

## Articles

**Ab initio Valence Bond Study on AB-type Molecules. A Description for XH (X = Li, Be, B, C, N, O, F) and XF (X = Li, Be, B)**

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*Ab initio* valence bond method is employed to quantitatively study the concepts of ionic resonance energy and ionicity of a chemical bond in the cases of hydrides XH (X = Li, Be, B, C, N, O, F) and fluorides XF (X = Li, Be, B). By establishing the relationship between resonance and stability, and comparing the calculated ionicities with Pauling's earlier estimations in the above diatomic molecules, the merits of Pauling's classical resonance theory were demonstrated at the *ab initio* level.

**Keywords** valence bond theory, ionicity, electronegativity

**Introduction**

The qualitative description of the bonding features of molecules is of basic interests to the structural chemists. In this important area, Pauling made the most outstanding contributions by proposing and developing a series of concepts, such as resonance, hybridization, electronegativity as well as covalent character and ionicity of a chemical bond.<sup>1</sup> These intuitive and fundamental concepts have given remarkable impetus to the development of chemistry. With the advent of the modern computational chemistry, it is valuable to justify these concepts with *ab initio* valence bond (VB) approaches, advantages of which have been demonstrated by the recent studies on the breaking and forming of chemical bonds.<sup>2-9</sup> Concerning the AB-type diatomic molecules of only a single bond, Pauling suggested that one might describe each of them either with two resonant VB structures (A-B, A<sup>+</sup>B<sup>-</sup> or A<sup>-</sup>B<sup>+</sup>, depending on the relative electronegativities of two atoms A and B) or with a covalent bond of partial ionic characters. As the core of the resonance theory, Pauling also proposed that the resonance between the two VB structures will stabilize the molecule. If one of the two extreme structures is of a larger bond energy than the other, the more stable resonance structure is supposed to contribute more to the ground state than the less stable one. Clearly, the resonance of the two resonance structures will result in the actual bond energy of the ground state stronger than that of any individual resonance structure. In an attempt to investigate the resonance

effect of VB structures at *ab initio* VB level, in this work we will evaluate the ionic resonance energies and the ionicities of hydrides XH (X = Li, Be, B, C, N, O, F) and fluorides XF (X = Li, Be, B) based on a spin-free VB theory, called bonded tableau unitary group approach (BTUGA).<sup>10-16</sup> Furthermore, a careful description about the bonding features of these diatomic molecules will be presented.

**Methodology***Bonded tableau unitary group approach (BTUGA)*

As a simple spin-free VB method, BTUGA<sup>10-16</sup> is identical to the classical Heitler-London-Slater-Pauling (HLSP) approach and a bonded tableau (BT), which is a state function of a system and used to describe a resonance structure, is equivalent to an HLSP wavefunction. Thus, BTUGA is much closer to classical concepts and ideas of chemistry than any other many-body theory based on the molecular orbital (MO) theory. For an N electron system, a BT is defined as

$$\begin{aligned}\Phi^{[\lambda]}(k) &= A_k e_{11}^{[\lambda]} \Omega(k) \\ &= A_k e_{11}^{[\lambda]} [u_1(1)u_2(2)\cdots u_N(N)]\end{aligned}\quad (1)$$

where  $A_k$  is a normalization constant,  $e_{11}^{[\lambda]}$  is a standard projection operator of symmetric group for the irreducible representation and  $u_i$  is a one-electron basis function. Also, if the spin quantum number of the system is  $S$ ,  $[\lambda] = [2^{\frac{N}{2}-S}, 1^{2S}]$  is an irreducible representation of permutation group  $S_N$ . In fact, the above BT corresponds to a VB structure where two one-electron bases  $u_{2i-1}$  and  $u_{2i}$  overlap to form a bond ( $i \leq N/2 - S$  and if  $u_{2i-1} = u_{2i}$ , the 'bond' is a lone electron pair) and the last  $2s$  one-electron orbitals are unpaired. As a consequence, the wavefunction of the system can be expressed as a superimposition of all possible BTs (or resonance structures), namely

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$$\Psi_i = \sum_{k=1}^M C_{ik} \Phi_i(k) \quad (2)$$

The structural weight of a BT  $\Phi_i(k)$  in the  $\Psi_i$  can be defined as

$$T_i(k) = \sum_{l=1}^M C_{ik} C_{il} S_{kl} \quad (3)$$

where  $S_{kl}$  is the overlap integral between BTs  $\Phi_i(k)$  and  $\Phi_i(l)$ .

