

# chemical principles revisited

Edited by  
**DAN KALLUS**  
Midland Senior High School  
906 W. Illinois  
Midland, TX 79705  
  
**RUSSELL D. LARSEN**  
Texas Tech University  
Lubbock, TX 79409



## Principles of Electronegativity

### II. Applications

**R. T. Sanderson<sup>1</sup>**

Arizona State University, Tempe, AZ

This is the second of two articles on electronegativity (1).

8. *Equalization of electronegativities always places partial charges on the initially neutral atoms, which can very easily be determined from the initial atomic electronegativities and the electronegativity of the compound.*

The partial charge on a combined atom is defined as the ratio of the change in electronegativity it underwent in forming the compound to the change it would have undergone had it acquired unit (negative or positive) charge. For the current relative compactness scale of electronegativity, the change corresponding to the acquisition of unit charge is  $\Delta S_i = 1.57 \times S^{1/2}$ . (This was originally based on assumption of a particular charge in NaF molecule and assumption that electronegativity changes linearly with charge.) The electronegativity change in forming the compound is simply the difference between the molecular value,  $S_m$ , and the original atomic electronegativity.

For example, consider a molecule of phosphorus oxyfluoride,  $\text{POF}_3$ . The electronegativities and  $\Delta S_i$  values are: P, 2.515, 2.490; O, 3.654, 2.490; F, 4.000, 3.140. The molecular electronegativity,  $S_m$ , of  $\text{POF}_3$  is the fifth root of the atomic electronegativity product,  $2.515 \times 3.654 \times 4.000^3$ , which is 3.580. In combining to form  $\text{POF}_3$ , P has changed from 2.515 to 3.580, or by 1.065. If P had lost an electron completely, it would have changed in electronegativity by 2.490. The partial charge is defined as the ratio of the change in electronegativity in forming the compound to the unit charge change:  $\delta_P = 1.065/2.490 = 0.428$ . Similarly,  $\delta_O = (3.580 - 3.654)/3.00a = -0.025$ . For fluorine,  $\delta_F = (3.580 - 4.000)/3.140 = -0.134$ . If correct, these must add to zero for the molecule:  $0.428 - 0.025 - 3 \times 0.134 = -0.001$ .

It must be recognized that any assignment of atomic charges to the individual atoms in a complex cloud of electrons in which the nuclei are imbedded is quite arbitrary and likely to be controversial. Theorists sometimes find it convenient to assign different charges to different like atoms within a molecule, which implies the uneven sharing of bonding

electrons between like atoms differing in relative position. The method described here, on the other hand, assigns the same partial charge to each atom of the same kind within a molecule, regardless of its location. For example, all four hydrogen atoms are assigned the same charge in  $\text{CH}_3\text{OH}$ , wherein the different behavior of the hydroxyl hydrogen must then be ascribed to its different position rather than a difference in charge. There is no possibility of resolving the controversy herein. Let us simply recognize that different methods, all arbitrary, provide different values.

"Validity" implies utility. The partial charges described herein have the advantage of remarkable consistency with experienced chemical intuition, as will be detailed presently. In addition, partial charges are indispensable in the calculation of bond energy, also to be described, and it is useful to regard them as an index of the condition of a combined atom with respect to charge. One might imagine that each atomic nucleus within the compound is able to identify what part of the surrounding electronic cloud belongs to it. For example, the partial charges in NaCl are 0.605 and -0.605. One can imagine that the sodium nucleus recognizes ownership of 10.395 electrons and the chlorine nucleus, 17.605 electrons.

Despite the demonstrated value of partial charge in interpreting chemistry (2-4), some might question the evaluation since it is based on somewhat arbitrary electronegativity values, on the validity of the principle of electronegativity equalization, and on a rather arbitrary definition of partial charge. Is there some independent way of evaluating such charges? Fortunately, there is. Anticipating a later discussion of the calculation of polar bond energy, it has been found that the energy of a polar covalent bond,  $E$ , can be determined a weighted blend of a covalent contribution and an ionic contribution:

$$E = t_c E_c + t_i E_i$$

In this equation,  $E_c$  is a covalent energy calculated purely from experimental data,  $E_i$ , the ionic energy depends solely on Coulomb's law and the experimental bond length, and  $t_i$  and  $t_c$  are the ionic and covalent blending coefficients, weighting the relative contributions of ionicity and cova-

