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Topological Research on Lattice Energies for Inorganic Compounds

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A novel connectivity index ${}^{m}G$ and its converse index ${}^{m}G'$ based on adjacency matrix of molecular graphs are proposed as follows: ${}^{m}G = \Sigma\,(g_i g_j g_k \cdots)^{0.5}$, ${}^{m}G' = \Sigma\,(g_i g_j g_k \cdots)^{-0.5}$. The g_i element of adjacency matrix is defined as $g_i=(1+m_i^{1.7}).X_i^{0.3}/(1+r_i)$, where m_i,X_i,r_i, are the charge number, the electronegativity and Goldschmidt ionic radius of atom *i* respectively. By using the connectivity index ${}^{m}G$ and its converse index ${}^{m}G'$, the multiple linear regression and multiple nonlinear regression can provide high-quality QSPR models for the lattice energies of 318 inorganic compounds. The results imply that the lattice energies may be expressed as a linear or nonlinear combination of the connectivity indices ${}^{0}G$,${}^{1}G$,${}^{0}G'$ and ${}^{1}G'$. For the nonlinear model, the correlation coefficient *r* and the standard error *s* are 0.9998 and 217.6 kJ.mol^{-1}, respectively. The cross-validation by using the leave-one-out method demonstrates that the models are highly reliable from the point of view of statistics.

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 papers[4-11] about the QSPR/

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QSAR studies of inorganic compounds, due to the complexity of inorganic-compound composition.

The lattice energy of an inorganic ionic crystal is a dominant term in the thermodynamic analysis of the existence and stability of an ionic crystal. It is one of the most important quantities in indicating the structure, character, and behavior (reactivity) of solids. Although lattice energy can be determined experimentally from the Born-Haber-Fajans thermochemical cycle, direct experimental determination is generally not possible since, in practice, the crystalline solid dissociates into atoms but not gaseous ions, as it is required in the lattice energy evaluation. Therefore, its indirect experimental determination, computation, or estimation is of considerable interest in modern materials science. Theoretical studies on lattice energy have been carried out almost since the beginning of 1900s, and a variety of estimation methods for lattice energies were available.[12~29]

In recent years, Feng et al.[7,9-11] and Xu et al.[8] etc., by using various model parameters, have developed some QSPR/QSAR models to estimate the lattice energies of inorganic compounds. In this study, the ionic polarization force parameter g_i is defined based on ionic radii, electronegativity, ionic charge. A now topological index ${}^mG$ and its converse index ${}^mG'$ are proposed based on the randic's index and g_i. The connectivity index ${}^mG$ together with ${}^mG'$ has good correlations for lattice energies of inorganic ionic crystals.

2. METHODS

Ionic crystals are made up of positive and negative ions, and the strongest interactions result from the nearest oppositely charged ions. The lattice energy contribution originates mainly from these nearest interactions, and the sum of the lattice energies of these interacting ion pairs is affected by the ionic radius, electronegativity, ionic charge. As mentioned above the polarization force parameter g_i is defined as:

$$g_i=(1+m_i^{1.7}).X_i^{0.3}/(1+r_i) \qquad (1)$$

where m_i, X_i , r_i are the charge number, the electronegativity[30] and Goldschmidt[31] ionic radius of atom i respectively. For ions of different atoms and ions of the same atom with different charges, the g_i are different. The g_i of 78 ions are calculated and listed in Table 1.

Table 1. Ionic polarization force parameters

No	Ionic	r_i	X_i	m_i	g_i	No	Ionic	r_i	X_i	m_i	g_i
1	Ag^+	1.13	1.93	1	1.1437	40	Nd^{3+}	1.15	1.14	3	3.6152
2	Al^{3+}	0.55	1.61	3	5.5618	41	Ni^{2+}	0.78	1.91	2	2.8985
3	As^{3+}	0.69	2.18	3	5.5866	42	P^{5+}	0.17	2.19	5	17.7613
4	Au^{3+}	1.37	2.54	3	1.1162	43	Pb^{2+}	1.32	2.33	2	2.3605

5	B^{3+}	0.20	2.04	3	7.7126	44	Pb^{4+}	0.84	2.33	4	8.0947
6	Ba^{2+}	1.38	0.89	2	1.7240	45	Pd^{2+}	0.80	2.20	2	2.9905
7	Be^{2+}	0.34	1.57	2	3.6304	46	Pr^{3+}	1.12	1.13	3	3.6566
8	Bi^{3+}	1.20	2.02	3	4.1945	47	Rb^{+}	1.49	0.82	1	0.7568
9	Ca^{2+}	1.05	1.00	2	2.0727	48	Rh^{3+}	0.75	2.28	3	5.4681
10	Cd^{2+}	0.99	1.69	2	2.4992	49	Sb^{3+}	0.90	2.05	3	4.8783
11	Ce^{3+}	1.19	1.12	3	3.5303	50	Sb^{5+}	0.62	2.05	5	12.5759
12	Co^{2+}	0.82	1.88	2	2.8214	51	Sc^{3+}	0.83	1.36	3	4.4782
13	Co^{3+}	0.65	1.88	3	5.4734	52	Si^{4+}	0.40	1.90	4	10.0071
14	Cr^{2+}	0.89	1.66	2	2.6173	53	Sm^{3+}	1.13	1.17	3	3.6777
15	Cr^{3+}	0.65	1.66	3	5.2728	54	Sn^{2+}	1.02	1.96	2	2.5740
16	Cs^{+}	1.70	0.79	1	0.6902	55	Sn^{4+}	0.74	1.96	4	8.1271
17	Cu^{+}	0.96	1.90	1	1.2371	56	Sr^{2+}	1.18	0.95	2	1.9193
18	Cu^{2+}	0.72	1.90	2	2.9949	57	Ti^{2+}	0.76	1.54	2	2.7481
19	Dy^{3+}	1.07	1.22	3	3.8321	58	Ti^{3+}	0.70	1.54	3	5.0038
20	Er^{3+}	1.04	1.24	3	3.9074	59	Ti^{4+}	0.64	1.54	4	8.0209
21	Fe^{2+}	0.83	1.83	2	2.7834	60	Tl^{+}	1.49	2.04	1	0.9948
22	Fe^{3+}	0.67	1.83	3	5.3643	61	Tl^{3+}	1.05	2.04	3	4.5147
23	Ga^{3+}	0.62	1.81	3	5.5117	62	Tm^{3+}	1.04	1.25	3	3.9169
24	Gd^{3+}	1.11	1.20	3	3.7408	63	V^{2+}	0.88	1.63	2	2.6169
25	Ge^{2+}	0.65	2.01	2	3.1751	64	V^{3+}	0.75	1.63	3	4.9444
26	Hg^{2+}	1.12	2.00	2	2.4675	65	V^{5+}	0.36	1.63	5	13.9844
27	Ho^{3+}	1.05	1.23	3	3.8789	66	Y^{3+}	0.95	1.22	3	4.0679
28	In^{3+}	0.92	1.78	3	4.6272	67	Zn^{2+}	0.83	1.65	2	2.6982
29	K^{+}	1.33	0.82	1	0.8088	68	Zr^{4+}	0.80	1.33	4	6.9935
30	La^{3+}	1.15	1.10	3	3.5766	69	Br^{-}	1.96	2.96	1	0.9357
31	Li^{+}	0.70	0.98	1	1.1694	70	Cl^{-}	1.81	3.16	1	1.0051
32	Mg^{2+}	0.75	1.31	2	2.6329	71	F^{-}	1.33	3.98	1	1.2991
33	Mn^{2+}	0.91	1.55	2	2.5372	72	H^{-}	2.08	2.20	1	0.8226
34	Mn^{3+}	0.62	1.55	3	5.2611	73	I^{-}	2.20	2.66	1	0.8382
35	Mn^{4+}	0.52	1.55	4	8.6709	74	N^{3-}	1.71	3.04	3	3.8494
36	Mo^{3+}	0.69	2.16	3	5.5712	75	O^{2-}	1.35	3.44	2	2.6193
37	Mo^{4+}	0.65	2.16	4	8.8239	76	S^{2-}	1.82	2.58	2	2.0023
38	Mo^{6+}	0.41	2.16	6	19.6856	77	Se^{2-}	1.93	2.55	2	1.9204
39	Na^{+}	0.98	0.93	1	0.9883	78	Te^{2-}	2.12	2.10	2	1.7014