The normalization condition requires

$$\sum_{k=1}^M T_i(k) = 1 \quad (4)$$

where  $M$  is the number of linearly independent BTs.

### Ionic Resonance Energy and Ionicity

The resonance structures of an AB-type molecule can be classified by three sets, namely A-B,  $A^- B^+$  and  $A^+ B^-$ , which can be represented with I, II and III, respectively. We define the ionic resonance energy  $\Delta$  as:

$$\Delta = D(I + II + III) - D(I) \quad (5)$$

where  $D(I + II + III)$  is the dissociation energy derived from the calculations with all three sets of VB structures, and  $D(I)$  is the dissociation energy estimated without taking the interaction of the ionic structure into account, *e. g.*,  $D(I)$  is the dissociation energy of the covalent structure I.

According to Pauling's postulation, we may describe the single bond in AB as a covalent bond with partial ionic characters. In the VB calculations, VB structures II ( $A^- B^+$ ) and III ( $A^+ B^-$ ) represent two kinds of ionic VB structures

where the directions of the electron transfer are opposite to each other. As a result, pure ionicity of the bond can be obtained by the following two steps: (1) to evaluate the structural weights of II and III after performing the VB calculation with all three types of VB structures; (2) to normalize the covalent weight and finally derive the ionicity. Therefore we define the ionicity of the bond A—B as:

$$f = \frac{|T_{II} - T_{III}|}{T_I + |T_{II} - T_{III}|} \quad (6)$$

where  $T_I$ ,  $T_{II}$  and  $T_{III}$  are the structural weights of the sets I, II and III, respectively.

### Computational details

In this work, the 6-31G basis set was used. To reduce the VB computation efforts, we employed the frozen-core approximation by freezing the 1s orbitals of the atoms other than hydrogen. In the VB wavefunctions, atomic hybrid orbitals (AHOs) are taken as one-electron orbitals to ensure an unambiguous definition of a covalent or an ionic bond. Five atomic hybrid orbitals are adopted in VB calculations and they are denoted as X(2s), X(2p<sub>x</sub>), X(2p<sub>y</sub>), X(2p<sub>z</sub>) and H(1s), and are represented by using Arabic numbers 1 to 5, respectively. The number of the overall canonical configurations of the symmetry of the ground state is 8, 14, 19, 15, 14, 10, 8 for XH (X = Li, Be, B, C, N, O, F), respectively, and the bonded tableaux which contribute to the ground states are listed in Table 1. To check whether the 3BTs, *e. g.*, the first column of the bonded tableaux are good enough to describe the ground states of these hydrides, we performed multi BT (MBT) calculations with all possible BTs to compare with the 3BT calculations.

**Table 1** Bonded tableaux which contribute to ground states

Molecule	VB structure	Bonded tableau
LiH	Li-H	4 5     1 5
	Li <sup>+</sup> H <sup>-</sup>	5 5
	Li <sup>-</sup> H <sup>+</sup>	1 1     2 2     3 3     4 4     1 4
BeH	Be-H	1 1     4 4     1 5     4 5     2 2     3 3   5   5   4   1   5   5
	Be <sup>+</sup> H <sup>-</sup>	5 5     5 5   1   4
	Be <sup>-</sup> H <sup>+</sup>	1 1     4 4     2 2     2 2     3 3     3 3   4   1   1   4   1   4
BH	B-H	4 4     2 2     3 3     1 1     2 2     3 3   1 5   1 5   1 5   4 5   4 5   4 5
	B <sup>+</sup> H <sup>-</sup>	5 5     5 5     5 5     5 5     5 5   1 4   1 1   4 4   2 2   3 3
	B <sup>-</sup> H <sup>+</sup>	2 2     3 3     1 1     1 1     1 1     2 2     2 2     4 4   1 4   1 4   4 4   2 2   3 3   4 4   3 3   3 3