<sup>1</sup> Present address: 4725 Player Drive, Ft. Collins, CO 80525.

lence to the total bond energy,  $E$ . The sum of  $t_c$  and  $t_i$  is 1.000. Normally,  $t_i$  is calculated from partial charges, as half the difference between them. But if the above equation for polar bond energy is rearranged, we have

$$t_i = (E - E_c)/(E_i - E_c)$$

Thus if we take the experimental value of  $E$  and calculate the values of  $E_c$  and  $E_i$ , both solely dependent on experimentally determined quantities, it is possible to calculate  $t_i$  independently, and from it, the partial charges. Representative calculations of partial charge by this method are presented in Table 1. The agreement with values calculated from electronegativities is excellent, as well it might, since the reverse procedure, the calculation of polar bond energy, is absolutely dependent on accuracy in partial charge values. The latter calculation has been performed successfully for thousands of bonds.

#### 9. Properties of compounds are reasonably and logically consistent with the partial charges on their atoms.

Let us consider the general implications of partial charge. Any atom will tend to be more oxidizing, a better electron pair acceptor, and more acidic, the higher its positive partial charge. The higher its negative partial charge, the less oxidizing, the more reducing, the better its electron pair donating ability, and the more basic it will be. Application of these concepts to binary compounds of the active nonmetals has proven especially useful. These bear a general resemblance to one another no matter which nonmetal is involved. Oxides, sulfides, selenides, fluorides, chlorides, bromides, and iodides all tend to form relatively stable, high-melting, nonvolatile, nonmolecular solids when the nonmetal bears a high negative charge in the compound. Consequently, they tend to be basic, good electron-pair donors, and nonoxidizing. As the partial charge on the nonmetal becomes less negative, however, these properties change. The compounds tend to become lower melting, more volatile, less basic, and less effective as electron-pair donors. Then, with relatively low negative partial charge, compounds become still more volatile, less stable, more acidic, and stronger oxidizing agents.

Hydrogen provides an especially useful example, for it is intermediate in electronegativity and thus capable of oxidizing and reducing, but it is neither acidic nor basic. In its

binary compounds, therefore, it can become partially negative or partially positive. In the former role it acts more as a nonmetal, and in the latter role, more as a metal, by forming compounds of positive hydrogen. When hydrogen combines with elements much lower in electronegativity, it becomes highly negative, forms nonmolecular solids, is strongly reducing, and generally basic. As the negative charge on hydrogen becomes less, hydrogen compounds become more volatile but remain reactive toward compounds of positive hydrogen such as water. Negative hydrogen can form complexes by acting as an electron-pair donor, forming complex hydrides, such as  $\text{NaBH}_4$ . Protonic or positive hydrogen, for example the proton, can form complexes by acting as electron-pair acceptor, such as in  $\text{NH}_4^+$  ion. Consequently the complex formed by combination of hydride ion with proton is molecular hydrogen,  $\text{H}_2$ , which tends to be a product of any reaction between a compound of negative hydrogen and a compound of positive hydrogen. Hydrogen acquires partial positive charge in combination with more electronegative atoms, making it a potential proton donor, an acid, volatile, and to some extent oxidizing. There is no better basis for classification of hydrogen compounds than according to the partial charge on hydrogen.

The binary chemistry of oxygen is similarly well served by partial charges, which are negative in all combinations except with fluorine. The old rule that metal oxides tend to be basic and nonmetal oxides, acidic, is readily explained. Metals are much less electronegative than oxygen, allowing it to become highly negative in the oxide, and highly negative oxygen is always strongly basic. Nonmetals tend to be high in electronegativity and therefore to allow only a small negative charge on oxygen. This corresponds to an acidic oxide. The more polar bonds corresponding to highly negative oxygen also are associated with high melting, nonvolatile, nonmolecular solids. Otherwise, only molecules or very unstable polymers are possible when the charge on oxygen is low, and these oxides tend to be volatile or easily volatilized.

These illustrations are just a few out of hundreds of existing examples of correlation of partial charge with the physical and chemical properties of compounds (3).

