Topological Research on Molar Diamagnetic Susceptibilities for Inorganic Compounds

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For predicting the molar diamagnetic susceptibilities of inorganic compound, a novel connectivity index ^mQ based on adjacency matrix of molecular graphs is proposed as follows: $^mQ = \Sigma (q_i \cdot q_j \cdot q_k \cdots)^{0.5}$. The g_i of adjacency matrix is defined as $q_i = (n_i^{0.5} - 0.93)^4 \cdot E_i^{0.5}/Z_i^{0.5}$, where Z_i, n_i, E_i are the valence, the outer electronic shell primary quantum number, and the average energy of atomic valence Orbital of atom i respectively. The excellent QSPR models for the molar diamagnetic susceptibilities can be constructed from ^0Q and ^1Q 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 0.9864, 0.9886, 5.40 cgs, 4.94 cgs, 9.03% and 8.60%, respectively, for 206 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 molar diamagnetic susceptibility of inorganic compound. Both MLR and NN methods can provide acceptable models for the prediction of the molar diamagnetic susceptibilities. The NN model for the standard entropy appears more reliable than the MLR model.

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1. INTRODUCTION

The application of graph theoretical concepts for the description of chemical structures has evolved from the description of physical properties of alkanes by using relatively simple topological indices to the combined use of more potent descriptors to predict complex physicochemical and biological properties of structurally diverse data sets of organic compounds.[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.

The diamagnetic susceptibility χ of compounds is an important physicochemical property. When a material is placed in a magnetic field H, a magnetization (magnetic moment per unit volume) M is induced in the material which is related to H by $M=\kappa H$[11-14], where κ is called the volume susceptibility. Since H and m have the same dimensions, κ is dimensionless. A more useful parameter is the molar susceptibility χ_m, defined by

$$\chi_m = \kappa V_m = \kappa \, M/\rho \qquad (1)$$

where V_m is the molar volume of the substance, M the molar mass, and ρ the mass density. When the cgs system is used, the customary units for χ_m are $cm^3 \, mol^{-1}$; the corresponding SI units are $m^3 \, mol^{-1}$.

Substances that have no unpaired electron orbital or spin angular momentum generally have negative values of χ_m and are called diamagnetic. Their molar susceptibility varies only slightly with temperature. Substances with unpaired electrons, which are termed paramagnetic, have positive χ_m and show much stronger temperature dependence, varying roughly as $1/T$. The net susceptibility of a paramagnetic substance is the sum of the paramagnetic and diamagnetic contributions, but the former almost always dominates. A substance for which one has $\chi_m < 0$ is diamagnetic, and its molar diamagnetic susceptibility can be obtained from the Langevin-Pauli formula.[11-14]

There has been a continued interest in chemistry, based on the theoretical and practical importance of this property, for the determination and prediction of diamagnetic susceptibility of compounds.[14] For many years, experimental and theoretical efforts in the field of diamagnetic susceptibility of compounds are devoted to the determination of this property by different ways in complex systems.[15-18]

The interest in theoretical treatments for magnetic susceptibility dates from the beginning of the twentieth century. Magnetic susceptibilities of stable organic species have long been observed to be approximately fit by a sum of atomic contribution, which was so-called

Pascal's constants,[13,14] which has been successful in the prediction of diamagnetic susceptibilities of organic compounds and is used even today.[14] A subsequent expansion, motivated by the simple quantum chemical treatment, was developed by Hameka[19-23] to describe diamagnetic susceptibilities of several classes of organic compounds. In Hameka's approach not only atomic contributions are considered, but also contributions coming from bonds and bond-bond interactions are included. But a large number of experimental values of diamagnetic susceptibilities are needed in order to obtain those large families of parameters. In some simple cases the theoretical calculation of diamagnetic susceptibility seems to be attractive, but most of the results thus obtained are quantitatively incomparable with the experimental value[24]. Subsequent studies include quantum chemical approaches such as the path-integral formulation of quantum mechanics, Weizsäcker energy of many-electron systems, and density-functional methods,[25-28] integrated molecular transform,[29] or graph theoretical concepts.[30-35]

The diamagnetic property of a compound is determined mainly by its molecular structure other than the bulk as a whole.[36] Hence, the application of graph theory in this connection may be of some merits, though the structures here are approximately represented by the graphs without taking into account of the geometrical details. In fact, many attempts have been made in this direction, from the Wiener[37] or Randić index[38] for alkanes, through the more sophisticated connectivity indices by Kier and Hall,[30,39] for both alkanes and aliphatic alcohols, to the cluster expansion method,[31,40]. As can be seen, a tendency in the construction of new topological indices is followed[41] as the incorporation of more electronic structure information into a graph to get so-called chromograph; therefore the elements other than C, N, O, F, C1, etc. can be fully described, and the method can be largely extended to fit the use for the inorganic or organometallic compounds. [4-10, 32]

In recent years, Qing Z. L., [42] Feng C. J.[43] etc., by using various model parameters, have developed some QSPR/QSAR models to estimate the diamagnetic susceptibilities of Alkali and Alkaline earth metal compounds. In this study, the magnetic valence q_i is defined based on the average energy of atomic valence Orbital, outer electronic shell primary quantum number, and valence. A new topological index is proposed based on the Kier-Hall[30] index and q_i. The connectivity index has a good correlation for the diamagnetic susceptibilities of inorganic solid compounds.

