2486	6.7845	5.3062	137.3	129.3	-8.0	129.9	-7.4
448	TmF_3	3.2660	4.8990	3.5683	2.7830	3.2339	115.6	116.0	0.4	114.3	-1.3
449	Tm_2O_3	4.6330	5.4495	5.2476	6.7814	5.3086	139.8	129.4	-10.4	129.9	-9.9
450	UBr_3	2.6533	6.0663	3.4320	2.6294	3.4228	192.0	198.2	6.2	194.5	2.5
451	UCl_3	2.8772	5.5655	3.4682	2.6712	3.3692	159.0	165.2	6.2	163.3	4.3
452	UF_3	3.2054	4.9971	3.5713	2.7902	3.2256	123.4	122.8	-0.6	121.3	-2.1
453	UH_3	3.7559	4.3229	3.5587	2.7756	3.2425	63.7	69.7	6.0	66.0	2.3
454	UI_3	2.4880	6.5190	3.3739	2.5623	3.5125	224.0	227.4	3.4	222.6	-1.4
455	UN	1.9106	2.1889	2.2564	3.8163	2.3583	62.4	59.3	-3.1	56.6	-5.8
456	U_2S_3	4.1099	6.1099	5.1339	6.5228	5.5191	188.4	184.5	-3.9	190.5	2.1
457	U_3Bi_4	5.5592	8.8412	8.0809	16.2942	8.8375	342.9	340.8	-2.1	341.2	-1.7
458	UBr_4	3.3750	7.5078	4.3247	3.9115	4.0905	238.0	242.8	4.8	240.1	2.1
459	UC	2.1361	1.9578	2.4083	5.7716	2.7722	59.2	59.2	0.0	55.7	-3.5
460	UCl_4	3.6736	6.8401	4.3730	3.9736	4.0265	198.5	199.0	0.5	199.3	0.8
461	UF_4	4.1111	6.0822	4.5104	4.1506	3.8549	151.7	143.0	-8.7	148.2	-3.5
462	UO_2	2.8452	3.1832	3.2510	5.0569	3.1640	77.0	75.9	-1.1	70.8	-6.2
463	US_2	2.5772	3.4926	3.1713	4.8516	3.2979	110.4	103.1	-7.3	102.2	-8.2
464	UBr_5	4.0881	8.9858	5.1925	5.3016	4.7156	293.0	289.6	-3.4	287.5	-5.5
465	UCl_5	4.4614	8.1512	5.2528	5.3858	4.6418	242.7	235.0	-7.7	233.5	-9.2
466	UCl_6	5.2426	9.4853	6.1301	6.9537	5.1771	285.8	272.0	-13.8	264.6	-21.2
467	UO_3	4.0000	4.0000	4.4472	8.8493	4.0681	96.1	92.8	-3.3	96.5	0.4
468	US_3	3.5981	4.4641	4.3276	8.4900	4.2403	138.5	132.7	-5.8	138.3	-0.2
469	VBr_2	2.1309	4.3170	2.5092	1.5044	2.6589	125.6	131.1	5.5	131.2	5.6
470	V_2C	3.0230	3.0840	3.1018	4.4396	3.6039	59.9	69.5	9.6	67.4	7.5
471	VCl_2	2.2802	3.9831	2.5333	1.5283	2.6173	97.1	109.0	11.9	109.6	12.5
472	VF_2	2.4990	3.6042	2.6020	1.5964	2.5057	79.5	80.4	0.9	79.3	-0.2
473	VI_2	2.0207	4.6188	2.4704	1.4660	2.7286	146.5	150.8	4.3	149.9	3.4
474	VO	1.8660	2.1547	1.9723	1.9449	2.0566	38.9	44.2	5.3	43.2	4.3
475	VCl_3	3.1213	5.2426	3.4313	2.5858	3.4806	131.0	142.3	11.3	140.9	9.9
476	VF_3	3.4495	4.6742	3.5343	2.7009	3.3322	97.1	99.8	2.7	97.7	0.6
477	VI_3	2.7321	6.1962	3.3369	2.4803	3.6286	203.1	204.6	1.5	200.1	-3.0
478	VN	2.1547	1.8660	2.2194	3.6942	2.4362	37.3	35.5	-1.8	32.5	-4.8
479	V_2O_3	5.0000	5.0000	5.1796	6.5814	5.4700	98.3	96.0	-2.3	92.5	-5.8
480	V_2S_3	4.5981	5.4641	5.0601	6.3142	5.7015	127.7	137.7	10.0	137.1	9.4
481	VC	2.4090	1.6690	2.3503	5.5120	2.9028	27.6	35.9	8.3	34.2	6.6
482	VF_4	4.3840	5.7934	4.4525	3.9639	4.0364	121.4	121.2	-0.2	126.2	4.8
483	VO_2	3.1180	2.8944	3.1931	4.8294	3.3130	51.5	53.2	1.7	46.9	-4.6
484	V_2O_4	6.2361	5.7889	6.3862	9.6589	6.6260	103.0	107.7	4.7	105.5	2.5
485	V_2O_5	7.4495	6.6330	7.5674	13.0538	7.6606	131.0	123.0	-8.0	123.8	-7.2
486	WCl_4	3.7413	6.7523	4.3398	3.8712	4.1331	198.3	193.8	-4.5	194.7	-3.6
487	WF_4	4.1789	5.9944	4.4772	4.0436	3.9569	152.8	137.7	-15.1	142.8	-10.0