Continued

Molecule	VB structure	Bonded tableau									
CH	C-H	11	11	33	33	33	33	44	44	25	25
		25	45	15	15	25	45	15	25	4	2
		4	2	2	1	4	2	2	1		
CH	C <sup>+</sup> H <sup>-</sup>	55	55	55	55						
		11	33	12	24						
		2	2	4	1						
CH	C <sup>-</sup> H <sup>+</sup>	11	11	33							
		33	44	44							
		2	2	2							
NH	N-H	11	11	22	33						
		22	33	44	44						
		45	45	15	15						
	N <sup>+</sup> H <sup>-</sup>	55	55	55	55	55	55				
		11	11	22	33	22	33				
		22	33	44	44	14	14				
NH	N <sup>-</sup> H <sup>+</sup>	11	11								
		22	33								
		44	44								
OH	O-H	11	11	22	22						
		22	22	44	44						
		45	35	35	15						
		3	4	1	3						
	O <sup>+</sup> H <sup>-</sup>	55	55	55	55	55					
		11	11	22	22	22					
OH	O <sup>-</sup> H <sup>+</sup>	11									
		22									
		44									
FH	F-H	11	22								
		22	33								
		33	44								
		45	15								
	F <sup>+</sup> H <sup>-</sup>	55	55	55	55	55					
		11	11	11	22	22					
FH	F <sup>-</sup> H <sup>+</sup>	11									
		22									
		33									

Xiamen package<sup>17</sup> was used for all VB calculations in this paper. The experimental values were taken as the equilibrium bond lengths of the diatomic molecules studied in this paper, which are listed in Table 2.

**Table 2** Experimental bond lengths ( $10^{-1}$  nm).

LiH	BeH	BH	CH	NH	OH	FH	LiF	BeF	BF
1.595	1.343	1.233	1.120	1.038	0.971	0.917	1.564	1.361	1.311

## Results and discussion

*Energies and structural weights of XH* (X = Li, Be, B, C, N, O, F)

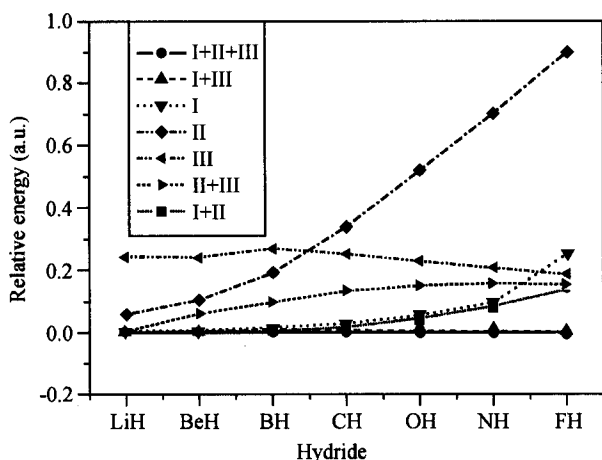
The total energies of the MBT and the 3BT calculations are listed in Table 3. Furthermore, MP2 and HF energies are presented for comparisons. It is clear from Table 3 that the

3BT energies are even lower than the MP2 energies and essentially identical with the MBT energies in the cases of AB-type molecules. In other words, using only 3BTs can recover the electron correlation energies completely. Thus, the following results and discussions based on the 3BT calculations are reliable and convincing.

**Table 3** Total energies obtained from 3BT, MBT, MP2 and HF calculations.

Molecule	Energy (a. u.)			
	3BT	MBT	MP2	HF
LiH	-7.99495	-7.99496	-7.99141	-7.97927
BeH	-15.15514	-15.15514	-15.15876	-15.14298
BH	-25.12121	-25.12121	-25.14680	-25.10897
CH	-38.26499	-38.26499	-38.33762	-38.25167
NH	-54.88588	-54.88588	-54.90622	-54.83562
OH	-75.37961	-75.37961	-75.45144	-75.36326
FH	-100.00222	-100.00222	-100.11108	-99.98341