2. MOLECULAR DESCRIPTORS

The diamagnetic susceptibility for atom or ion is dependent on the electron number and the attracting electron ability of atomic nucleus, and that the electron number and the

attracting electron ability of atomic nucleus is mainly affected by the atomic valence orbital average energy, valence, and outer electronic shell primary quantum number. So, it is considered that the atomic valence orbital average energy, valence, and outer electronic shell primary quantum number are the main factors of affecting on the diamagnetic susceptibility for atom or ion. By the optimizing, the magnetic valence q_i is can be defined as:

$$q_i = (n_i^{0.5} - 0.93)^4 \cdot E_i^{0.5} / Z_i^{0.5} \qquad (2)$$

where Z_i, n_i, E_i are the absolute value of valence, the atomic outer electronic shell primary quantum number, and the atomic valence orbital average energy of atom i respectively.

$$E_i = \Sigma n_j E_j / \Sigma n_j \qquad (3)$$

Fro example Pb, $6s^2(10.0)6p^2(7.42)$, $E_{Pb}=(2\times10.0000+2\times7.4200)/(2+2)=8.7100$, $q_{Pb}=(6^{0.5}-0.93)^4 \cdot 8.7100^{0.5}/2^{0.5}=11.1246$. The E_i of 41 elements and the q_i of 52 ions are calculated and listed in Table 1 and Table 2.

Table 1. The average energy of atomic valence Orbital (E)

No	element	E_i	No	element	E_i	No	element	E_i
1	Ag	9.7800	15	Cu	10.1570	29	O	18.5670
2	Al	9.0567	16	F	23.2290	30	P	12.7800
3	As	12.6860	17	Ga	9.3330	31	Pb	8.7100
4	Au	10.9300	18	Ge	11.1000	32	Rb	4.1800
5	B	11.3667	19	H	13.6000	33	S	13.6670
6	Ba	5.2100	20	Hg	10.0000	34	Sb	11.1840
7	Be	9.3200	21	I	13.3860	35	Se	13.2000
8	Bi	9.1740	22	In	8.5967	36	Si	10.8250
9	Br	15.3000	23	K	4.3400	37	Sn	9.6700
10	C	13.9500	24	La	5.6367	38	Sr	5.7000
11	Ca	6.1100	25	Li	5.3900	39	Tl	7.3700
12	Cd	8.9900	26	Mg	7.6500	40	Zn	9.3900
13	Cl	16.2860	27	N	16.8200	41	Zr	7.7250
14	Cs	3.8900	28	Na	5.1400			

Table 2. the magnetic valence q_i

No	ionic	q_i	No	ionic	q_i	No	ionic	q_i
1	Ag^+	9.0998	19	Cs^+	10.5139	36	N^{5+}	0.1008
2	Al^{3+}	0.7190	20	F^-	0.2649	37	Na^+	0.9382
3	As^{3+}	2.6955	21	Ga^{3+}	2.3120	38	O^{2-}	0.1675
4	Au^+	17.6239	22	Ge^{2+}	3.0880	39	P^{5+}	0.6616
5	B^{3+}	0.1070	23	Ge^{4+}	2.1836	40	Pb^{2+}	11.1246

6	Ba^{2+}	8.6039	24	H^-	0.0001	41	Rb^+	5.9491
7	Be^{2+}	0.1187	25	H^+	0.0001	42	S^{2-}	1.0818
8	Bi^{3+}	9.3220	26	Hg^+	11.9200	43	S^{6+}	0.6246
9	Br^-	5.1272	27	Hg^{2+}	11.9200	44	Sb^{3+}	5.6183
10	Br^{5+}	2.2930	28	I^-	10.6461	45	Se^{4+}	2.3812
11	C^{4-}	0.1027	29	I^{5+}	4.7611	46	Si^{4+}	0.6808
12	C^{4+}	0.1027	30	In^{3+}	4.9257	47	Sn^{2+}	6.3983
13	Ca^{2+}	2.2911	31	K^+	2.7307	48	Sn^{4+}	4.5242
14	Cd^{2+}	6.1692	32	La^{3+}	7.3071	49	Sr^{2+}	4.9123
15	Cl^-	1.6700	33	Li^+	0.1276	50	Tl^+	14.4719
16	Cl^{5+}	0.7468	34	Mg^{2+}	0.8093	51	Zn^{2+}	2.8402
17	Cl^{7+}	0.6312	35	N^{3+}	0.1302	52	Zr^{4+}	4.0437
18	Cu^+	4.1775						

Inorganic solid compound are made up of positive and negative ions. The diamagnetic property of a compound is determined mainly by its molecular structure. The different compounds have different molecular structure. Based on adjacency matrix of molecular graphs, the novel connectivity index ^mQ can be defined as follows:

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

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

$$^0Q = \Sigma(q_i)^{0.5} \qquad (5)$$
$$^1Q = \Sigma(q_i.q_j)^{0.5} \qquad (6)$$

In expressions (5), the "Σ" is the sum of atomic of inorganic compound chemical formula. In expressions (6), the "Σ" is the sum of chemical single bonds of chemical formula. For example, the $^0Q, ^1Q$ of are calculated as follows:

For $Pb_3(PO_4)_2$, it can be treated as consisting of three Pb^{2+}, two P^{5+} and eight O^{2-}, it contains six Pb-O single bonds and ten P-O single bonds, so:

$^0Q = 3 \times (11.1246)^{0.5} + 2 \times (0.6616)^{0.5} + 8 \times (0.1675)^{0.5} = 14.9070$

$^1Q = 6 \times (11.1246 \times 0.1675)^{0.5} + 10 \times (0.6616 \times 0.1675)^{0.5} = 11.5193$

the $^0Q, ^1Q$ of 206 inorganic compounds are calculated, and listed in Table 3.