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

$${}^{m}G=\Sigma(g_i.g_j.g_k\ldots)^{0.5} \quad (2)$$

$${}^{m}G'=\Sigma(g_i.g_j.g_k\ldots)^{-0.5} \quad (3)$$

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

$${}^{0}G=\Sigma(g_i)^{0.5} \quad (4)$$

$${}^{1}G=\Sigma(g_i.g_j)^{0.5} \quad (5)$$

$${}^{0}G'=\Sigma(g_i)^{-0.5} \quad (6)$$

$${}^{1}G'=\Sigma(g_i.g_j)^{-0.5} \quad (7)$$

In expressions (4) and (6), the "Σ" is the sum of atomic of inorganic compound chemical formula. In expressions (5) and (7), the "Σ" is the sum of chemical single bonds of chemical formula. For example, the ${}^0G$, ${}^1G$, ${}^0G'$, and ${}^1G'$ of $Ba_4NaSb_3O_{12}$ are calculated as follows:

For $Ba_4NaSb_3O_{12}$, it can be treated as consisting of four Ba^{2+}, one Na^+, three Sb^{5+} and twelve O^{2-}, it contains eight Ba-O single bonds, one Na-O single bonds and fifteen Sb-O single bonds, so:

${}^0G=4\times1.7240^{0.5}+0.9883^{0.5}+3\times12.5759^{0.5}+12\times2.6193^{0.5}=36.3060$

${}^1G=8\times(1.7240\times2.6193)^{0.5}+(0.9883\times2.6193)^{0.5}+15\times(12.5759\times2.6193)^{0.5}=104.6993$

${}^0G'=4\times1.7240^{-0.5}+0.9883^{-0.5}+3\times12.5759^{-0.5}+12\times2.6193^{-0.5}=12.3129$

${}^1G'=8\times(1.7240\times2.6193)^{-0.5}+(0.9883\times2.6193)^{-0.5}+15\times(12.5759\times2.6193)^{-0.5}=6.9998$

The ${}^0G$, ${}^1G$, ${}^0G'$, and ${}^1G'$ of 318 inorganic compounds are calculated and listed in Table 2.

Table2. The calculated and Experimental Lattice Energies of 318inorganic compounds ($kJ.mol^{-1}$)

No	Substance	${}^0G$	${}^1G$	${}^0G'$	${}^1G'$	U(ref)	U(pred)	Er.	ref
1	LiF	2.2211	1.2325	1.8021	0.8113	1049	1025	24	32
2	NaF	2.1339	1.1331	1.8832	0.8825	930	941	-11	32
3	KF	2.0391	1.0250	1.9893	0.9756	829	848	-19	32
4	RbF	2.0097	0.9915	2.0269	1.0085	795	818	-23	32
5	CsF	1.9705	0.9469	2.0811	1.0561	759	778	-19	32
6	LiCl	2.0839	1.0841	1.9222	0.9224	864	897	-33	32
7	NaCl	1.9967	0.9967	2.0033	1.0033	790	817	-27	32
8	KCl	1.9019	0.9016	2.1094	1.1091	720	725	-5	32
9	RbCl	1.8725	0.8722	2.1469	1.1466	695	695	0	32
10	CsCl	1.8333	0.8329	2.2011	1.2006	670	654	16	32
11	LiBr	2.0487	1.0460	1.9586	0.9560	820	863	-43	32
12	NaBr	1.9615	0.9617	2.0397	1.0399	754	783	-29	32
13	KBr	1.8666	0.8699	2.1458	1.1496	691	691	0	32
14	RbBr	1.8372	0.8415	2.1833	1.1884	668	661	7	32
15	CsBr	1.7981	0.8036	2.2375	1.2444	647	620	27	32
16	LiI	1.9969	0.9900	2.0170	1.0101	764	813	-49	32
17	NaI	1.9097	0.9102	2.0981	1.0987	705	733	-28	32
18	KI	1.8148	0.8233	2.2042	1.2146	650	640	10	32
19	RbI	1.7855	0.7965	2.2418	1.2556	632	610	22	32
20	CsI	1.7463	0.7606	2.2960	1.3148	613	567	46	32
21	BeF_2	4.1849	4.3434	2.2796	0.9209	3526	3505	21	32
22	MgF_2	3.9022	3.6988	2.3710	1.0814	2978	3012	-34	32
23	CaF_2	3.7192	3.2818	2.4493	1.2188	2651	2678	-27	32
24	SrF_2	3.6649	3.1581	2.4765	1.2666	2513	2575	-62	32
25	BaF_2	3.5925	2.9930	2.5163	1.3364	2373	2435	-62	32
26	$BeCl_2$	3.9105	3.8205	2.5197	1.0470	3033	3141	-108	32
27	$MgCl_2$	3.6278	3.2536	2.6112	1.2294	2540	2681	-141	32
28	$CaCl_2$	3.4448	2.8868	2.6895	1.3856	2271	2363	-92	32
29	$SrCl_2$	3.3905	2.7779	2.7167	1.4399	2170	2264	-94	32
30	$BaCl_2$	3.3181	2.6327	2.7565	1.5193	2069	2128	-59	32
31	$BeBr_2$	3.8400	3.6861	2.5924	1.0852	2914	3047	-133	32
32	$MgBr_2$	3.5572	3.1391	2.6839	1.2742	2451	2595	-144	32
33	$CaBr_2$	3.3743	2.7852	2.7622	1.4362	2134	2280	-146	9
34	$SrBr_2$	3.3200	2.6802	2.7894	1.4924	2040	2182	-142	9
35	$BaBr_2$	3.2476	2.5401	2.8292	1.5747	1995	2046	-51	32