#### 10. Partial charges on atoms in polyatomic ions can also be useful in explaining the properties of these ions.

Just as there is only one electronegativity for which the

**Table 1. Representative Partial Charges (A) Calculated from Electronegativity and Related Concepts and (B) from Experimental Quantities Only<sup>a</sup>**

A	B	A	B	A	B
$\text{BaF}_2(\text{c})$	1.16	1.16	$\text{CO}_2(\text{g})$	0.22	0.22
$\text{SrCl}_2(\text{c})$	0.96	0.96	$\text{PBr}_3(\text{g})$	0.20	0.19
$\text{CaBr}_2(\text{c})$	0.76	0.76	$\text{SO}_2(\text{g})$	0.17	0.17
$\text{RbBr}(\text{c})$	0.79	0.80	$\text{HCl}(\text{g})$	0.16	0.16
$\text{CsI}(\text{g})$	0.76	0.76	$\text{H}_2\text{O}(\text{g})$	0.12	0.12
$\text{KCl}(\text{g})$	0.76	0.76	$\text{NO}_2(\text{g})$	0.11	0.12
$\text{NaF}(\text{c})$	0.69	0.71	$\text{NO}(\text{g})$	0.08	0.08
$\text{LiBr}(\text{g})$	0.54	0.54	$\text{NH}_3(\text{g})$	0.06	0.06
$\text{AlBr}_3(\text{g})$	0.50	0.49	$\text{CS}_2(\text{g})$	0.05	0.05
$\text{TlI}_4(\text{g})$	0.49	0.47	$\text{H}_2\text{S}(\text{g})$	0.05	0.05
$\text{MgI}_2(\text{g})$	0.47	0.46	$\text{SbH}_3(\text{g})$	0.04	0.04
$\text{SiCl}_4(\text{g})$	0.44	0.47	$\text{PH}_3(\text{g})$	0.02	0.02
$\text{SiO}_2(\text{c})$	0.40	0.40	$\text{CH}_4(\text{g})$	0.01	0.01
$\text{BeBr}_2$	0.40	0.40	$\text{GeH}_4(\text{g})$	0.00	0.00
$\text{CF}_4(\text{g})$	0.37	0.37	$\text{H}_2\text{Te}(\text{g})$	0.00	0.00
$\text{InBr}_3(\text{g})$	0.33	0.35	$\text{PH}_3(\text{g})$	-0.01	-0.01
$\text{ZnCl}_2(\text{g})$	0.33	0.33	$\text{CH}_4(\text{g})$	-0.05	-0.05
$\text{BiCl}_3(\text{g})$	0.34	0.33	$\text{NO}_2(\text{g})$	-0.05	-0.06
$\text{GeCl}_4(\text{g})$	0.27	0.29	$\text{SO}_3(\text{g})$	-0.06	-0.06
$\text{HF}(\text{g})$	0.25	0.25	$\text{AsH}_3(\text{g})$	-0.07	-0.07
$\text{P}_4\text{O}_6(\text{g})$	0.25	0.25	$\text{ZnI}_2(\text{g})$	-0.08	-0.08

<sup>a</sup> Partial charge is on atom in boldface.

partial charges in a compound will add to zero, so there is only one electronegativity for which the partial charges in a polyatomic ion will add up to the charge on the ion. This principle has been used to calculate the electronegativities and partial charges in polyatomic cations and anions (5). Such information can be extremely useful in interpretations of common chemistry. For example, there is no obvious difference in hydrogen or in oxygen to be recognized from the equation,



However, this autoionization becomes far more meaningful if viewed in terms of partial charges. On H they are  $\text{H}_3\text{O}^+$ , 0.352;  $\text{H}_2\text{O}$ , 0.124; and  $\text{OH}^-$ , -0.351. The oxygen charges are  $\text{H}_3\text{O}^+$ , -0.056;  $\text{H}_2\text{O}$ , -0.248;  $\text{OH}^-$ , -0.649. The electronegativities from which these charges are calculated are  $\text{H}_3\text{O}^+$ , 3.483;  $\text{H}_2\text{O}$ , 2.906;  $\text{OH}^-$ , 1.705. Since these ions are hydrated in solution, the partial charges just given may be modified, but these figures suffice to allow ready distinction among the three species with respect to their chemical properties. Protonic activity must be greater in  $\text{H}_3\text{O}^+$ , less in  $\text{H}_2\text{O}$ , and absent from  $\text{OH}^-$ . Basicity, on the other hand, must be much greater for  $\text{OH}^-$ , less in  $\text{H}_2\text{O}$ , and absent from  $\text{H}_3\text{O}^+$ . The striking differences between aqueous acids and aqueous bases can be much better understood if students are familiar with the chemical consequences of partial charges and with the partial charges on the species just discussed.