3. DATA SET

The QSPR treatment started with the assembly of the data set. The experimental molar diamagnetic susceptibilities, χ_m, data were compiled from Ref.43 and Ref.44. A total of 206 inorganic compounds with extensive structural diversity were selected as the data set (see

Table 3). 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, sulfide, and hydroxide. The structures include 41 elements and 52 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 (a statistical analysis software). The regression of molar diamagnetic susceptibilities, χ_m, versus ^0Q and ^1Q resulted in a two-parameter model with the correlation coefficient r of 0.9864. The model is shown as follows:

$$-\chi_m \times 10^{-6} (cgs) = 0.1362 + 11.7718\,^0Q + 0.4606\,^1Q \qquad (7)$$

$n=206$, $r=0.9864$, $r^2= 0.9730$, $s= 5.40$ cgs, $F= 3654.99$

The results of t-test show that these variables in these models are significant. The model (7) explains more than 97.3% of the variance in the experimental values of molar diamagnetic susceptibilities, χ_m, for these inorganic compounds. The calculated results from Eq. (7) for 206 inorganic compounds are shown in Table 3 (Cal.1). The average absolute deviation is 4.31 cgs. The calculated molar diamagnetic susceptibility versus experimental data is shown in Figure 1.

Finally, the model(7) above generated for 206 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 0.9859(0.9864), 5.47(5.40) cgs, 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.
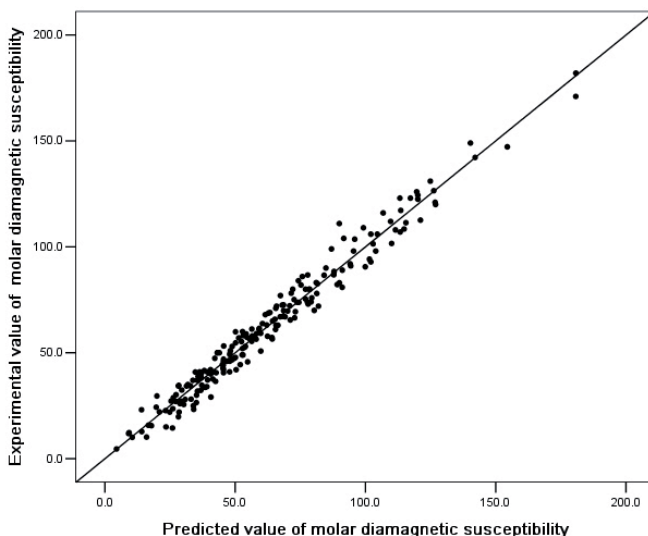
Figure 1. Plot of calculated vs experimental values of molar diamagnetic susceptibilities, MLR model

5. ARTIFICIAL NEURAL NETWORK MODELS

Artificial neural network (NN) is a 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[45,46] include QSAR/QSPR studies, spectroscopy (IR, NMR, and UV spectra), 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 ^0Q and ^1Q. The data set was divided into three data sets: training, test, and validation. The training, test, and validation sets represented 50% (103data points), 30% (62data points), and 20%(41data 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.
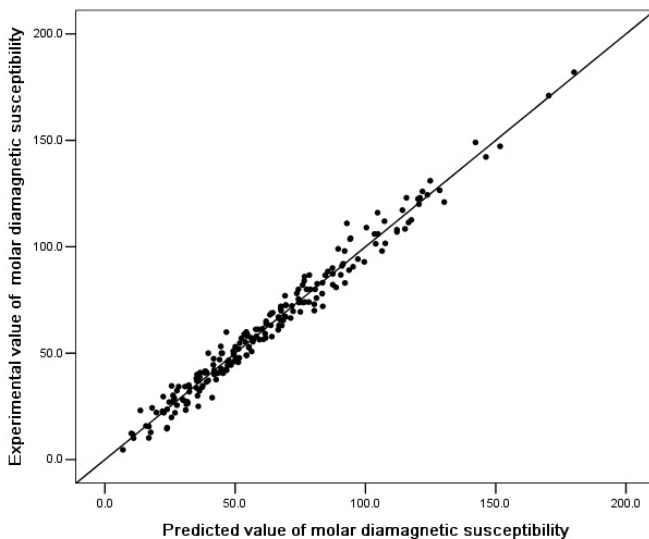
Figure 2. Plot of predicted vs experimental values of molar diamagnetic susceptibility, NN model

To find the optimal number of hidden neurons, neural network training with a 2:h:1 architecture was carried out. After examining neural nets with various numbers of hidden nodes, we found that 4 offered the most accurate results, and we therefore employ a 2:4:1 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 5.05 cgs, 4.63 cgs and 4.90 cgs, respectively. The predicted values for 206 inorganic compounds are shown in Table 3 (Cal.2). The r, standard deviation and average absolute deviation between predicted and experimental values for the 206 inorganic compounds are 0.9886 and 4.94 cgs, 3.97 cgs.