36	BeI_2	3.7364	3.4888	2.7094	1.1465	2813	2909	-96	32
37	MgI_2	3.4537	2.9711	2.8008	1.3463	2340	2467	-127	32
38	CaI_2	3.2707	2.6361	2.8791	1.5174	2087	2156	-69	32
39	SrI_2	3.2165	2.5367	2.9063	1.5768	1976	2058	-82	32
40	BaI_2	3.1441	2.4042	2.9461	1.6638	1890	1922	-32	32
41	BeO	3.5238	6.1674	1.1427	0.6486	4443	4359	84	32
42	MgO	3.2410	5.2522	1.2342	0.7616	3791	3738	53	32
43	CaO	3.0581	4.6601	1.3125	0.8584	3401	3328	73	32
44	SrO	3.0038	4.4843	1.3397	0.8920	3223	3204	19	32
45	BaO	2.9314	4.2500	1.3795	0.9412	3054	3038	16	32
46	BeS	3.3204	5.3922	1.2315	0.7418	3770	3842	-72	9
47	MgS	3.0376	4.5921	1.3230	0.8711	3238	3280	-42	9
48	CaS	2.8547	4.0744	1.4013	0.9817	2966	2906	60	9
49	SrS	2.8004	3.9207	1.4285	1.0202	2779	2793	-14	9
50	BaS	2.7280	3.7158	1.4683	1.0765	2643	2640	3	9
51	CuCl	2.1148	1.1151	1.8965	0.8968	996	925	71	32
52	AgCl	2.0720	1.0722	1.9325	0.9327	918	886	32	32
53	Al_2O_3	9.5720	22.9008	2.7017	1.5720	15111	15361	-250	9
54	AgF	2.2092	1.2189	1.8124	0.8204	974	1013	-39	32
55	AgBr	2.0367	1.0345	1.9689	0.9667	905	852	53	32
56	AgI	1.9850	0.9791	2.0273	1.0213	892	802	90	32
57	TiF_2	3.9373	3.7789	2.3580	1.0585	2757	3075	-318	9
58	VF_2	3.8972	3.6876	2.3729	1.0847	2770	3003	-233	9
59	CrF_2	3.8974	3.6879	2.3728	1.0846	2939	3004	-65	32
60	MnF_2	3.8724	3.6310	2.3825	1.1016	2803	2959	-156	9
61	FeF_2	3.9479	3.8031	2.3541	1.0518	2967	3093	-126	32
62	CoF_2	3.9593	3.8290	2.3501	1.0447	3042	3113	-71	32
63	NiF_2	3.9821	3.8810	2.3421	1.0307	3089	3154	-65	32
64	CuF_2	4.0101	3.9450	2.3326	1.0140	3102	3203	-101	32
65	ZnF_2	3.9222	3.7445	2.3635	1.0682	3053	3048	5	32
66	$TiCl_2$	3.6629	3.3240	2.5981	1.2034	2514	2740	-226	32
67	VCl_2	3.6228	3.2437	2.6130	1.2332	2593	2672	-79	32
68	$CrCl_2$	3.6230	3.2439	2.6130	1.2331	2601	2673	-72	32
69	$MnCl_2$	3.5980	3.1939	2.6227	1.2524	2551	2630	-79	32
70	$FeCl_2$	3.6735	3.3453	2.5943	1.1957	2641	2757	-116	32
71	$CoCl_2$	3.6848	3.3680	2.5902	1.1876	2706	2776	-70	32
72	$NiCl_2$	3.7076	3.4138	2.5822	1.1717	2786	2814	-28	32
73	$CuCl_2$	3.7357	3.4701	2.5727	1.1527	2824	2860	-36	32
74	TiI_2	3.4888	3.0354	2.7878	1.3178	2342	2524	-182	32
75	VI_2	3.4487	2.9621	2.8027	1.3504	2470	2459	11	32
76	CrI_2	3.4489	2.9623	2.8026	1.3503	2440	2459	-19	32
77	MnI_2	3.4239	2.9166	2.8123	1.3715	2388	2418	-30	9
78	FeI_2	3.4994	3.0548	2.7839	1.3094	2491	2541	-50	32
79	CoI_2	3.5108	3.0756	2.7799	1.3005	2561	2559	2	32
80	NiI_2	3.5336	3.1174	2.7719	1.2831	2637	2596	41	32
81	CuI_2	3.5616	3.1688	2.7624	1.2623	2694	2640	54	9
82	TlF	2.1372	1.1368	1.8800	0.8797	850	944	-94	32
83	TlCl	1.9999	0.9999	2.0001	1.0001	751	820	-69	32
84	TlBr	1.9647	0.9648	2.0364	1.0365	734	786	-52	32
85	TlI	1.9129	0.9131	2.0949	1.0951	710	736	-26	32
86	Tl_2O	3.6132	3.2284	2.6231	1.2390	2575	2661	-86	32
87	Tl_2S	3.4098	2.8226	2.7120	1.4171	2258	2306	-48	32
88	Tl_2Se	3.3805	2.7643	2.7269	1.4470	2326	2253	73	9
89	Tl_2Te	3.2991	2.6019	2.7719	1.5373	2172	2099	73	32
90	TlF_3	5.5441	7.2653	3.1027	1.2388	5431	5704	-273	9
91	$TlCl_3$	5.1325	6.3907	3.4629	1.4083	5278	5113	165	32
92	$TlBr_3$	5.0267	6.1659	3.5720	1.4596	5146	4962	184	9