A related example is the relationship of the strengths of oxygen acids to the partial charge on oxygen in the anion. The partial charge is not the sole factor, but it is interesting that the following partial charges on oxygen are calculated:  $\text{ClO}_4^-$ , -0.211;  $\text{NO}_3^-$ , -0.286;  $\text{CH}_3\text{COO}^-$ , -0.376;  $\text{CO}_3^{2-}$ , -0.566;  $\text{PO}_4^{3-}$ , -0.664. These exhibit an inverse relationship between the strength of the acid and the negative charge on oxygen in the anion. Aqueous acidity involves a competition between two bases, water, which normally is present in large excess, and the anion of the acid molecule. If the anion of the acid can acquire protons despite the abundance of competitive water molecules, this signifies that the acid is weak. Similarly, if the anion of the acid is unable to compete with water molecules for the proton, the acid loses most or all of its protons to the water and is called strong. To the extent that the basic ability of the anion depends on its relative attraction for the proton, as measured by the partial charge

of its oxygen atoms, the latter provides both a guide to and an explanation of the observed differences. Here  $\text{ClO}_4^-$  with lowest negative charge on oxygen corresponds to  $\text{HClO}_4$ , perchloric acid, the strongest acid. Nitric acid is strong, acetic acid weak, carbonic acid weaker, and  $\text{HPO}_4^{2-}$  weakest of all. Hydrolysis of salts can similarly be explained.

### 11. Partial charges from electronegativity equalization are indispensable for the accurate calculation of the energy of a polar covalent bond.

This is perhaps the most important application of electronegativity, for it opens up a vast new potential for student understanding. Bond energies and atomization energies have of course long been available from standard heats of formation, but the latter have been mere numbers in a table for the students, who have been provided with no real understanding. Now they can learn the fundamental origin of such numbers along with the atomic origin of bond energies, the reasons for the direction of chemical reactions, and gain many useful insights about chemistry that were previously unavailable.

Three books (5, 6) have described the results of polar bond energy calculations in considerable detail, but a brief review should be helpful here. Although there is no direct way of calculating the energy of a polar covalent bond, a valuable description of such a bond is available from the assumption that its energy is intermediate between two extremes. One is the nonpolar covalent form, which pictures the two electrons of the bond as being exactly evenly shared, and the other, an ionic form which assumes complete transfer of one electron. In fact, the actual bond energy is, as previously stated, a weighted blend of the two extremes. If the bonding electrons are evenly shared, the covalent energy is simply the geometric mean of the two homonuclear bond energies,  $E_h(\text{A})$  and  $E_h(\text{B})$ , corrected for any difference between the sum of the covalent radii  $R_c$  and the observed bond length,  $R_o$ :

$$E_c = R_c [E_h(\text{A}) \times E_h(\text{B})]^{1/2} / R_o$$

If the sharing of bonding electrons is completely uneven, creating unit charges on the two atoms, then the ionic energy would be  $33200/R_o$ , where 33200 is the factor to convert the energy to kilocalories per mole when  $R_o$  is measured in picometers. If kilojoules per mole are preferred, the factor 33200 is simply multiplied by 4.184.

$$E_i = 33200/R_o$$

The actual energy of a polar covalent bond, assumed to be intermediate between these two extremes, is then, where  $t_c$  and  $t_i$  are the covalent and ionic blending coefficients,

$$E = t_c E_c + t_i E_i$$

In words, a polar covalent bond is described as having a total energy that is a weighted blend of a covalent and an ionic contribution. If the bond were gray, it could be described as formed by combination of white covalence and black ionicity. The exact shade of gray could be represented in terms of the exact relative quantities of white and black needed to produce that gray, as determined by the blending coefficients. These blending coefficients,  $t_c$  and  $t_i$ , total 1.000, and  $t_i$  the