488	WO_2	2.9129	3.0954	3.2178	4.9266	3.2477	50.5	70.1	19.6	64.8	14.3
489	WBr_5	4.1623	8.9057	5.1582	5.1711	4.8345	272.0	284.6	12.6	283.5	11.5
490	WCl_5	4.5355	8.0711	5.2185	5.2533	4.7589	217.6	229.9	12.3	229.5	11.9
491	WBr_6	4.8749	10.4127	6.0189	6.6678	5.3990	314.0	332.5	18.5	335.3	21.3
492	WO_3	4.0801	3.9258	4.4083	8.6204	4.1761	75.9	86.9	11.0	89.0	13.1
493	YCl_3	3.0157	5.3607	3.4663	2.6667	3.3750	136.8	150.3	13.5	148.5	11.7
494	YF_3	3.3439	4.7923	3.5693	2.7854	3.2311	100.0	107.9	7.9	106.0	6.0
495	YI_3	2.6265	6.3142	3.3719	2.5579	3.5185	207.2	212.4	5.2	207.3	0.1
496	YN	2.0491	1.9841	2.2544	3.8098	2.3623	37.7	44.4	6.7	40.8	3.1
497	Y_2O_3	4.7889	5.2361	5.2496	6.7873	5.3040	99.1	113.1	14.0	111.9	12.8
498	$YbCl_2$	2.1213	4.2426	2.5400	1.5386	2.5997	130.6	127.0	-3.6	127.1	-3.5
499	YbS	1.5731	2.5689	1.9391	1.8786	2.1293	69.1	76.4	7.3	79.1	10.0
500	Yb_2O_3	4.6330	5.4495	5.2464	6.7780	5.3113	133.1	129.4	-3.7	129.9	-3.2
501	Zn_3As_2	4.3869	5.7002	5.0432	6.1703	5.8344	168.2	158.8	-9.4	159.7	-8.5
502	$ZnBr_2$	2.1309	4.3170	2.5034	1.4957	2.6743	138.5	131.4	-7.1	131.7	-6.8
503	$ZnCl_2$	2.2802	3.9831	2.5276	1.5195	2.6324	108.4	109.3	0.9	110.1	1.7
504	ZnF_2	2.4990	3.6042	2.5963	1.5872	2.5202	73.7	80.6	6.9	79.8	6.1
505	ZnI_2	2.0207	4.6188	2.4647	1.4575	2.7444	161.1	151.1	-10.0	150.5	-10.6
506	ZnO	1.8660	2.1547	1.9666	1.9337	2.0685	43.7	44.4	0.7	43.5	-0.2
507	ZnS	1.7321	2.3094	1.9267	1.8552	2.1561	57.7	58.5	0.8	59.2	1.5
508	ZnSe	1.6406	2.4457	1.9129	1.8280	2.1882	70.3	69.1	-1.2	71.1	0.8
509	ZnTe	1.5731	2.5689	1.8902	1.7832	2.2432	77.9	78.4	0.5	81.9	4.0
510	$ZrBr_4$	3.5298	7.3246	4.3049	3.8511	4.1547	224.0	229.0	5.0	226.5	2.5
511	ZrC	2.2910	1.7746	2.3884	5.6824	2.8157	33.3	44.8	11.5	41.8	8.5
512	$ZrCl_4$	3.8284	6.6569	4.3531	3.9123	4.0897	181.6	185.2	3.6	186.2	4.6
513	ZrI_4	3.3094	7.9282	4.2273	3.7527	4.2636	260.0	267.6	7.6	265.9	5.9
514	ZrO_2	3.0000	3.0000	3.2311	4.9788	3.2136	50.4	61.8	11.4	55.4	5.0
515	ZrS_2	2.7321	3.3094	3.1514	4.7766	3.3496	78.3	89.0	10.7	86.7	8.4
516	ZrSi	2.1180	1.8944	2.4660	6.0761	2.6333	58.2	56.0	-2.2	50.9	-7.3
517	Ag_2CrO_4	6.5878	7.9182	6.9267	9.6836	6.9560	217.6	187.7	-29.9	206.7	-10.9
518	Ag_2SO_4	6.7924	7.8169	6.7828	8.8358	7.4774	200.4	179.8	-20.6	197.2	-3.2
519	$AgBrO_3$	4.7279	5.4940	5.0497	7.1363	5.1967	151.9	130.1	-21.8	138.3	-13.6
520	$AgClO_3$	4.8572	5.3976	4.9421	6.6084	5.5551	142.0	124.5	-17.5	129.0	-13.0
521	$AgIO_3$	4.6325	5.5811	5.1719	7.7358	4.8557	149.4	134.6	-14.8	146.5	-2.9
522	$AlPO_4$	6.5689	5.5731	6.2683	9.3632	6.8694	90.8	87.7	-3.1	85.7	-5.1
523	$BaSO_4$	6.2346	6.0689	6.1403	9.1722	7.0419	132.2	127.4	-4.8	128.0	-4.2
524	$Ca_3(PO_4)_2$	13.4265	12.8783	13.2978	17.8921	14.4443	236.0	239.7	3.7	236.8	0.8
525	$CaSO_4$	6.3936	5.8094	6.1551	9.2012	7.0113	106.5	108.5	2.0	107.2	0.7
526	$CdSO_4$	6.3021	5.9456	6.1546	9.2004	7.0122	123.0	118.5	-4.5	118.1	-4.9
527	$CoSO_4$	6.3936	5.8094	6.1251	9.1423	7.0743	118.0	109.6	-8.4	108.0	-10.0
528	Cs_2SO_4	6.6822	8.1188	6.7195	8.7737	7.5787	211.9	200.1	-11.8	219.4	7.5
529	$CuSO_4$	6.3936	5.8094	6.1388	9.1694	7.0449	109.2	109.1	-0.1	107.7	-1.5
530	Fe_2SiO_4	7.0230	7.0840	6.9799	8.2175	7.8408	145.2	137.2	-8.0	136.9	-8.3
531	$FeMoO_4$	6.0492	5.9999	6.3466	10.4826	6.3085	129.3	125.5	-3.8	130.8	1.5
532	$FeSO_4$	6.3936	5.8094	6.1159	9.1244	7.0943	107.5	110.0	2.5	108.3	0.8
533	$FeWO_4$	5.9461	6.0805	6.3506	10.5066	6.2969	131.8	133.4	1.6	138.7	6.9
534	K_2CuCl_4	5.1087	9.6400	5.6739	2.7554	5.8671	270.7	272.9	2.2	265.0	-5.7