93	TiO_2	6.0690	18.3343	1.5889	0.8727	12054	11923	131	9
94	PbF_2	3.8159	3.5023	2.4056	1.1421	2543	2857	-314	32
95	$PbCl_2$	3.5415	3.0807	2.6457	1.2984	2282	2534	-252	32
96	$PbBr_2$	3.4710	2.9723	2.7185	1.3457	2230	2449	-219	32
97	PbI_2	3.3675	2.8132	2.8354	1.4219	2177	2324	-147	32
98	PbO	3.1548	4.9731	1.2688	0.8043	3520	3546	-26	9
99	PbS	2.9514	4.3481	1.3576	0.9200	3161	3105	56	9
100	PbSe	2.9222	4.2582	1.3725	0.9394	3144	3041	103	9
101	PbTe	2.8408	4.0080	1.4175	0.9980	3039	2860	179	9
102	PbF_4	7.4042	12.9712	3.8609	1.2335	9468	9727	-259	9
103	PbO_2	6.0820	18.4185	1.5872	0.8687	11682	11973	-291	9
104	AlF_3	5.7777	8.0639	3.0561	1.1161	6252	6269	-17	32
105	$AlCl_3$	5.3660	7.0932	3.4163	1.2688	5513	5638	-125	32
106	$AlBr_3$	5.2602	6.8437	3.5254	1.3151	5360	5476	-116	32
107	AlI_3	5.1049	6.4774	3.7008	1.3895	5227	5240	-13	32
108	$TiBr_2$	3.5923	3.2071	2.6708	1.2472	2430	2653	-223	32
109	TiO	3.2762	5.3659	1.2211	0.7455	3811	3816	-5	32
110	TiS	3.0728	4.6915	1.3099	0.8526	3357	3351	6	9
111	TiF_3	5.6563	7.6488	3.0791	1.1767	5665	5977	-312	9
112	$TiCl_3$	5.2446	6.7280	3.4394	1.3377	5153	5367	-214	32
113	$TiBr_3$	5.1388	6.4914	3.5484	1.3865	5023	5211	-188	32
114	TiI_3	4.9835	6.1439	3.7238	1.4649	4971	4982	-11	9
115	Ti_2O_3	9.3291	21.7218	2.7477	1.6573	14487	14617	-130	25
116	TiF_4	7.3912	12.9119	3.8626	1.2392	9908	9688	220	32
117	$TiCl_4$	6.8424	11.3576	4.3428	1.4088	9129	8734	395	9
118	$TiBr_4$	6.7013	10.9581	4.4883	1.4601	9059	8491	568	32
119	TiI_4	6.4942	10.3715	4.7222	1.5427	8918	8137	781	32
120	CuF	2.2520	1.2677	1.7764	0.7888	1088	1054	34	9
121	CuBr	2.0795	1.0759	1.9329	0.9295	978	891	87	32
122	CuI	2.0278	1.0183	1.9913	0.9820	966	840	126	32
123	Cu_2O	3.8429	3.6002	2.4160	1.1111	3189	2939	250	32
124	Cu_2S	3.6395	3.1477	2.5049	1.2708	2865	2570	295	32
125	Cu_2Se	3.6103	3.0826	2.5198	1.2976	2936	2515	421	9
126	CdF_2	3.8604	3.6037	2.3873	1.1100	2830	2937	-107	32
127	HgF_2	3.8504	3.5808	2.3913	1.1171	2780	2919	-139	9
128	VO	3.2361	5.2362	1.2361	0.7639	3863	3727	136	32
129	MnO	3.2113	5.1559	1.2457	0.7758	3745	3672	73	32
130	FeO	3.2868	5.4002	1.2173	0.7407	3865	3839	26	32
131	CoO	3.2981	5.4370	1.2132	0.7357	3910	3864	46	32
132	NiO	3.3209	5.5108	1.2053	0.7259	4010	3915	95	32
133	CuO	3.3490	5.6017	1.1957	0.7141	4050	3977	73	32
134	ZnO	3.2611	5.3170	1.2267	0.7523	3971	3782	189	32
135	CdO	3.1993	5.1171	1.2504	0.7817	3806	3645	161	9
136	HgO	3.1893	5.0846	1.2545	0.7867	3907	3623	284	9
137	GeO	3.4003	5.7677	1.1791	0.6935	3919	4089	-170	9
138	SnO	3.2228	5.1931	1.2412	0.7702	3652	3697	-45	9
139	PdO	3.3477	5.5975	1.1962	0.7146	3736	3974	-238	9
140	$MnBr_2$	3.5275	3.0816	2.6954	1.2980	2482	2545	-63	32
141	MnS	3.0079	4.5078	1.3345	0.8873	3415	3220	195	9
142	MnSe	2.9786	4.4147	1.3494	0.9061	3330	3154	176	9
143	MnTe	2.8972	4.1553	1.3945	0.9626	3207	2969	238	9
144	MnF_3	5.7130	7.8430	3.0681	1.1475	6012	6114	-102	9
145	$MnCl_3$	5.3014	6.8988	3.4283	1.3046	5556	5494	62	9
146	MnO_2	6.1815	19.0628	1.5754	0.8393	13150	12355	795	9
147	MgSe	3.0084	4.4971	1.3379	0.8895	3365	3213	152	9
148	MgTe	2.9270	4.2330	1.3829	0.9450	3202	3026	176	9
149	$ScBr_3$	5.0181	6.1410	3.5740	1.4656	4761	4942	-181	32

150	YBr_3	4.9188	5.8529	3.5972	1.5377	4435	4716	-281	9
151	$LaBr_3$	4.7931	5.4881	3.6302	1.6399	4280	4421	-141	9
152	$CeBr_3$	4.7808	5.4525	3.6336	1.6506	4418	4391	27	9
153	$CdCl_2$	3.5860	3.1699	2.6274	1.2619	2565	2610	-45	32
154	$CdBr_2$	3.5155	3.0584	2.7002	1.3079	2517	2525	-8	32
155	CdI_2	3.4119	2.8947	2.8171	1.3818	2455	2398	57	32
156	CdS	2.9959	4.4740	1.3393	0.8941	3460	3196	264	9
157	CdSe	2.9667	4.3815	1.3542	0.9129	3310	3130	180	9
158	$CoCl_2$	3.6848	3.3680	2.5902	1.1876	2695	2776	-81	9
159	$CoBr_2$	3.6143	3.2496	2.6629	1.2309	2643	2689	-46	32
160	CoI_2	3.5108	3.0756	2.7799	1.3005	2531	2559	-28	9
161	CoS	3.0947	4.7536	1.3020	0.8415	3653	3395	258	9
162	CoSe	3.0655	4.6554	1.3170	0.8592	3611	3326	285	9
163	$ZnCl_2$	3.6478	3.2937	2.6037	1.2144	2748	2714	34	32
164	$HgCl_2$	3.5760	3.1497	2.6315	1.2699	2664	2593	71	32
165	$SnCl_2$	3.6095	3.2170	2.6182	1.2434	2310	2650	-340	32
166	$FeBr_2$	3.6030	3.2276	2.6670	1.2393	2515	2670	-155	9
167	$NiBr_2$	3.6371	3.2937	2.6550	1.2144	2721	2726	-5	32
168	$CuBr_2$	3.6652	3.3480	2.6454	1.1947	2774	2771	3	32
169	$ZnBr_2$	3.5772	3.1779	2.6764	1.2587	2689	2628	61	32
170	$HgBr_2$	3.5054	3.0389	2.7042	1.3162	2639	2508	131	32
171	$SnBr_2$	3.5390	3.1038	2.6909	1.2887	2256	2564	-308	32
172	ZnI_2	3.4737	3.0078	2.7933	1.3299	2619	2500	119	32
173	HgI_2	3.4019	2.8763	2.8211	1.3907	2624	2382	242	32
174	SnI_2	3.4354	2.9377	2.8078	1.3616	2206	2437	-231	32
175	FeS	3.0834	4.7215	1.3061	0.8472	3506	3372	134	9
176	CoS	3.0947	4.7536	1.3020	0.8415	3653	3395	258	9
177	NiS	3.1175	4.8182	1.2941	0.8302	3694	3441	253	9
178	CuS	3.1456	4.8976	1.2845	0.8167	3795	3496	299	9
179	ZnS	3.0577	4.6487	1.3155	0.8605	3674	3320	354	9
180	SnS	3.0194	4.5404	1.3300	0.8810	3201	3243	-42	9
181	Ag_2O	3.7573	3.4616	2.4880	1.1555	2910	2836	74	32
182	Ag_2S	3.5539	3.0266	2.5768	1.3216	2677	2473	204	32
183	Ag_2Te	3.4433	2.7899	2.6368	1.4337	2600	2263	337	32
184	AlH_3	5.0793	6.4170	3.7317	1.4025	5969	5201	768	32
185	$AsBr_3$	5.2655	6.8589	3.5245	1.3122	5365	5487	-122	32
186	AsI_3	5.1102	6.4918	3.6999	1.3864	5295	5251	44	32
187	AuBr	2.0238	1.0219	1.9803	0.9785	1059	841	218	32
188	AuCl	2.0591	1.0592	1.9440	0.9441	1066	874	192	32
189	AuH	1.9635	0.9582	2.0491	1.0436	1108	782	326	32
190	AuI	1.9720	0.9672	2.0388	1.0339	1070	790	280	32
191	BaH_2	3.1270	2.3818	2.9667	1.6794	2133	1901	232	32
192	BeH_2	3.7193	3.4563	2.7299	1.1573	3306	2887	419	32
193	$BiCl_3$	5.0558	6.1599	3.4806	1.4611	4707	4936	-229	32
194	CaH_2	3.2537	2.6116	2.8997	1.5317	2406	2136	270	32
195	$CeCl_3$	4.8866	5.6512	3.5245	1.5926	4348	4535	-187	32
196	CeI_3	4.6255	5.1606	3.8090	1.7440	4061	4179	-118	32
197	Cr_2O_3	9.4478	22.2981	2.7246	1.6145	14957	14981	-24	32
198	$CrBr_2$	3.5524	3.1298	2.6857	1.2780	2536	2587	-51	32
199	$CrCl_3$	5.3040	6.9065	3.4278	1.3031	5529	5500	29	32
200	CrF_3	5.7156	7.8517	3.0676	1.1463	6065	6120	-55	32
201	CrI_3	5.0429	6.3069	3.7123	1.4270	5294	5109	185	32
202	CrN	4.2582	13.5157	0.9452	0.6659	8358	8779	-421	32
203	Cs_2O	3.2800	2.6891	3.0253	1.4875	2063	2247	-184	32
204	Cs_2S	3.0765	2.3511	3.1141	1.7013	1850	1901	-51	32
205	CsH	1.7378	0.7535	2.3063	1.3271	653	558	95	32
206	Cu_2Te	3.5289	2.9015	2.5648	1.3786	2683	2358	325	32