6. RESULTS AND DISCUSSION

Diamagnetic susceptibilities of various organic compounds have been investigated using the connectivity indices by Kier et al,[39] the topological sub structural molecular design approach by Estrada et al.[33-35] In most of the cases, up to seven different kinds of indices have been employed for a good linear fitting of the experimental data. But the large families of variables used in the correlation need more experimental χ_m values, which may not be the cases in practice. On the other hand, until now, the method is only limited to the organic compounds. As for the inorganic compounds, intrinsic difficulty arises. But on our indices, no confinement is imposed at the point.

The q_i defined in this paper is various for different ions due to various the valences, the average energy of atomic valence Orbital and the outer electronic shell primary quantum number. For the different ions having the same valence and outer electronic shell primary quantum number, the q_i is unequal due to their different atomic valence orbital average energy, For example, the q_i of Ag^+ and Rb^+ are 9.0998 and 5.9491, respectively, in other words, the q_i is different. Even for the ions of the different valence states of the same element, the q_i are also different. For example the q_i of Cl^-, Cl^{5+} and Cl^{7+} are 1.6700, 0.7468 and 0.6312. So, the q_i can reflect the characteristic of different ion.

Due to inorganic compound are made up of positive and negative ions, their diamagnetic susceptibilities is affected by the average energy of atomic valence Orbital, valence, and outer electronic shell primary quantum number. So the diamagnetic susceptibility is affect by the g_i of positive and negative ions. The diamagnetic property of a compound is determined mainly by its molecular structure. The different compounds have different molecular structure, namely, different adjacency matrix of molecular graphs, their ^mQ are different. Based expression (4) and expression (5), ^0Q is the sum of atomic q_i square root of inorganic compound chemical formula, and ^1G is the sum of chemical single bonds of chemical formula. So ^0Q and ^1Q contain atomic and bonds contributions to diamagnetic susceptibility of the compound. From the model (7), it can be known that the contribution coming from atoms or ions is dominating.

The theoretical prediction of the molar diamagnetic susceptibility 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 (7) is excellent, and the correlation coefficient r is 0.9864. The estimated molar diamagnetic susceptibilities of 206 inorganic compounds are listed in Table 3 (Cal.1). As

shown in Table 3 (Cal.1), our calculated values agree well with the available experimental values. The average error of 206 inorganic solid compounds is 9.03 % (13.66 % for $-\chi_m \times 10^{-6} < 50$ cgs, 6.18% for $100 > -\chi_m \times 10^{-6} > 50$ cgs, 5.04% for $-\chi_m \times 10^{-6} > 100$ cgs). The NN model developed for the prediction of molar diamagnetic susceptibility performed better than the MLR model and the correlation coefficient r and the RMS errors are 0.9886 and 4.94 cgs. The predicted molar diamagnetic susceptibilities of 206 inorganic compounds from the NN model are listed in Table 3 (Cal.2). The average prediction errors of 206 compounds is 8.80%(13.22% for $-\chi_m \times 10^{-6} < 50$ cgs, 5.81% for $100 > -\chi_m \times 10^{-6} > 50$ cgs, 4.47% for $-\chi_m \times 10^{-6} > 100$ cgs). The results show that the current method is more effective than the literature methods[35,36] for complex inorganic compounds .

7. CONCLUSION

A novel connectivity index ^mQ is proposed from the magnetic valence q_i, for predicting the molar diamagnetic susceptibility of inorganic compound. The excellent QSPR model for the molar diamagnetic susceptibilities can be constructed from ^0Q and ^1Q, by using MLR method and NN method. The correlation coefficient r, standard error, and average relative error of the MLR model and NN model are 0.9864, 0.9886, 5.40 cgs, 4.94 cgs, 9.03 % and 8.60%, respectively, for the 206 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 molar diamagnetic susceptibility of inorganic compound. Both MLR and NN methods can provide acceptable models for the prediction of the molar diamagnetic susceptibility. The NN model for the molar diamagnetic susceptibilities appears to be more reliable than the MLR model.

8. ACKNOWLEDGEMENT

Table3. The calculated and experimental molar diamagnetic susceptibilities of 206 inorganic compounds