535	K_2SiF_6	7.6042	10.9515	7.5710	4.9417	7.4785	226.0	248.2	22.2	237.4	11.4
536	K_2SnCl_6	6.6569	12.3137	7.4947	5.1313	7.3406	366.5	349.1	-17.4	357.2	-9.3
537	K_2SO_4	6.9417	7.4831	6.7603	8.8138	7.5124	175.6	159.3	-16.3	174.4	-1.2
538	Li_2SiO_3	6.2910	5.7746	5.6895	6.0281	6.1264	79.8	77.9	-1.9	83.4	3.6
539	Li_2SO_4	7.5275	6.6547	6.7678	8.8212	7.5006	115.1	97.1	-18.0	106.9	-8.2
540	$LiNO_3$	5.7321	4.5774	4.5755	4.8385	7.4409	90.0	77.3	-12.7	91.1	1.1
541	$Mg(NO_3)_2$	10.4641	8.1547	8.5206	10.0223	14.4291	164.0	155.2	-8.8	171.1	7.1
542	Mg_2SiO_4	7.2910	6.7746	7.0229	8.3018	7.7481	95.1	110.4	15.3	109.0	13.9
543	$MgSO_4$	6.5275	5.6547	6.1374	9.1665	7.0480	91.6	96.5	4.9	94.7	3.1
544	$Na_2B_4O_7$	14.2898	12.2779	12.0904	12.1648	16.1295	189.5	180.9	-8.6	177.9	-11.6
545	Na_2MoO_4	6.8162	7.2946	7.0186	10.1991	6.6836	159.7	147.6	-12.1	165.9	6.2
546	Na_2SiO_3	5.9240	6.2241	5.7096	6.0479	6.0952	113.9	112.9	-1.0	121.4	7.5
547	Na_2SO_3	5.7510	6.3439	5.6853	5.9526	6.1741	145.9	126.7	-19.2	134.6	-11.3
548	Na_2SO_4	7.1605	7.1041	6.7879	8.8409	7.4694	149.6	132.1	-17.5	144.3	-5.3
549	Na_2WO_4	6.7131	7.3753	7.0227	10.2231	6.6720	161.5	155.5	-6.0	173.5	12.0
550	Na_3AlF_6	8.5032	11.8887	8.3687	4.5976	7.9906	238.5	249.4	10.9	230.3	-8.2
551	$NaBO_2$	4.2307	3.9319	3.6762	3.4419	4.6563	73.5	61.5	-12.0	61.8	-11.7
552	$NaNbO_3$	4.9119	5.1376	5.1297	7.5184	4.9698	117.0	103.9	-13.1	110.7	-6.3
553	$NaNO_2$	3.9712	4.0908	3.5141	2.9647	5.4082	103.8	92.1	-11.7	103.1	-0.7
554	Na_2SiF_6	7.8230	10.5726	7.5986	4.9640	7.4262	207.1	220.9	13.8	212.3	5.2
555	$NiSO_4$	6.3021	5.9456	6.1326	9.1572	7.0581	92.0	119.3	27.3	118.7	26.7
556	Pb_2SiO_4	6.6003	7.8296	7.0482	8.3514	7.6954	186.6	186.0	-0.6	194.0	7.4
557	$PbMoO_4$	5.8379	6.3727	6.3807	10.5496	6.2358	166.1	149.8	-16.3	159.1	-7.0
558	$PbSiO_3$	4.9456	5.3021	5.0717	6.3983	5.6474	109.6	115.1	5.5	115.3	5.7
559	$PbSO_4$	6.1822	6.1822	6.1500	9.1914	7.0216	148.5	134.3	-14.2	136.2	-12.3
560	Rb_2SO_4	6.7924	7.8169	6.7417	8.7955	7.5422	197.4	181.2	-16.2	198.7	1.3
561	Sr_2SiO_4	6.8402	7.3566	7.0491	8.3533	7.6935	153.1	154.6	1.5	157.3	4.2
562	$SrSiO_3$	5.0656	5.0656	5.0722	6.3993	5.6464	96.7	99.4	2.7	97.2	0.5
563	$SrSO_4$	6.3021	5.9456	6.1505	9.1923	7.0206	117.0	118.6	1.6	118.2	1.2
564	Tl_2SO_4	6.5966	8.3963	6.7445	8.7983	7.5377	230.5	215.3	-15.2	235.3	4.8
565	Zn_2SiO_4	7.0230	7.0840	7.0284	8.3127	7.7364	131.4	135.4	4.0	135.5	4.1
566	$ZnCO_3$	5.4472	4.7872	4.8276	5.4593	6.6068	82.4	84.8	2.4	85.1	2.7
567	$ZnSO_4$	6.3936	5.8094	6.1402	9.1720	7.0421	110.5	109.0	-1.5	107.6	-2.9
568	$ZrSiO_4$	6.2910	5.7746	6.3264	9.4240	6.8130	116.7	107.2	-9.5	104.0	-12.7
569	$CaCO_3$	5.4472	4.7872	4.8425	5.4885	6.5760	88.0	84.2	-3.8	84.0	-4.0
570	Ca_2SiO_4	7.0230	7.0840	7.0582	8.3711	7.6748	120.5	134.3	13.8	134.7	14.2
571	$MgSiO_3$	5.2910	4.7746	5.0590	6.3735	5.6738	67.9	77.3	9.4	73.2	5.3
572	$Fe(AlO_2)_2$	7.1754	6.8868	7.0587	8.2812	7.7501	113.5	119.8	6.3	117.8	4.3
573	$FeTiO_3$	4.9841	5.0491	5.1441	6.7497	5.4105	106.4	99.4	-6.9	97.9	-8.4
574	$MgCO_3$	5.5811	4.6325	4.8248	5.4539	6.6127	69.0	72.3	3.3	72.4	3.4
575	$FeSiO_3$	5.1570	4.9293	5.0376	6.3314	5.7201	95.9	90.7	-5.2	87.3	-8.6
576	Be_2SiO_4	7.7405	6.4076	6.8659	7.9937	8.1084	64.3	81.2	16.9	78.9	14.6
577	$CaSiO_3$	5.1570	4.9293	5.0767	6.4082	5.6371	87.5	89.3	1.8	86.0	-1.5
578	$MnSiO_3$	5.1570	4.9293	5.0710	6.3969	5.6489	102.5	89.5	-13.0	86.2	-16.3
579	$FeCO_3$	5.4472	4.7872	4.8033	5.4117	6.6590	95.5	85.7	-9.8	86.8	-8.7
580	$AlK(SO_4)_2$	12.9169	11.5895	12.1743	18.3035	14.1386	204.6	214.4	9.8	211.8	7.2
581	$Ca_2MgSi_2O_7$	12.3140	11.8586	12.1172	14.7447	13.3486	208.2	212.8	4.6	209.7	1.5