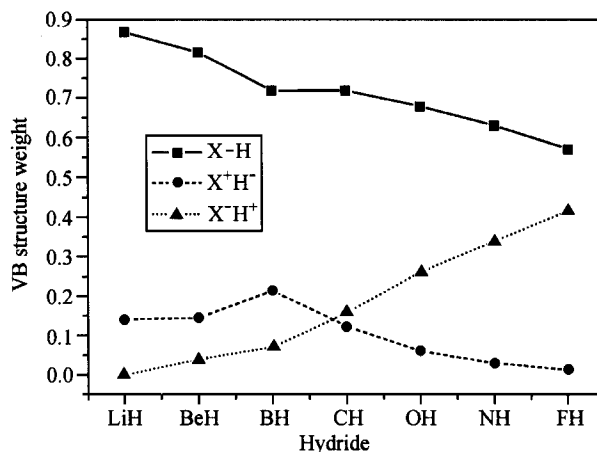
To explore the relationship between resonance and stability in the hydrides, we performed VB calculations with selected VB structures in the following seven cases: (1) 1BT with structure I; (2) 1BT with structure II; (3) 1BT with structure III; (4) 2BT with structures II + III; (5) 2BT with structures I + II; (6) 2BT with structures I + III; (7) 3BT with structures I + II + III. Fig. 1 shows the trends of energy variations based on the various VB calculations relative to the 3BT energies. The structural weights derived from the 3BT calculations are pictorial in Fig. 2.



**Fig. 1** Relative energies of XH ( $X = \text{Li, Be, B, C, N, O, F}$ ) with various resonance structures. Energies of I + II + III are set to zero as reference.

It can be generally summarized from Fig. 1 that the resonance among VB structures will stabilize molecules, which is in accordance with Pauling's ideas. Fig. 1 clearly manifests that in all the seven hydrides, the covalent resonance structure is of lower energy than the ionic structures. For the molecules LiH, BeH and BH, the energy of the ionic structure II ( $X^+H^-$ ) is lower than that of III ( $X^-H^+$ ). Corre-

spondingly, the structural weights are of the order I ( $X-H$ ) > II ( $X^+H^-$ ) > III ( $X^-H^+$ ), *e. g.*, normally the more stable the resonance structure is, the larger the structural weight is, or, the more the resonance structure will contribute to the ground state of the molecule. On the other side, the larger structural weight of II ( $X^+H^-$ ) compared with III ( $X^-H^+$ ) as shown in Fig. 2 implies that the electronegativities of the atoms Li, Be and B are lower than that of the hydrogen atom. Therefore, we can use two resonance structures I ( $X-H$ ) and II ( $X^+H^-$ ) to describe the molecules LiH, BeH and BH.



**Fig. 2** VB structural weights versus various diatomic molecules.

In contrast to the cases of LiH, BeH and BH, for the molecules NH, OH and FH, the energies of III ( $X^-H^+$ ) are lower than those of II ( $X^+H^-$ ). Correspondingly, the structural weight of I ( $X-H$ ) is the largest and the structural weight of II ( $X^+H^-$ ) is the smallest. This result is also in agreement with the conventional electronegativity rule, *e. g.*, the electronegativities of the atoms N, O and F are higher than that of the hydrogen atom. We can thus employ the resonance structures of I ( $X-H$ ) and III ( $X^-H^+$ ) to describe the molecules NH, OH and FH. Among the hydrides of the second row elements, CH is of some specific features. From Fig. 2, we can find that the structural weights of  $C^-H^+$  and  $C^+H^-$  are comparable in magnitude. This result implies the closeness of the electronegativities of C and H and thus all three resonance structures (one covalent and two ionic) are necessary to reasonably describe the electronic structure of CH.

#### *Ionic resonance energies and ionicity in hydrides of XH ( $X = \text{Li, Be, B, C, N, O, F}$ )*

The ionic resonance energies and the ionicities of the seven hydrides derived from Eqs. (5) and (6) are listed in Table 4, where results based on Pauling's formulation are also shown for comparisons. Noticeably, there is a significant discrepancy between our quantitative data and Pauling's qualitative estimations. The reason is that in Pauling's formulation the ionic resonance energy and the ionicity of a