No	compound	^0Q	^1Q	$-\chi_m(10^{-6}cm^3.mol^{-1})$				
				Exp.	Cal1.	Er1.	Cal2.	Er2.
1	AgBr	5.2809	6.8306	61.0	65.4	4.4	66.2	5.2
2	AgCl	4.3089	3.8983	49.0	52.7	3.7	54.1	5.1
3	AgF	3.5313	1.5526	36.5	42.4	5.9	38.8	2.3
4	AgI	6.2794	9.8426	80.0	78.6	-1.4	78.5	-1.5
5	Al$_2$O$_3$	2.9237	2.0822	37.0	35.5	-1.5	35.9	-1.1
6	AsBr$_3$	8.4348	11.1527	106.0	104.6	-1.4	104.4	-1.6
7	AsCl$_3$	5.5187	6.3650	72.5	68.0	-4.5	69.1	-3.4
8	AsI$_3$	11.4303	16.0708	142.2	142.1	-0.1	145.5	3.3
9	As$_2$S$_3$	6.4039	10.2458	70.0	80.2	10.2	80.0	10.0
10	AuCl	5.4904	5.4251	67.0	67.3	0.3	68.7	1.7
11	AuI	7.4609	13.6977	91.0	94.3	3.3	90.6	-0.4
12	BCl$_3$	4.2040	1.2682	59.9	50.2	-9.7	46.5	-13.4
13	BaBr$_2$	7.4619	13.2837	92.0	94.1	2.1	91.1	-0.9
14	BaCl$_2$	5.5178	7.5812	72.6	68.6	-4.0	69.2	-3.4
15	BaF$_2$	3.9626	3.0194	51.0	48.2	-2.8	49.1	-1.9
16	BaI$_2$	9.4589	19.1414	124.4	120.3	-4.1	123.3	-1.1
17	BaO	3.3425	2.4010	29.1	40.6	11.5	40.9	11.8
18	BaO$_2$	3.7518	2.5685	40.6	45.5	4.9	45.2	4.6
19	BeCl$_2$	2.9291	0.8905	26.5	35.0	8.5	31.7	5.2
20	BeO	0.7538	0.2820	11.9	9.1	-2.8	10.6	-1.3
21	BiF$_3$	4.5972	4.7143	61.2	56.4	-4.8	57.7	-3.5
22	Bi$_2$O$_3$	7.3342	7.4974	83.0	89.9	6.9	91.7	8.7
23	Bi$_2$S$_3$	9.2267	19.0537	123.0	117.5	-5.5	120.5	-2.5
24	CaBr$_2$	6.0423	6.8548	73.8	74.4	0.6	75.7	1.9
25	CaCl$_2$	4.0982	3.9121	54.7	50.2	-4.5	51.6	-3.1
26	CaF$_2$	2.5430	1.5581	28.0	30.8	2.8	29.9	1.9
27	CaI$_2$	8.0393	9.8775	109.0	99.3	-9.7	100.1	-8.9
28	CaO	1.9229	1.2390	15.0	23.3	8.3	23.7	8.7
29	CdBr$_2$	7.0125	11.2482	87.3	87.9	0.6	87.1	-0.2
30	CdCl$_2$	5.0684	6.4195	68.7	62.8	-5.9	63.6	-5.1
31	CdF$_2$	3.5132	2.5567	40.6	42.7	2.1	43.1	2.5
32	CdI$_2$	9.0095	16.2084	117.2	113.7	-3.5	113.8	-3.4
33	CdO	2.8931	2.0331	30.0	35.1	5.1	35.3	5.3
34	CdS	3.5239	5.1668	50.0	44.0	-6.0	44.9	-5.1
35	CsBr	5.5068	7.3421	67.2	68.3	1.1	69.0	1.8
36	CsCl	4.5348	4.1903	56.7	55.4	-1.3	56.8	0.1
37	CsF	3.7572	1.6689	44.5	45.1	0.6	41.5	-3.0
38	CsI	6.5054	10.5798	82.6	81.6	-1.0	81.1	-1.5
39	Cs$_2$S	7.5251	6.7451	104.0	91.8	-12.2	94.0	-10.0
40	CuBr	4.3082	4.6281	49.0	53.0	4.0	54.2	5.2
41	CuCl	3.3362	2.6413	40.0	40.6	0.6	41.8	1.8
42	CuI	5.3067	6.6689	63.0	65.7	2.7	66.5	3.5
43	GaCl$_3$	5.3974	5.8949	63.0	66.4	3.4	67.6	4.6
44	Ga$_2$S$_3$	6.1613	9.4890	80.0	77.0	-3.0	77.1	-2.9
45	GeO	2.1665	1.4384	28.8	26.3	-2.5	26.6	-2.2
46	GeS	2.7974	3.6555	40.9	34.8	-6.1	36.4	-4.5
47	GeCl$_4$	6.6468	7.6384	72.0	81.9	9.9	83.2	11.2
48	GeF$_4$	3.5364	3.0422	50.0	43.2	-6.8	44.6	-5.4