207	CuH	2.0192	1.0088	2.0016	0.9913	1254	831	423	32
208	$DyCl_3$	4.9653	5.8878	3.5031	1.5286	4529	4724	-195	32
209	$ErCl_3$	4.9844	5.9454	3.4982	1.5138	4591	4769	-178	32
210	Fe_2O_3	9.4875	22.4907	2.7172	1.6007	14774	15103	-329	32
211	$FeCl_3$	5.3238	6.9662	3.4241	1.2920	5436	5544	-108	32
212	Ga_2O_3	9.5507	22.7975	2.7055	1.5791	15220	15296	-76	32
213	$GaBr_3$	5.2496	6.8128	3.5274	1.3210	5569	5453	116	32
214	$GaCl_3$	5.3554	7.0612	3.4183	1.2746	5665	5614	51	32
215	GaF_3	5.7670	8.0275	3.0580	1.1211	6238	6244	-6	32
216	GaI_3	5.0943	6.4482	3.7027	1.3957	5496	5217	279	32
217	$GdCl_3$	4.9418	5.8173	3.5093	1.5471	4495	4668	-173	32
218	$HoCl_3$	4.9772	5.9237	3.5001	1.5193	4572	4752	-180	32
219	$InBr_3$	5.0530	6.2423	3.5663	1.4418	5117	5021	96	32
220	$InCl_3$	5.1588	6.4699	3.4572	1.3911	5183	5173	10	32
221	InI_3	4.8977	5.9082	3.7417	1.5233	5001	4796	205	32
222	K_2O	3.4170	2.9109	2.8418	1.3741	2232	2420	-188	32
223	K_2S	3.2136	2.5451	2.9306	1.5717	1979	2073	-94	25
224	KH	1.8063	0.8157	2.2145	1.2260	713	632	81	32
225	$LaCl_3$	4.8989	5.6882	3.5211	1.5822	4242	4564	-322	32
226	LaH_3	4.6122	5.1459	3.8364	1.7490	4493	4172	321	32
227	LaI_3	4.6378	5.1943	3.8056	1.7327	3986	4208	-222	32
228	LaN	3.8532	11.1315	1.0385	0.8085	6793	7322	-529	32
229	Li_2O	3.7812	3.5002	2.4674	1.1428	2814	2864	-50	32
230	Li_2S	3.5778	3.0603	2.5562	1.3071	2472	2500	-28	32
231	LiH	1.9884	0.9808	2.0273	1.0196	918	804	114	32
232	MgH_2	3.4366	2.9434	2.8214	1.3590	2718	2446	272	32
233	Mn_2O_3	9.4427	22.2733	2.7256	1.6163	15035	14966	69	32
234	$MoBr_4$	6.8397	11.4935	4.4718	1.3921	9500	8862	638	32
235	$MoCl_3$	5.3680	7.0992	3.4160	1.2678	5253	5642	-389	32
236	$MoCl_4$	6.9808	11.9126	4.3264	1.3431	9603	9113	490	32
237	$ZrBr_4$	6.5137	10.2322	4.5133	1.5637	7984	7980	4	32
238	$ZrCl_4$	6.6548	10.6053	4.3679	1.5087	8144	8212	-68	32
239	ZrF_4	7.2036	12.0566	3.8876	1.3271	8971	9121	-150	32
240	ZrI_4	6.3066	9.6845	4.7472	1.6521	7801	7641	160	32
241	Na_2O	3.6067	3.2179	2.6296	1.2430	2478	2653	-175	32
242	Na_2S	3.4033	2.8135	2.7185	1.4217	2203	2299	-96	32
243	Na_2Te	3.2927	2.5935	2.7784	1.5423	2095	2092	3	32
244	NaH	1.9011	0.9017	2.1084	1.1090	807	725	82	32
245	$NdCl_3$	4.9091	5.7187	3.5182	1.5738	4415	4589	-174	32
246	$PdBr_2$	3.6639	3.3455	2.6459	1.1956	2751	2769	-18	32
247	$PdCl_2$	3.7344	3.4675	2.5731	1.1536	2818	2858	-40	32
248	PdI_2	3.5604	3.1665	2.7628	1.2632	2760	2638	122	32
249	$PrCl_3$	4.9199	5.7515	3.5153	1.5648	4387	4615	-228	32
250	PrI_3	4.6588	5.2521	3.7997	1.7136	4101	4257	-156	32
251	Rb_2O	3.3583	2.8159	2.9169	1.4205	2161	2347	-186	32
252	Rb_2S	3.1549	2.4620	3.0057	1.6247	1949	2000	-51	32
253	RbH	1.7769	0.7890	2.2521	1.2674	684	601	83	32
254	$RhCl_3$	5.3461	7.0332	3.4200	1.2796	5665	5594	71	32
255	$SbBr_3$	5.1106	6.4094	3.5542	1.4042	4776	5149	-373	32
256	$SbCl_3$	5.2164	6.6431	3.4451	1.3548	4857	5304	-447	32
257	SbF_3	5.6280	7.5522	3.0849	1.1917	5324	5909	-585	32
258	SbI_3	4.9553	6.0664	3.7296	1.4836	4692	4921	-229	32
259	Sc_2O_3	9.0877	20.5493	2.7987	1.7519	13708	13867	-159	32
260	$ScCl_3$	5.1239	6.3649	3.4649	1.4140	4901	5094	-193	32
261	ScF_3	5.5355	7.2359	3.1046	1.2438	5540	5682	-142	32
262	ScN	4.0782	12.4557	0.9822	0.7226	7506	8135	-629	32
263	$SmCl_3$	4.9254	5.7680	3.5138	1.5603	4450	4628	-178	32