**Table 4** Ionic resonance energies (kJ/mol) and ionicities of bond X—H

Molecule	Ionic resonance energy			Ionicities of bond X—H		
	VB calculations		Pauling's formulation	VB calculations		Pauling's formulation
	3BT	MBT	$\Delta = 30(X_A - X_B)^2$	3BT	MBT	$1 - e^{-\frac{1}{4}(X_A - X_B)^2}$
LiH	17.6146	26.7358	151.8792	0.140	0.149	0.250
BeH	18.1167	14.2674	45.1872	0.113	0.142	0.086
BH	43.8902	38.7438	12.5520	0.167	0.170	0.0025
CH	75.6467	72.6382	20.0832	0.045	0.048	0.039
NH	141.7958	140.3732	101.6712	0.228	0.229	0.183
OH	252.7136	253.7596	246.0192	0.328	0.344	0.380
FH	394.1328	391.2877	453.1272	0.420	0.419	0.594

diatomic molecule solely depend on the absolute difference between the two atomic electronegativities, whereas the determination of the electronegativities is of some arbitrariness in many ways. Moreover, the theoretical formulations of the relationship between the ionic resonance energy or the ionicity and the electronegativities may be not as simple as Pauling's formulations. However, generally our results do support Pauling's theory that the ionic resonance energy in a diatomic molecule increases with the increasing of the absolute difference between the electronegativities of the atoms X and H.

Regarding the ionicity of the bond X—H, except for B—H, our VB results show a similar trend of variation with the data obtained from Pauling's formulation. Among the seven hydrides, the VB result for the ionicity of C—H is in the best agreement with Pauling's estimation, and the difference between them is only 0.006 and 0.009 in the cases of 3BT and the MBT calculations, respectively. Since the C—H bond is of the smallest ionicity and the covalency is as high as about 95%, we can anticipate that the electronegativity of hydrogen should be very close to that of carbon, as Pauling pointed out, and the C—H bond is a typical covalent bond.

As for the bonding feature of LiH, detailed calculations and analyses with the 6-311G\*\* basis set were available,<sup>3</sup> where the ionicity of the chemical bond in LiH was shown to be about 0.130, close to the present value 0.140 or 0.149 with the 6-31G basis set. Therefore we believe that the present results are reliable. In this specific case, Pauling's theory predicted that the ionicity of the LiH molecule was 0.250, higher than our results. In the previous work,<sup>3</sup> we have shown that the high dipole moment of LiH mainly results from the high polarizability of the lithium atom.

For the bond of F—H, our calculations indicate that the ionic character is about 0.42. In his famous book,<sup>1</sup> Pauling suggested another two schemes to make a rough determination about the bond types of the halogen hydrides. One scheme is to compare the energy curves of the covalent bond as well as the ionic bond of the halogen hydrides. The other scheme is to analyze the electric dipole moments  $\mu$ , *i. e.* ionicity =  $\mu/er_0$ , where  $r_0$  is the equilibrium internuclear distance of the molecule under consideration. According to the former scheme, Pauling concluded that the ionic charac-

ter of F—H bond was 0.50, whereas, according to the latter scheme, the value was 0.45. In Table 3, the value 0.594 was nevertheless derived from the formulation  $I = 1 - e^{-\frac{1}{4}(X_A - X_B)^2}$ .

The disagreement between our results and Pauling's estimations is the most remarkable in the case of BH. According to our *ab initio* VB calculations, we believe that the bond of B—H has a considerable ionic character although in Pauling's work the ionicity of the BH molecule is negligible. In the electronegativity scale of Pauling, the difference between the values of the atoms B and H is only 0.1. Although there is a possibility that the electronegativity of boron is overestimated, the abnormality of the ionicity of BH compared with those of others such as BeH and CH is still short of reasonable explanations and needs further studies.

#### Energies and structural weights of XF (X = Li, Be, B)

Similar to the calculations of the hydrides, we performed VB calculations on some fluorides to investigate the relationship between the structural weights and the stabilities as well as the relationship between the ionicities and the electronegativities. Table 5 gave the 3BT energies and the structural weights for the fluorides LiF, BeF and BF. The individual energies of the resonance structures I, II and III together with the Hartree-Fock and the MP2 energies are also listed for comparisons. Although the 3BT energies are lower than the HF energies, they are much higher than the MP2 energies. This comparison implies that the 3BT can only recover a small part of electron correlation energies. Moreover, for the molecules LiF, BeF and BF, the  $\pi$ -symmetry covalent VB structural weights are remarkable, showing that the  $\pi$ -electron interaction plays an essential role in the formation of the chemical bonds in fluorides.