**Table 2. The Polar Covalent Atomization Energy of Sodium Chloride**

#### Basic Data

	Na	Cl
Homonuclear covalent bond energy, $E_h$ (kcal/mol)	16.4	58.0
Nonpolar covalent radius, pm	153.9	99.4 (sum, $R_c = 253.3$ )
Electronegativity, $S$	0.835	3.475
Change in $s$ with unit charge: $\Delta S_i = 1.57 S^{1/2}$	1.435	2.927
Bond length, pm, in NaCl molecule: 236.1; in solid: 281.4 ( $= R_o$ )		
NaCl solid: coordination 4, Madelung constant 1.748, repulsion coefficient 0.88.		

#### Calculations

- (1) Compound electronegativity,  $S_m = (S_{\text{Na}}S_{\text{Cl}})^{1/2} = (0.835 \times 3.475)^{1/2} = 1.703$
- (2) Partial Charges:  $\delta_{\text{Na}} = (S_m - S_{\text{Na}})/\Delta S_i = (1.703 - 0.835)/1.435 = 0.605$   
 $\delta_{\text{Cl}} = (S_m - S_{\text{Cl}})/\Delta S_i = (1.703 - 3.475)/2.927 = -0.605$
- (3) Mean  $E_h$  (NaCl) =  $[E_h(\text{Na}) \times E_h(\text{Cl})]^{1/2} = (16.4 \times 58.0)^{1/2} = 30.8 \text{ kcal/mol}$
- (4) Max. covalent energy:  $E_c (\text{NaCl}) = E_h \times R_c/R_o = 30.8 \times 253.3/236.1 = 33.1 \text{ kcal}$
- (5) Max. ionic energy:  $E_i (\text{NaCl}) = 33200/R_o = 33200/236.1 = 140.6 \text{ kcal}$
- (6) Blending coefficients: ionic:  $t_i = (\delta_{\text{Na}} - \delta_{\text{Cl}})/2 = (0.605 - (-0.605))/2 = 0.605$   
 covalent:  $t_c = 1.000 - t_i = 0.395$
- (7) Polar covalent bond energy of NaCl:  $E = t_c E_c + t_i E_i = (0.395 \times 33.1) + (0.605 \times 140.6) = 13.1 + 85.1 = \text{calculated value: } 98.2; \text{ experimental value: } 98 \text{ kcal/mol}$
- (8) Max.  $E_c (\text{NaCl(s)})$ :  $E_c = 4 \times 30.8 \times 253.3/281.4 = 110.9 \text{ kcal/mol}$
- (9) Max.  $E_i (\text{NaCl(s)})$ :  $E_i = 33200 \times 1.748 \times 0.88/281.4 = 181.5 \text{ kcal/mol}$
- (10) Atomization Energy of NaCl(s):  $E = (0.395 \times 110.9) + (0.605 \times 181.5) = 43.8 + 109.8 = \text{calculated value: } 153.6; \text{ experimental value: } 153.0 \text{ kcal/mol}$

ionic value is one-half the difference between the two partial charges,  $\delta_A$  and  $\delta_B$ :

$$t_i = (\delta_A - \delta_B)/2$$

Out of thousands of illustrative examples is chosen here that of NaCl, both gas and solid, for which a sample calculation is provided in Table 2. First it is important to call attention to the condition of the atoms in sodium and chlorine as they occur in their standard states, for each of these must be atomized in order to permit their atoms to combine as NaCl.

The electronic structure of an atom of sodium, here represented as 2-8-1, shows that there is but one electron in the outermost shell beyond the neon structure. Such an electron characteristically is held only loosely, allowing the atom of sodium to be relatively large and providing three more orbitals into which a bonding electron may become delocalized. In the vapor, sodium is mostly monatomic, but near the condensation temperature its atoms tend to a slight degree to combine into the diatomic molecules that can be expected when each atom has one half-filled outer orbital and therefore the capacity to form one covalent bond. The atomization energy of  $\text{Na}_2$  is only about 8 kcal per mole of atoms. However, when the vapor is cooled, it condenses to form liquid and then solid sodium, in which each interior atom is at the center of a cube of other atoms, with eight atoms thus in direct contact with it. This condensation is made possible by the existence of the three vacant orbitals also in the outer shell of the sodium atom, and the atomization energy of the solid metal is 25.8 kcal. The metallic condition is thus about three times more stable than the diatomic molecular form, which accounts very well for the existence of sodium under ordinary conditions as solid metal. Delocalization of the bonding electrons as in all metals permits much closer association of atoms than would be possible just by forming normal covalent bonds as when the bonding electrons are localized. Such delocalization also accounts for those special properties that characterize the metallic state. Here the principal point is that it will cost 25.8 kcal per mole of sodium atoms to liberate them for reaction.