264	$SnBr_4$	6.7200	11.0304	4.4860	1.4505	8852	8542	310	32
265	$SnCl_4$	6.8611	11.4326	4.3405	1.3995	8930	8785	145	32
266	SrH_2	3.1994	2.5131	2.9269	1.5917	2265	2038	227	32
267	TiH_2	3.4717	3.0071	2.8083	1.3302	2864	2503	361	32
268	TiN	4.1989	13.1664	0.9567	0.6836	8033	8567	-534	32
269	$TmCl_3$	4.9868	5.9526	3.4976	1.5119	4608	4775	-167	32
270	TmI_3	4.7257	5.4358	3.7821	1.6557	4340	4412	-72	32
271	V_2O_3	9.3025	21.5924	2.7531	1.6672	14520	14534	-14	32
272	VBr_2	3.5523	3.1296	2.6858	1.2781	2534	2586	-52	32
273	VBr_3	5.1255	6.4527	3.5511	1.3948	5224	5182	42	32
274	VCl_3	5.2313	6.6879	3.4420	1.3457	5329	5337	-8	32
275	VI_3	4.9702	6.1073	3.7265	1.4736	5136	4953	183	32
276	VN	4.1856	13.0880	0.9594	0.6877	8233	8520	-287	32
277	YCl_3	5.0246	6.0663	3.4881	1.4836	4524	4864	-340	32
278	YH_3	4.7379	5.4879	3.8035	1.6400	4910	4462	448	32
279	YI_3	4.7635	5.5396	3.7726	1.6247	4258	4498	-240	32
280	BN	4.7391	16.3462	0.8698	0.5506	10911	10471	440	9
281	AlN	4.3203	13.8810	0.9337	0.6484	8405	8999	-594	9
282	CaSe	2.8255	3.9901	1.4162	1.0025	2862	2844	18	32
283	$MgAl_2O_4$	12.8130	28.1530	3.9359	2.3336	19128	19133	-5	9
284	$FeAl_2O_4$	12.8587	28.3010	3.9190	2.3127	19216	19240	-24	9
285	$CaMoO_4$	12.3502	47.7444	3.3915	1.6939	29521	29240	281	9
286	$SrMoO_4$	12.2960	47.5687	3.4187	1.7276	29403	29121	282	9
287	$ZrSiO_4$	12.2816	37.5988	3.1658	1.7159	24058	24022	36	9
288	YVO_4	12.2302	40.0538	3.2348	1.7452	25846	25256	590	9
289	Ce_2O_2S	8.4097	17.4810	3.0069	2.0676	12131	11839	292	9
290	YPO_4	12.7050	43.8963	3.2046	1.6521	27207	27416	-209	9
291	$LaFeO_3$	9.0626	20.4276	2.8142	1.7805	13364	13781	-417	25
292	$LaMnO_3$	9.0402	20.3190	2.8184	1.7883	13487	13712	-225	25
293	$LaCrO_3$	9.0428	20.3313	2.8179	1.7874	13678	13720	-42	25
294	$LaCoO_3$	9.0860	20.5414	2.8098	1.7725	13805	13854	-49	25
295	$LaAlO_3$	9.1048	20.6327	2.8064	1.7661	13856	13912	-56	25
296	$NdFeO_3$	9.0727	20.4770	2.8113	1.7752	13854	13813	41	25
297	$CaSiO_3$	9.4584	25.1390	2.8644	1.6396	16439	16531	-92	25
298	$MgSiO_3$	9.6413	25.7311	2.7861	1.5429	16725	16932	-207	25
299	Ba_2SiO_4	12.2631	28.9789	4.3109	2.6636	19300	19195	105	25
300	Ca_2SiO_4	12.5165	29.7990	4.1768	2.4980	19831	19825	6	25
301	Mg_2SiO_4	12.8823	30.9833	4.0202	2.3045	20697	20691	6	25
302	$YAlO_3$	9.2305	21.2430	2.7735	1.7051	14570	14308	262	28
303	$ZnFe_2O_4$	12.7485	27.8076	3.9438	2.3530	18972	18914	58	28
304	$PrMnO_3$	9.0612	20.4211	2.8126	1.7775	14084	13778	306	25
305	$Y_3Al_5O_{12}$	37.2635	86.6299	11.0222	6.6872	58006	57449	557	25
306	$Y_3Fe_5O_{12}$	37.0523	85.6045	11.0608	6.7588	56504	56636	-132	25
307	$Ba_2In_2O_5$	15.0203	29.3884	5.5424	3.6058	20065	19861	204	25
308	$CaMgSiO_4$	12.6994	30.3912	4.0985	2.4012	20364	20260	104	25
309	$Ca_2Fe_2O_5$	15.6037	31.8108	5.3421	3.3174	21811	21664	147	25
310	Al_2SiO_5	15.9722	43.3798	4.2536	2.3533	28687	28331	356	25
311	$CaMgSi_2O_6$	19.0997	50.8701	5.6504	3.1825	33324	33192	132	25
312	$LiAlSi_2O_6$	19.4771	54.1584	5.6883	2.9200	34815	35301	-486	25
313	$NaAlSi_2O_6$	19.3899	54.0173	5.7694	2.9701	35020	35166	-146	25
314	$CaAl_2Si_2O_8$	25.4306	68.5187	7.1179	3.9929	45005	44714	291	25
315	$KAlSi_3O_8$	25.6953	74.3427	7.4274	3.8169	47626	48036	-410	25
316	$Ba_4NaSb_3O_{12}$	36.3060	104.6993	12.3129	6.9998	64996	64918	78	25
317	$Ba_4LiSb_3O_{12}$	36.3933	104.8404	12.2318	6.9496	65181	65146	35	25
318	$Sr_4NaSb_3O_{12}$	36.5956	105.6366	12.1537	6.8030	65481	66027	-546	25

3. REGRESSION ANALYSIS

The experimental values of 318 inorganic-compounds lattice energies (U) are taken from Ref.9, Ref.25, Ref.28 and Ref.32, and listed in Table 2. Only multiple regression analysis (MRA) is used to construct the prediction models in this study, because the results obtained by using approach MRA are good enough.