582	$Fe_3Al_2Si_3O_{12}$	20.7805	19.5199	20.2291	25.3892	22.7896	336.3	349.0	12.7	337.0	0.7
583	$CaAl_2Si_2O_8$	13.7574	12.4359	13.2883	17.2485	14.8658	199.3	209.2	9.9	197.0	-2.3
584	$LiAlSi_2O_6$	10.7367	9.4152	10.0458	12.8794	11.2769	154.4	143.7	-10.7	143.0	-11.4
585	$CaAl_2SiO_6$	10.4664	9.6613	10.1931	12.8032	11.2665	144.5	163.7	19.2	159.7	15.2
586	$CaMg(CO_3)_2$	11.0283	9.4196	9.4708	10.1710	14.3035	155.2	175.1	19.9	166.7	11.5
587	$Ca_2Al_2SiO_7$	12.3324	11.8160	12.1745	14.7662	13.3042	204.4	208.8	4.5	204.2	-0.2
588	$KAlSi_3O_8$	13.7348	12.6040	13.1372	17.3210	14.8822	232.9	220.3	-12.6	214.4	-18.5
589	$CaMgSiO_4$	7.1570	6.9293	7.0405	8.3365	7.7115	112.1	122.3	10.3	121.8	9.8
590	$NaAlSiO_4$	7.2622	6.8654	6.9606	8.4441	7.6620	124.4	115.8	-8.6	118.2	-6.1