The electronic structure of an atom of chlorine, 2-8-7, shows us that one outer vacancy remains per atom, which means one half-filled outer orbital able to form one covalent bond. The condition of chlorine in its standard state is therefore as diatomic molecules,  $\text{Cl}_2$ , which have such low intermolecular attraction that under ordinary conditions chlorine is a gas. We can predict that a much higher effective nuclear charge in chlorine compared to sodium should make its atoms smaller, radius 99.4 ppm compared to 153.9 pm for sodium, and more electronegative, 3.475 for chlorine but only 0.835 for sodium. The dissociation energy of chlorine molecules has been measured as 58.0 kcal per mole, which corresponds to 29 kcal per mole of atoms for the atomization energy. Before sodium and chlorine atoms can combine, it is thus apparent that it will be necessary to invest 25.8 kcal for the sodium and 29.0 kcal for the chlorine, totalling 54.8 kcal per mole of NaCl. The NaCl formula is easily predicted from the monovalence of both sodium and chlorine atoms.

Let us suppose first that the two atoms are alike in electronegativity and therefore form a nonpolar covalent bond. The energy would then be simply the geometric mean of the two homonuclear energies, 16.4 kcal for Na and 58.0 for Cl, or 30.8 kcal per mole of NaCl. This is for the molecular form, consisting of NaCl molecules in the gaseous state. Clearly this is not nearly enough to pay off the investment of 54.8 kcal. Therefore if the bonds were nonpolar, there would be no incentive to form molecules, nor would a solid form either because there would be no attraction between molecules except weak van der Waals forces. In fact, sodium chloride would decompose spontaneously to the elements with evolu-

tion of energy. (In a similar manner, it has been shown that neither hydrogen nor carbon would burn if they were of the same electronegativity as oxygen.)

As shown in Table 2, however, the actual electronegativity difference between sodium and chlorine produces partial charges of 0.605 on Na and -0.605 on Cl. At the observed bond length in the gaseous molecule, which is considerably shorter than the sum of the two nonpolar radii, the energy if nonpolar would be 33.1 kcal as shown. If the bond were ionic, however, the energy is calculated to be 140.6 kcal. As a result of the electronegativity difference, the covalent energy is reduced from 33.1 to 13.1, or by 20 kcal. The ionic contribution that replaces this 20 kcal, however, is 85.1 kcal. Consequently, the actual polar bond energy is 98.2 kcal per mole, allowing a profit of the difference between it and the 54.8 kcal investment. *It is characteristic of ionic energy that it is always greater than that portion of the covalent energy that it replaces.* Thus a difference in electronegativity is often the principal driving force in the reaction. The importance of electronegativity difference can hardly be overestimated.

The idea that NaCl is not the perfect example of an ionic compound as it has been claimed to be over these many years does not sit well with those who find new ideas disturbing. In general, the calculation of partial charge from electronegativity equalization suggests that no binary compound is completely ionic. However, we also know that NaCl is normally nonmolecular, not gaseous, and should account for this also. As shown in Table 2, by assuming that the NaCl molecules attract one another through their partial charges and condense to a nonmolecular solid in which all outermost electrons are involved in the covalent bonding and the ionic energy can be calculated as for the older "ionic model," the atomization energy of the solid is found to be in excellent agreement with the experimental value. Thus the solid state is about 55 kcal per mole more stable than the molecular gaseous state, which accounts very well for the preference for the solid condition.