Linear regression analysis is carried by SPSS. The results of the best subsets regression of U versus ${}^0G$, ${}^1G$, ${}^0G'$, and ${}^1G'$ show: if only the index ${}^1G$ is used, a good correlation for the U of the 318 can be obtained, and the correlation coefficient r is 0.9987. When the index ${}^0G$ is included, the model can be significantly improved (r = 0.9993); whereas the results obtained by using three-parameters, ${}^1G$, ${}^0G$, and ${}^1G'$, as well as four-parameters, ${}^1G$, ${}^0G$, ${}^1G'$, and ${}^0G'$ are better than the results of single-parameter and two-parameters (r = 0.9995 and 0.9996, respectively). Four models are shown as follows:

$$U=641.688+633.310\,{}^1G \qquad (8)$$

$r = 0.9987$, $r^2 = 0.9974$, $s = 503.60$, $F = 118971.0$, $N = 318$

$$U=-88.043+525.426\,{}^1G+ 325.266\,{}^0G \qquad (9)$$

$r = 0.9993$, $r^2 =0.9986$, $s = 365.16$, $F = 113280.1$, $N = 318$

$$U=185.578+487.076\,{}^1G+ 558.961\,{}^0G-829.699\,{}^1G' \qquad (10)$$

$r = 0.9995$, $r^2 =0.9991$, $s = 293.46$, $F = 116993.6$, $N = 318$

$$U=153.238+502.937\,{}^1G+ 51.140\,{}^0G-1076.505\,{}^1G'+177.442\,{}^0G' \qquad (11)$$

$r = 0.9996$, $r^2 =0.9992$, $s =280.98$, $F = 95718.9$, $N = 318$

If the nonlinear regression analysis is carried by SPSS, the best nonlinear model by using four parameters is shown as follows:

$$U=-315.953+831.216\,{}^1G^{0.896}+ 44.576\,{}^0G^{1.644}-140.712\,{}^1G'^{2.150}+110.096\,{}^0G'^{1.474} \qquad (12)$$

$r = 0.9998$, $r^2 =0.9995$, $s =217.6$, $F = 159603.7$, $N = 318$

The results of t-test show that these variables in these models are significant. Obviously, five models are excellent QSPR models without exception. The model (12) explains more than 99.95% of the variance in the experimental values of U for these inorganic compounds. The calculated results from Eq. (12) for 318 inorganic compounds show in Table 2. that the average absolute deviation is 156.78 kJ. mol^{-1}. The calculated U versus experimental data is shown in Figure 1. Fig.1 shows that the model (12) is quite excellent.

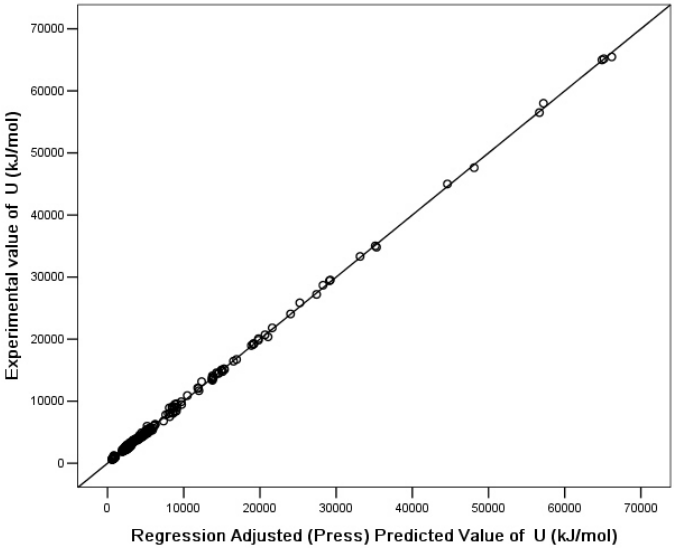

Figure 1. A plot of calculated versus experimental U for 318 inorganic compounds.

Finally, the models above generated for 318 inorganic compounds are 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 shown in Table 3. This table reveals that the results of the cross-validations for each model are very close to the normal results of the models, which means that the models constructed in this work are stable.

Table3. Statistics of MLR and Leave-One-Out Cross-Validation for the Five Models

properties	r	r^2	s	r_{cv}	r_{cv}^2	s_{cv}
Model (8)	0.9987	0.9974	503.60	0.9986	0.9972	521.99
Model (9)	0.9993	0.9986	365.16	0.9992	0.9985	381.29
Model (10)	0.9995	0.9991	293.46	0.9995	0.9990	303.36
Model (11)	0.9996	0.9992	280.98	0.9995	0.9991	295.53
Model (12)	0.9998	0.9995	217.63	0.9997	0.9995	226.15

4. RESULTS AND DISCUSSION

The g_i defined in this paper are different for ions of different elements due to their different electronegativities. Even for the ions of the different valence states of the same element, the g_i are also different. Therefore, the g_i can reflect the characteristics of different ions.

In inorganic compounds, the lattice energy is positively correlated with the number of ions of chemical formula. The topological indices ${}^0G$ and ${}^0G'$ are proportional to the number of ions of chemical formula, so the lattice energy is positively correlated with ${}^0G$ and ${}^0G'$. The more chemical single bonds there are in inorganic compound, the greater lattice energy the compound has, so the lattice energy is positively correlated with ${}^1G$ and ${}^1G'$ too. This fact is in agreement with the results of the regression analysis. Among the ${}^1G$, ${}^1G'$, ${}^0G$, and ${}^0G'$, the index ${}^1G$ has the best correlation with the lattice energy, r=0.9987, When the index ^{0}G is included, the double-parameter model can be significantly improved (r = 0.9993). In the two models, the coefficients of ${}^0G$ and ${}^1G$ are all positive. However in the three-parameter model, ${}^1G$, ${}^0G$, and ${}^1G'$,(r=0.9995), as well as four-parameters model, ${}^1G$,${}^0G$,, ${}^1G'$, and ${}^0G'$(r=0.9996), the coefficients of both ${}^1G$ are negative. The results show that the infection factors contained in index ${}^1G'$ are different from indices ${}^1G$, ${}^0G$ *and* ${}^0G'$. Index ${}^1G$ together with ${}^0G$, ${}^1G'$and ${}^0G'$ reflects the essential influencing factor of lattice energy.

The estimated lattice energies of 318 inorganic compounds containing 282 binary ionic crystals and 36 complex ionic crystals are listed in Table 2. As shown in Table 2, our calculated values agree well with the available experimental values. The average error of 318 crystals is 4.28 %(5.18% for U<5000 kJ mol^{-1}, 2.32% for U>5000 kJ mol^{-1}). The average error of 36 complex ionic crystals is only 0.82%. If the regression is carried only for the experimental values of 36 complex ionic crystals, the best linear and nonlinear three-parameter models are shown as:

$$U=486.290+505.221{}^1G+622.675{}^0G-886.78{}^0G' \quad (13)$$

r=0.9999, r^2=0.9997, s=292.12, F=36722.6, N=36

$$U=-96.116+650.806{}^1G^{0.955}+138.916{}^0G^{1.322}-31.395{}^0G'^{\,2.114} \quad (14)$$

r=0.9999, r^2=0.9998, s=218.23, F=65807.1, N=36

The average errors of the estimated lattice energies of 36 complex ionic crystals are 1.08% and 0.67% for linear model (13) and nonlinear model (14), respectively. The results show that the current method is more effective than literature methods[7-11,23,25-26,28] for complex ionic crystals.