REFERENCES

(1). Kier L. B., Hall H. Molecular Connectivity in Chemistry and Drug Research. New York: Academic Press , 1976, 181

(2). Balaban, A. T. Applications of Graph in Chemistry. *J. Chem. Inf. Comput. Sci.* **1985**,25,334-343.

(3). Balaban, A. T. Chemical Graphs: Looking Back and Glimpsing Ahead. *J. Chem. Inf. Comput. Sci*. **1995**,35,339-350.

(4). Mu L. L.; Feng C. J.. Topological Research on Standard Entropies of Alkali and Alkaline Earth Metal Compounds. *Chin. J. Chem. Phys.* **2003**, 16, 19-24

(5). Feng C. J.. The Connection Index of Average Energy Level for Valence Electron and its Applications. *Chin. J. Chem. Phys*. **2000**, 13, 66-70

(6). Xu S. Y.; Tang J. H.. The Topological Index ^{m}F Electronegativity and its Calculation of Physical and Chemical Properties of Inorganic Compounds. *Chin. J. Chem. Phys*. **2003**, 16, 203-208

(7). Feng C. J.. Studies on the Relationships between the Quantitative Structure and Physico-Chemical Properties for the Inorganic Compounds. *Chin. J. Anal. Sci*. **2002**, 18, 27-32

(8). Feng C. J.. Estimating and Predicting Lattice Energies of Inorganic Compounds with Connectivity Indices. *Chin. J. Mol. Sci*. **1999**, 15, 223-228

(9). Feng C. J.; Chen Y. A Novel Structural Parameter for QSPR Study of Halides. *Chin. J. Mol. Sci*. **2000**, 16, 177-183

(10) Mu,L.L.; Feng C.J., He H. M.. Topological Research on Lattice Energies for Inorganic Compounds. *MATCH Commun. Math. Comput. Chem*. 2006,56, 97-111

(11) David R. L.; Grace B.; Lev I. B.; Robert N. G.; Henry V. K.; Kozo K.; Gerd R.; Dana L. R.; Daniel Z. *CRC Handbook of Chemistry and Physics*. 85th ed; CRC Press; Boca Raton, FL,**2002**;pp5-5 to 5-60

(12) John A. Dean; *Langes Handbook of Chemistry*, 15th ed; McGRAW-HILL, INC; **1999**; pp6.81-6.123

(13) Wagman, D. D.; Evans, W. H.; Parker, V. B.; Schumm, R. H.; Nutall, R. L. *Selected Values of Chemical Thermodynamic Properties*; U. S. Department Commerce, National Bureau of Standards: Washington, DC, **1982**.