49	GeI$_4$	14.5290	19.2860	171.0	180.1	9.1	169.7	-1.3
50	GeO$_2$	2.2962	2.4191	34.3	28.3	-6.0	30.7	-3.6
51	Hg$_2$Cl$_2$	9.4896	29.7666	120.0	125.6	5.6	120.0	0.0
52	Hg$_2$F$_2$	7.9344	19.0279	106.0	102.3	-3.7	103.1	-2.9
53	HgBr$_2$	7.9812	15.6354	94.2	101.3	7.1	96.7	2.5
54	HgCl$_2$	6.0371	8.9233	82.0	75.3	-6.7	75.6	-6.4
55	HgF$_2$	4.4819	3.5539	57.3	54.5	-2.8	55.8	-1.5
56	HgO	3.8618	2.8260	46.0	46.9	0.9	47.4	1.4
57	HgS	4.4926	7.1819	55.4	56.3	0.9	56.6	1.2
58	InBr$_3$	9.0124	15.0763	107.0	113.2	6.2	111.6	4.6
59	InCl$_3$	6.0962	8.6043	86.0	75.9	-10.1	76.4	-9.6
60	In$_2$S$_3$	7.5591	13.8503	98.0	95.5	-2.5	91.7	-6.3
61	KBr	3.9168	3.7418	49.1	48.0	-1.1	49.4	0.3
62	KCl	2.9448	2.1355	38.8	35.8	-3.0	36.3	-2.5
63	KF	2.1672	0.8505	23.6	26.0	2.4	23.8	0.2
64	KI	4.9153	5.3918	63.8	60.5	-3.3	61.6	-2.2
65	K$_2$S$_5$	8.5054	7.7647	98.0	103.8	5.8	105.8	7.8
66	K$_2$S$_4$	7.4654	6.6829	89.0	91.1	2.1	93.3	4.3
67	K$_2$S$_3$	6.4253	5.6011	80.0	78.4	-1.6	80.4	0.4
68	K$_2$S$_2$	5.3852	4.5193	71.0	65.6	-5.4	67.3	-3.7
69	K$_2$S	4.3451	3.4375	60.0	52.9	-7.1	54.1	-5.9
70	La$_2$O$_3$	6.6341	6.6379	78.0	81.3	3.3	83.0	5.0
71	LiBr	2.6215	0.8088	34.3	31.4	-2.9	28.3	-6.0
72	LiCl	1.6495	0.4616	24.3	19.8	-4.5	18.1	-6.2
73	LiF	0.8719	0.1839	10.1	10.5	0.4	11.0	0.9
74	LiH	0.3672	0.0036	4.6	4.5	-0.1	6.8	2.2
75	LiI	3.6200	1.1655	50.0	43.3	-6.7	39.6	-10.4
76	MgBr$_2$	5.4283	4.0740	72.0	65.9	-6.1	67.3	-4.7
77	MgCl$_2$	3.4842	2.3251	47.4	42.2	-5.2	41.6	-5.8
78	MgF$_2$	1.9290	0.9260	22.7	23.3	0.6	22.0	-0.7
79	MgI$_2$	7.4253	5.8706	111.0	90.2	-20.8	92.7	-18.3
80	MgO	1.3089	0.7364	10.2	15.9	5.7	16.7	6.5
81	NaBr	3.2329	2.1932	41.0	39.2	-1.8	38.9	-2.1
82	NaCl	2.2609	1.2517	30.2	27.3	-2.9	26.1	-4.1
83	NaF	1.4833	0.4985	15.6	17.8	2.2	16.8	1.2
84	NaI	4.2314	3.1604	57.0	51.4	-5.6	52.2	-4.8
85	Na$_2$O	2.3465	0.7928	19.8	28.1	8.3	25.4	5.6
86	Na$_2$O$_2$	2.7557	0.9603	28.1	33.0	4.9	29.8	1.7
87	Na$_2$S$_5$	7.1377	6.3421	99.0	87.1	-11.9	89.2	-9.8
88	Na$_2$S$_4$	6.0976	5.2603	84.0	74.3	-9.7	76.2	-7.8
89	Na$_2$S$_3$	5.0575	4.1785	68.0	61.6	-6.4	63.1	-4.9
90	Na$_2$S$_2$	4.0174	3.0967	53.0	48.9	-4.1	49.8	-3.2
91	Na$_2$S	2.9773	2.0149	39.0	36.1	-2.9	35.9	-3.1
92	PbBr$_2$	7.8640	15.1047	90.6	99.7	9.1	94.8	4.2
93	PbCl$_2$	5.9199	8.6205	73.8	73.8	0.0	74.2	0.4
94	PbF$_2$	4.3647	3.4333	58.1	53.1	-5.0	54.3	-3.8
95	PbI$_2$	9.8610	21.7654	126.5	126.2	-0.3	127.9	1.4
96	PbO	3.7446	2.7301	42.0	45.5	3.5	45.9	3.9
97	RbBr	4.7034	5.5229	56.4	58.0	1.6	59.0	2.6
98	RbCl	3.7314	3.1520	46.0	45.5	-0.5	46.9	0.9
99	RbF	2.9538	1.2554	31.9	35.5	3.6	32.3	0.4