Hundreds of examples involving most of the chemical elements attest to the general validity of these procedures,

**Table 3. Calculated and Experimental Atomization Energies (Kilocalories per Mole) of Representative Molecules**

cpmd	calc.	exp.	cpmd	calc.	exp.
HF	135.9	135.9	$\text{B}_2\text{O}_3$	653.8	652.5
$\text{AlOCl}$	251.7	250.6	HCl	103.7	103.2
HBr	87.3	87.4	$\text{NO}_2\text{Cl}$	255.9	258.2
$\text{NbF}_5$	676.5	682.5	$(\text{COOH})_2$	859.8	860.2
$\text{SO}_2$	218.2	217.6	$\text{BF}_3$	462.0	469.2
$\text{H}_2\text{O}$	225.6	221.6	$\text{MoO}_3$	424.2	422.1
$\text{AlB}_3\text{H}_{12}$	1120	1110	$\text{CH}_3\text{COCH}_3$	938.3	938.0
$\text{N}_2$	225.9	225.9	$\text{CS}_2$	276.8	275.7
$\text{ZnCl}_2$	157.0	157.4	$\text{BF}_2\text{OH}$	544.2	546.6
$\text{CO}_2$	382.6	384.6	$\text{SO}_2\text{Cl}_2$	329.4	330.3
$\text{SiO}_2$	301.8	303.4	$\text{TiCl}_2$	238.6	244.8
$\text{SiO}_2(\text{C})$	445.8	444.8	$\text{SOF}_2$	279.0	276.6
$\text{N}_2\text{O}$	267.6	266.1	$\text{B}_3\text{O}_3\text{F}_2\text{H}$	1151.7	1153.2
$\text{FeBr}_2$	164.0	164.0	NO	149.8	150.7
$\text{B}_3\text{N}_3\text{H}_6$	1194	1182	$\text{NbF}_5$	676.5	682.5
Lil	82.1	84.0	$\text{CH}_2=\text{CHCl}$	646.8	646.0
COS	327.3	330.2	$\text{BF}_2\text{F}$	404.2	401.5
$\text{P}_4\text{O}_6$	1214	1205	$\text{ZrCl}_4$	463.6	474.4
$\text{MgF}_2$	261.2	262.6	$\text{NH}_3$	280.2	280.2
$\text{CH}_3\text{CONH}_2$	832.7	832.8	$\text{BF}_2\text{Cl}$	418.7	415.8
$\text{NO}_2$	224.4	223.2	$\text{B}_2\text{H}_6$	566.6	576.5
$\text{CH}_4$	396.4	397.6	$\text{H}_2\text{SO}_4$	590.3	585.6
$\text{SiH}_2\text{Cl}_2$	347.6	345.2	$\text{O}_2$	118.9	119.1
$\text{PbI}_2$	97.2	98.0	$\text{TaCl}_2$	506.5	514.0
$\text{PCl}_3$	230.4	231.3	$\text{CH}_3\text{SCH}_3$	730.8	730.7
$(\text{C}_2\text{H}_5)_2\text{SO}$	1382.5	1381.5	$\text{ClO}_3\text{F}$	235.9	232.3
$\text{NH}_2\text{OH}$	342.4	341.9	$\text{WOF}_4$	676.2	676.7

which provides strong support for all the concepts and methods and electronegativity values employed in this work. Some representative examples of calculated atomization energies compared with experimental values are given in Table 3. It would seem unlikely that any teacher would wish to subject his students to a similarly complete analysis of the bonding in every compound included in their studies, but a few carefully presented examples should be invaluable in demonstrating the beautiful cause-and-effect relationships between the structure of atoms and the properties of their compounds. This provides, I believe, the closest approach to real understanding that has yet been available.

Use of these and closely related procedures has already provided simple and reasonable explanations of many previously puzzling chemical phenomena. These include at least partial answers to why nitrogen and oxygen are gaseous instead of being polymeric solids, why carbon dioxide is

gaseous but silicon dioxide solid, why the nitrogen oxides differ so much from the oxides of heavier elements of that group, why radius ratio data are invalid, why different oxides of the same element vary as they do in acid-base properties, why bond dissociation energies differ from contributing bond energies, how heats of formation are related to atomic structure, why fluorine seems anomalous among the halogens; and on and on. With electronegativity as a constant companion, chemistry can at last be taught as the beautifully integrated, logical, understandable science it really is.

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