The results for LiF show that the resonance structure  $\text{Li}^+ \text{F}^-$  is even more stable than the covalent structure and its structural weight is as high as 0.612. For the covalent VB structure LiF, the bonding electrons can occupy the orbitals either of  $\sigma$ -symmetry or of  $\pi$ -symmetry, and the weight of  $\sigma$ -type covalent structures is 0.138 while the weight of  $\pi$ -type covalent structures is 0.255. The VB calculations confirm us

that LiF is a typical ionic-type molecule.

**Table 5** Energies and structural weights

Molecule	Type	Energy (a. u.)	Structural weight	
			$\sigma$ -symmetry	$\pi$ -symmetry
LiF	I	-106.815436	0.138	0.255
	II	-106.883127	0.612	0.000
	III	-106.103133	-0.005	0.000
	I + II + III	-106.933899	0.745	0.255
	HF	-106.920890	—	—
	MP2	-107.056819	—	—
BeF	I	-114.035804	0.323	0.286
	II	-114.012635	0.413	0.000
	III	-113.079870	-0.022	0.000
	I + II + III	-114.115149	0.714	0.286
	HF	-114.086148	—	—
	MP2	-114.226000	—	—
BF	I	-124.015110	0.364	0.283
	II	-123.910555	0.353	0.000
	III	-123.032188	0.000	0.000
	I + II + III	-124.092552	0.717	0.283
	HF	-124.059560	—	—
	MP2	-124.227981	—	—

For BeF the ionic structural weight is smaller than that for LiF, which is consistent with the Pauling's electronegativity rules. The covalent structures make larger contribution to the ground state of BeF with the structural weights 0.323 and 0.286 for the  $\sigma$ - and  $\pi$ -type covalent bonds, respectively.

Due to the relatively higher electronegativity of the boron atom compared with lithium and beryllium, the covalent structures become dominant in the ground state of BF, although the ionic resonance structures still play an important role.

*Ionic resonance energies and ionicities of XF (X = Li, Be, B)*

The ionic resonance energies and the ionicities for the three fluorides are presented in Table 6. As in the pretext, the values estimated with Pauling's formulations are also listed in the table for comparison.

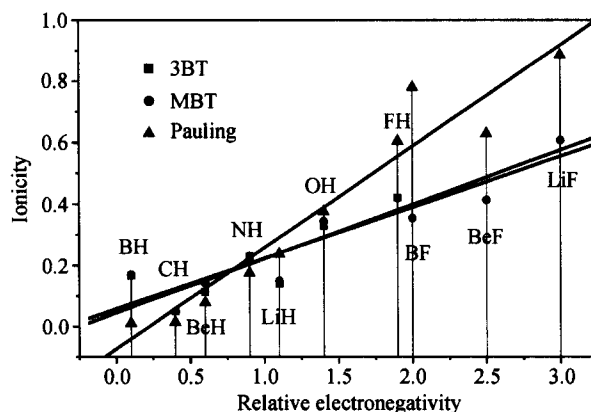
**Table 6** Ionic resonance energies ( $E_{\text{ion}}$ ) (kJ/mol) and ionicities ( $I$ )

Molecule	$E_{\text{ion}}$		$I$	
	VBSCF	$\Delta = 30(X_A - X_B)^2$	VBSCF	$1 - e^{-\frac{1}{4}(X_A - X_B)^2}$
LiF	311.0469	1129.6800	0.607	0.895
BeF	208.3339	782.4080	0.413	0.632
BF	203.3424	502.0800	0.353	0.790

From Table 6 we can find that the VB results are of the

same trend of variations as the values derived from the Pauling's formulation. This consistency suggests that qualitatively the formulations of Pauling  $\Delta = 30(X_A - X_B)^2$  and  $1 - e^{-\frac{1}{4}(X_A - X_B)^2}$  are still reasonable to some extent.

To generally explore the relationship between the ionicities and the relative electronegativities (or the absolute difference of electronegativities) in diatomic molecules graphically, we put the data for the seven hydrides and three fluorides together in Fig. 3, which shows that there approximately is a linear relationship between ionicities and the relative electronegativities.



**Fig. 3** Relationship between ionicities and relative electronegativities for diatomic molecules.

## Conclusion

Modern VB theory can not only provide a quantitative description of bonding features of molecules at *ab initio* level, but also provide an intuitive physical picture for the understanding of molecular structures. The present investigation on some diatomic molecules shows that the calculated resonance energy and the ionicity of a chemical bond possess similar properties to those obtained from Pauling's formulations.

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