100	RbI	5.7019	7.9583	72.2	70.9	-1.3	71.5	-0.7
101	Rb₂S₂	6.9583	6.1556	90.0	84.9	-5.1	87.0	-3.0
102	Rb₂S	5.9183	5.0738	80.0	72.1	-7.9	74.0	-6.0
103	SbBr₃	9.1633	16.1014	111.4	115.4	4.0	116.0	4.6
104	SbCl₃	6.2471	9.1893	86.7	77.9	-8.8	78.2	-8.5
105	SbF₃	3.9143	3.6599	46.0	47.9	1.9	49.3	3.3
106	SbH₃	2.4003	0.0711	34.6	28.4	-6.2	25.6	-9.0
107	SbI₃	12.1588	23.2017	147.2	154.0	6.8	150.9	3.7
108	Sb₂O₃	5.9684	5.8205	69.4	73.1	3.7	74.7	5.3
109	SeO₂	2.3616	2.5262	27.2	29.1	1.9	31.4	4.2
110	SiBr₄	9.8824	7.4733	126.0	119.9	-6.1	121.5	-4.5
111	SiC	1.1456	1.0577	12.8	14.1	1.3	17.4	4.6
112	SiO₂	1.6436	1.3508	29.6	20.1	-9.5	22.4	-7.2
113	SnCl₂	5.1141	6.5376	69.0	63.3	-5.7	64.1	-4.9
114	SnBr₄	11.1843	19.2651	149.0	140.7	-8.3	141.9	-7.1
115	SnO₂	2.9456	3.4821	41.0	36.4	-4.6	38.1	-2.9
116	SrBr₂	6.7450	10.0372	86.6	84.2	-2.4	84.2	-2.4
117	SrCl₂	4.8009	5.7284	61.5	59.3	-2.2	60.2	-1.3
118	SrF₂	3.2457	2.2815	37.2	39.4	2.2	39.5	2.3
119	SrI₂	8.7420	14.4633	112.0	109.7	-2.3	106.9	-5.1
120	SrO	2.6256	1.8142	35.0	31.9	-3.1	32.1	-2.9
121	SrO₂	3.0349	1.9817	32.3	36.8	4.5	36.1	3.8
122	TlCl	5.0965	4.9161	57.8	62.4	4.6	63.8	6.0
123	TlF	4.3189	1.9580	44.4	51.9	7.5	48.1	3.7
124	TlI	7.0670	12.4125	82.2	89.0	6.8	87.1	4.9
125	ZnCl₂	4.2699	4.3557	55.3	52.4	-2.9	53.7	-1.6
126	ZnF₂	2.7147	1.7348	34.3	32.9	-1.4	32.2	-2.1
127	ZnO	2.0946	1.3795	27.2	25.4	-1.8	25.7	-1.5
128	ZnS	2.7254	3.5057	25.0	33.8	8.8	35.6	10.6
129	ZrC	2.3314	2.5777	26.0	28.8	2.8	31.1	5.1
130	CsBrO₃	5.9846	4.4258	75.1	72.6	-2.5	74.2	-0.9
131	KBrO₃	4.3946	3.7750	52.6	53.6	1.0	55.0	2.4
132	NaBrO₃	3.7107	3.4951	44.2	45.4	1.2	46.9	2.7
133	TlBrO₃	6.5463	4.6556	75.9	79.3	3.4	80.8	4.9
134	Ag₂CO₃	7.5814	2.9938	80.9	90.8	9.9	88.3	7.4
135	BaCO₃	4.4815	2.9256	58.9	54.2	-4.7	53.2	-5.7
136	CaCO₃	3.0619	1.7636	38.2	37.0	-1.2	35.0	-3.2
137	CdCO₃	4.0321	2.5577	46.7	48.8	2.1	47.3	0.6
138	Cs₂CO₃	8.0333	3.1787	103.6	96.2	-7.4	93.8	-9.8
139	K₂CO₃	4.8532	1.8772	59.0	58.1	-0.9	54.5	-4.5
140	Li₂CO₃	2.2627	0.8170	27.0	27.1	0.1	24.6	-2.4
141	MgCO₃	2.4479	1.2610	32.4	29.5	-2.9	27.6	-4.8
142	Na₂CO₃	3.4855	1.3175	41.0	41.8	0.8	38.1	-2.9
143	PbCO₃	4.8836	3.2547	61.2	59.1	-2.1	58.6	-2.6
144	Rb₂CO₃	6.4264	2.5211	75.4	76.9	1.5	74.0	-1.4
145	SrCO₃	3.7646	2.3388	47.0	45.5	-1.5	43.9	-3.1
146	Tl₂CO₃	9.1567	3.6385	101.6	109.6	8.0	107.1	5.5
147	ZnCO₃	3.2336	1.9041	34.0	39.1	5.1	37.1	3.1
148	CsClO₃	5.3345	3.0955	65.0	64.4	-0.6	61.6	-3.4
149	KClO₃	3.7445	2.4447	42.8	45.3	2.5	44.4	1.6
150	NaClO₃	3.0606	2.1648	34.7	37.2	2.5	37.4	2.7