In addition, the current method is very simple comparing with literature methods[23,25-26,28], for the following reasons:

(a) In current method, the g_i of an ion can be easily calculated from the charge number, the electronegativity and Goldschmidt ionic radius of atom *i*. The electronegativity and Goldschmidt ionic radii for any atomic can obtained from the handbooks.

(b) The calculations of ${}^0G$, ${}^1G$, ${}^0G'$, and ${}^1G'$ of inorganic compounds are simple too. The ${}^0G$, and ${}^0G'$ are the summation of all the atoms of the chemical formula. The ${}^1G$, ${}^1G'$ are the summation of all chemical single bonds. For every ion, the numbers of chemical single bonds bonding to other ions equal to the charge numbers.

(c) The models can be used for calculating the lattice energies of binary ionic crystals and complex crystals.

5. CONCLUSION

A novel connectivity index ${}^mG$ and its converse index ${}^mG'$ are proposed for predicting the lattice energies of inorganic ionic compounds. The excellent QSPR models for the lattice energies can be constructed by using ${}^0G$, ${}^1G$, ${}^0G'$,and ${}^1G'$. For the nonlinear model, the correlation coefficient r, the standard error, and the average error of the nonlinear model are 0.9998, 217.6 kJ.mol^{-1} and 4.28%, respectively, for the 318 inorganic ionic crystals. However, the average error of 36 complex ionic crystals is only 0.82%. The cross-validation by using the leave-one-out method demonstrates that the models are highly reliable from the point of view of statistics. The results show that the current method is not only more effective, but also simpler than literature methods for estimating the lattice energies of inorganic ionic crystals, especially for estimating the lattice energies of complex ionic crystals.

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REFERENCES AND NOTES

(1) Trinajstic, N. *Chemical Graph Theory*, 2nd ed., CRC Press, Boca Raron, FL.**1992**.

(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) Yang, F.; Wang Z. D.; Huang, Y. P.; Ding X. R.. Modification of Wiener Index and Its Application. *J. Chem. Inf. Comput. Sci.* **2003**, 43, 753-756.

(5) Yang, F.; Wang Z. D.; Huang, Y. P.. Modification of Wiener Index .2 . *J Chem. Inf. Comput. Sci.* **2003**, 43, 1337-1341.

(6). Mu L. L.; Feng C. J.. Topological Research on Standard Entropies of Alkali and Alkaline Earth Metal Compounds. *Chin. J. Chem. Phys.* **2003**, 16(1), 19-24

(7). Feng C. J.. The connection index of average energy level for valence electron and its applications. *Chin. J. Chem. Phys*. **2000**, 13(1), 66-70

(8). Xu S. Y.; Tang J. H.. The topological index mF electronegativity and its calculation of physical and chemical properties of inorganic compounds. *Chin. J. Chem. Phys*. **2003**, 16(3), 203-208

(9). 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(1), 27-32

(10). Feng C. J.. Estimating and Predicting lattice energies of inorganic compounds with connectivity indices. *Chin. J. Mol. Sci*. **1999**, 15(4), 223-228

(11). Feng C. J.; Chen Y.. A novel structural parameter for QSPR study of halides. *Chin. J. Mol. Sci*. **2000**, 16(3), 177-183

(12). Altshuller A. P.. Lattice Energies and Related Thermodynamic Properties of the Alkali Metal Borohydrides and of the Borohydride Ion. *J. Am. Chem. Soc*. **1955**, 77(21), 5455-5457.

(13). Stokes R. H.. Crystal Lattice Energies and the Electrostatic Self Energies of Gaseous Ions. *J. Am. Chem. Soc.* **1964**, 86(6), 982-986.

(14). Gardner P. J. ; Finch A... Lattice Energies of Ionic Crystals. II. Some Group I-A and II-A Salts *J. Phys. Chem.* **1965**, 69(2), 384-389.

(15). D'Orazio L. A.; Wood R. H.. Thermodynamics of the Higher Oxides. I. The Heats of Formation and Lattice Energies of the Superoxides of Potassium, Rubidium, and Cesium. *J. Phys. Chem.* **1965**, 69(8), 2550-2557.

(16). D'Orazio L. A.; Wood R. H.. Thermodynamics of the Higher Oxides. II. Lattice Energies of the Alkali and Alkaline Earth Peroxides and the Double Electron Affinity of the Oxygen Molecule. *J. Phys. Chem.* **1965**, 69(8), 2558-2561.

(17). Brackett T. E., Brackett E. B.. The Lattice Energies of the Alkaline Earth Halides. *J. Phys. Chem.* **1965**, 69(10), 3611-3614.

(18). Jenkins H. D. B. Group 3 tetrahalide salts, lattice energies, and thermodynamic parameters. Tetrachloroaluminate(1-) and tetrachlorogallate(1-). *Inorg. Chem.* **1976**, 15(1), 241-243.

(19). Stevenson G. R.; Wiedrich C. R.. Anion-radical crystal lattice energies. *J. Am. Chem. Soc.* **1979**, 101(17), 5092-5094.

(20). Voogd J.; Derissen J. L., Duijneveldt F. B. V. Calculation of proton-transfer energies and electrostatic lattice energies of various amino acids and peptides using CNDO/2 and ab initio SCF methods. *J. Am. Chem. Soc.* **1981**, 103(26), 7701-7706.

(21). Stevenson G. R., Wiedrich C. R., Clark G. Crystal lattice energies of solid anion radical salts. *J. Phys. Chem.* **1981**, 85(4), 374-378.

(22) Glasser, L. Lattice Energies of Crystals with Multiple Ions: A Generalized Kapustinskii Equation *Inorg. Chem.* **1995**, 34, 4935-4936.

(23) 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.

(24). Abramov, Y. A.; Volkov, A.; Wu, G.; Coppens, P. Use of X-ray Charge Densities in the Calculation of Intermolecular Interactions and Lattice Energies: Application to Glycylglycine, DL-Histidine, and DL-Proline and Comparison with Theory. *J. Phys. Chem.* **2000**, 104(9), 2183-2188.

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

(26). 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.

(27). C. Mellot-Draznieks; S. Girard; G. Ferey. Novel Inorganic Frameworks Constructed from Double-Four-Ring (D4R) Units: Computational Design, Structures, and Lattice Energies of Silicate, Aluminophosphate, and Gallophosphate Candidates. *J. Am. Chem. Soc.* **2002**, 124(51),15326-15335.

(28). Liu D. T.; Zhang S. Y.; Wu Z. Lattice Energy Estimation for Inorganic Ionic Crystals. *Inorg. Chem.* **2003**, 42, 2465-2469

(29). S. Beaucamp; D. Mathieu; V. Agafonov. Parametrization of Semiempirical Models against ab Initio Crystal Data: Evaluation of Lattice Energies of Nitrate Salts. *J. Phys. Chem. B.* **2005**, 109(34),16469-16473.

(30). 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**;9-74

(31). Pan D. K.; Zhao D. C.; Zheng Z. X. *Material Structure.* 2nd ed., higher education Press, **1989**; A-8.(Chinese)

(32). 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**;12-23