(14) Robie, R. A.; Hemingway, B. S.; Fisher, J. R. *Thermodynamic Properties of Minerals and Related Substances at 298.15 K and 1 Bar (10^5 Pascals) Pressure and at Higher Temperatures*; Geological Survey Bulletin 1452; U. S. Government Printing Office: Washington, DC, **1978**.

(15) Saxena, S. K.; Chatterjee, N.; Fei, Y.; Shen, G. *Thermodynamic Data on Oxides and Silicates*; Springer: Berlin, **1993**.

(16) Scientific database, http://www.enginchem.csdb.cn/sdb_2004/all_thermochemistry.html

(17) Jenkins, H. D. B.; Roobottom. H. K.; Passmore, J.; Glasser, L. Relationships among Ionic Lattice Energies, Molecular (Formula Unit) Volumes, and Thermochemical Radii; *Inorg.Chem.* **1999**, 38, 3609-3620.

(18). Glasser, L.; Jenkins, H. D. B. Lattice Energies and Unit Cell Volumes of Complex Ionic Solids. *J. Am. Chem. Soc.* **2000**, 122, 632-638.

(19). Jenkins, H. D. B.; Tudela, D.; Glasser, L. Lattice Potential Energy Estimation for Complex Ionic Salts from Density Measurements. *Inorg. Chem.* **2002**, 41,2364-2367.

(20). Jenkins, H. D. B.; Glasser, L. Ionic Hydrates, $M_pX_q{\cdot}nH_2O$: Lattice Energy and Standard Enthalpy of Formation Estimation *Inorg. Chem.,* **2002**, *41*,4378-4388.

(21). Jenkins, H. D. B.; Roobottom, H. K.; Passmore, J., Estimation of Enthalpy Data for Reactions Involving Gas Phase Ions Utilizing Lattice Potential Energies: Fluoride Ion Affinities (FIA) and pF^- Values of $mSbF_5$(l) and $mSbF_5$(g) (m = 1, 2, 3), AsF_5(g), $AsF_5{\cdot}SO_2$(c). Standard Enthalpies of Formation: $\Delta_f H^o(Sb_mF_{5m+1}^-,g)$ (m = 1, 2, 3), $\Delta_f H^o(AsF_6^-,g)$, and $\Delta_f H^o(NF_4^+,g)$, *Inorg. Chem.,* **2003**, *42*,2886-2893.

(22). Christe, K. O.; Jenkins, H. D. B.Quantitative Measure for the "Nakedness" of Fluoride Ion Sources „*J. Am. Chem. Soc.,***2003**,*125*,9457-9461.

(23) Latimer, W. M. Methods of Estimating the Entropies of Solid Compounds, *J. Am. Chem. Soc.* **1951**, 73,1480-1482

(24) Fyfe, W. S.; Turner, F. J.; Verhoogen, J. *Metamorphic Reactions and Metamorphic Facies*; Geological Society of America: Boulder, CO, **1958**; Memoir 73.

(25) Jenkins, H. D. B.; Glasser, L. Standard Absolute Entropy, $S°_{298}$, Values from Volume or Density. 1.Inorganic Compounds, *Inorg. Chem.* **2003,** 42, 8702-8708

(26) Mu, L. L.; Feng, C. J. Topological Research on Standard Entropies of Alkali and Alkaline Earth Metal Compounds, *Chin. J. Chem. Phys.* **2003**, 16,19-24

(27) Feng, C. J. Topological Researches on the F Center Energy Bands, Lattice Energy and Standard Entropy of Alkaline Halides, *Chin. J. Struct. Chem.* **2004**, 23, 556-559

(28) Burns, J. A.; Whitesides, G. M. Feed Forward Neural Networks in Chemistry: Mathematical Systems for Classification and Pattern Recognition. *Chem. Re*V. **1993**, 93, 2583-2601.

(29) Svozil, D; Kvasnicka, V; Pospı´chal, J Introduction to Multilayer Feed Forward Neural Networks. *Chemometrics Intelligent Laboratory Systems* **1997**, *39*, 43-62.