151	Sr(ClO$_3$)$_2$	6.4003	5.3510	73.0	77.9	4.9	80.0	7.0
152	TlClO$_3$	5.8962	3.3253	65.5	71.1	5.6	68.2	2.7
153	CsClO$_4$	5.6741	3.6031	69.9	68.6	-1.3	67.4	-2.5
154	KClO$_4$	4.0840	2.9524	47.4	49.6	2.2	50.0	2.6
155	NaClO$_4$	3.4002	2.6725	37.6	41.4	3.8	42.5	4.9
156	Ba(OH)$_2$	3.7718	2.4091	53.2	45.6	-7.6	44.4	-8.8
157	Be(OH)$_2$	1.1831	0.2902	23.1	14.2	-8.9	13.7	-9.4
158	Ca(OH)$_2$	2.3522	1.2472	22.0	28.4	6.4	26.8	4.8
159	Cd(OH)$_2$	3.3223	2.0413	41.0	40.2	-0.8	38.6	-2.4
160	KOH	2.0718	0.6804	22.0	24.8	2.8	22.5	0.5
161	LiOH	0.7765	0.1503	12.3	9.3	-3.0	10.1	-2.2
162	Mg(OH)$_2$	1.7381	0.7445	22.1	20.9	-1.2	19.7	-2.4
163	NaOH	1.3879	0.4005	15.8	16.7	0.9	15.7	-0.1
164	Sr(OH)$_2$	3.0549	1.8224	40.0	36.9	-3.1	35.3	-4.7
165	Ba(IO$_3$)$_2$	9.7528	11.3312	122.5	120.2	-2.3	119.7	-2.8
166	Ca(IO$_3$)$_2$	8.3332	10.1692	101.4	102.9	1.5	103.5	2.1
167	Cd(IO$_3$)$_2$	9.3034	10.9633	108.4	114.7	6.3	114.6	6.2
168	CsIO$_3$	6.6523	5.7922	83.1	81.1	-2.0	83.2	0.1
169	KIO$_3$	5.0623	5.1414	63.1	62.1	-1.0	63.4	0.3
170	NaIO$_3$	4.3784	4.8615	53.0	53.9	0.9	55.0	2.0
171	Pb(IO$_3$)$_2$	10.1550	11.6603	131.0	125.0	-6.0	124.5	-6.5
172	Sr(IO$_3$)$_2$	9.0360	10.7444	108.0	111.5	3.5	111.6	3.6
173	TlIO$_3$	7.2140	6.0220	86.8	87.8	1.0	90.1	3.3
174	AgNO$_2$	4.1960	1.6776	42.0	50.3	8.3	46.5	4.5
175	KNO$_2$	2.8319	1.1193	23.3	34.0	10.7	30.8	7.5
176	NaNO$_2$	2.1480	0.8395	14.5	25.8	11.3	23.5	9.0
177	TlNO$_2$	4.9836	2.0000	50.8	59.7	8.9	56.1	5.3
178	AgNO$_3$	4.5619	1.8843	45.7	54.7	9.0	50.9	5.2
179	Ba(NO$_3$)$_2$	6.0238	3.7003	66.5	72.8	6.3	71.0	4.5
180	Hg$_2$(NO$_3$)$_2$	9.9957	18.8714	121.0	126.5	5.5	129.5	8.5
181	Hg(NO$_3$)$_2$	6.5431	4.1254	74.0	79.1	5.1	77.9	3.9
182	KNO$_3$	3.1978	1.3260	33.7	38.4	4.7	34.9	1.2
183	NaNO$_3$	2.5139	1.0461	25.6	30.2	4.6	27.5	1.9
184	Pb(NO$_3$)$_2$	6.4259	4.0295	74.0	77.6	3.6	76.4	2.4
185	RbNO$_3$	3.9844	1.6479	41.0	47.8	6.8	44.0	3.0
186	Sr(NO$_3$)$_2$	5.3070	3.1136	57.2	64.0	6.8	61.4	4.2
187	TlNO$_3$	5.3495	2.2066	56.5	64.1	7.6	60.6	4.1
188	BiPO$_4$	5.5037	5.4132	77.0	67.4	-9.6	68.9	-8.1
189	Pb$_3$(PO$_4$)$_2$	14.9070	11.5193	182.0	180.9	-1.1	179.5	-2.5
190	Ag$_2$SO$_4$	8.4606	4.4099	92.9	101.8	8.9	99.1	6.2
191	BaSO$_4$	5.3606	4.3417	65.8	65.2	-0.6	66.9	1.1
192	BeSO$_4$	2.7719	2.2227	37.0	33.8	-3.2	35.2	-1.8
193	CaSO$_4$	3.9410	3.1797	49.7	48.0	-1.7	49.2	-0.5
194	CdSO$_4$	4.9112	3.9738	59.2	59.8	0.6	61.2	2.0
195	Cs$_2$SO$_4$	8.9124	4.5948	116.0	107.2	-8.8	104.4	-11.6
196	Hg$_2$SO$_4$	9.3325	7.5927	123.0	113.5	-9.5	115.4	-7.6
197	HgSO$_4$	5.8799	4.7667	78.1	71.5	-6.6	73.4	-4.7
198	K$_2$SO$_4$	5.7324	3.2933	67.0	69.1	2.1	66.4	-0.6
199	Li$_2$SO$_4$	3.1418	2.2331	41.6	38.1	-3.5	38.4	-3.2
200	MgSO$_4$	3.3270	2.6771	42.0	40.5	-1.5	41.8	-0.2
201	Na$_2$SO$_4$	4.3646	2.7335	52.0	52.8	0.8	51.1	-0.9

202	PbSO$_4$	5.7627	4.6708	69.7	70.1	0.4	71.9	2.2
203	Rb$_2$SO$_4$	7.3055	3.9372	88.4	87.9	-0.5	85.2	-3.2
204	SrSO$_4$	4.6438	3.7549	57.9	56.5	-1.4	57.9	0.0
205	Tl$_2$SO$_4$	10.0358	5.0546	112.6	120.6	8.0	117.0	4.4
206	ZnSO$_4$	4.1127	3.3202	47.8	50.1	2.3	51.3	3.5

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