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Evaluation and Test of Pauling's Electronegativity Scale

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We first state simple rules which all electronegative scales must obey and apply these to Pauling's scale. Second, we investigate Pauling's bond energy−bond polarity equations and similar expressions that better reflect the additivity of energy. These relationships are then tested against many groups of molecules (including all of those previously tested by other research groups). Pauling χ is found to violate more than half of the elementary rules appropriate to χ scales. We also find that even the best form of the bond energy−bond polarity equation can only be satisfied by a very limited range of molecules and the form used by Pauling is only valid for a small number of bonds with low polarities.

Introduction

This article is divided into two parts. The first gives basic principles to which any electronegativity scale must conform and applies them to Pauling's scale. The second part focuses on Pauling's bond energy−bond polarity equations and how these have evolved to an improved form. Tests of these relationships are carried out for selected groups of molecules. These sets include all molecules previously employed to test Pauling's equations, and it also proves possible to predict the success of further tests that might be proposed for other molecules.

Electronegativity (χ) today faces the same problem it has for the past 50 years: can it be rigorously and usefully defined? Textbooks at the freshman, sophomore, and junior levels in colleges (as well as high schools) increasingly downplay the significance of this concept and generally include flawed and out-of-date accounts of the Pauling and Mulliken definitions.

Contemporary thinking centers on a quantum mechanical rationalization of chemical bonding but, unfortunately, there is no operator whose expectation value is electronegativity and the periodic table is similarly not derivable from Schrödinger's equation. Nevertheless, the periodic table remains the central chemical reference point and says that molecules are made out of atoms.[1] The name electronegativity and its association with an attracting power between atoms originated with J. J. Berzelius in 1811, and its continuous use since suggests that a true chemical entity is manifesting itself. In 1932 Pauling[2] was the first to assign quantitative values to a few elements and his scale (along with that of R. S. Mulliken,[3] 1934, 1935), initially enjoyed considerable enthusiastic support.

General Guidelines for an Acceptable Electronegativity Scale

1. A free atom definition. If properties of molecules or solids (e.g., bond energies, vibrational frequencies) are employed, the unavoidable spread of values among the chemically varying reference molecules greatly reduces the precision of χ values assigned to atoms. In exactly the same way that we obtain molecular and solid state information from the pattern of free atoms in the periodic table, one needs to obtain atomic χs from properties of free atoms. The possibility of doing this rests on the very well-known fact that the binding energy of atoms in molecules and the charge density in molecular bonds are a very small percentage of the total energies and total charge and therefore can be represented within the context of first-order perturbation theory, $E_1 = \int \varphi^\circ H^1 \varphi^\circ \, d\tau$, where φ° represents the free atom wave function and H^1 is the perturbing potential produced by molecular binding.

2. A precision of at least three significant figures is necessary to distiguish 30% of the main group elements and 75% of the transition metals. The transition metals have a smaller range of values than the main group elements but otherwise have similar magnitudes, thus further increasing the need for accuracy. The close-lying values originate from the complex screening effects of the 3d, 4d, 5d, and 4f orbitals and relativistic effects.[4]

3. Electronegativity is an energy per electron (measured in electronvolts). χ has continued to be associated with energy during the past 25 years (it is easy to include Allred and Rochow's definition in this category by simply imagining a radial integration of their force definition).

4. For main group atoms and most transition metals, all of their valence electrons must be included in the definition of χ. However, groups 8−11 transition elements (except Ru and Os)

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have maximum oxidation states which are lower than their group number, and these oxidation states correspond to the number of valence electrons to be counted in assigning their χ values.

5. Three main group requirements are interrelated: (a) the identification of χ with an atom's electron *attracting* power is generally equal to its electron *holding* power,[5] (b) noble gas atoms have only the holding ability,[5] and (c) χ magnitudes must parallel oxidation state limitations: seven main group atoms have oxidation state maxima that are less than the number of valence electrons: N, O, F, He, Ne, Ar, and Kr. These atoms must have the seven highest χs among the main group elements.

6. The metalloids are the well-known eight elements, B, Si, Ge, As, Sb, Te, Bi, and Po, that separate the metals from the nonmetals and must have a very narrow range of χ values that allows no overlap with metals or nonmetals. This establishes necessary and sufficient conditions for the χ values of these elements. Si has the lowest χ in the metalloid band, and this leads to the *Si rule*: All metals must have χ values which are less than or equal to that of Si.

7. For binary compounds, AB, χ_A and χ_B must quantify the definitions of ionic, covalent, and metallic bonds. That is, sums and differences of χ_As and χ_Bs must be able to distinguish between and quantify the sides of the binary bond triangle whose vertexes are labeled C (covalent), I (ionic), and M (metallic).

8. χ must have a quantum mechanically viable definition. That is, it must be compatible with the elementary quantum concepts (shell structure, quantum numbers, and energy levels) generally introduced in freshman chemistry textbooks to describe the electronic structure of atoms.

9. Because each row in the periodic table corresponds to filling a given shell as nuclear charge increases left to right, and because atoms increase in size down groups, all χ scales show a systematic increase left to right across rows and (except for relativistic effects) a general decrease down groups. This is the origin of the generally similar patterns found for *all* electronegativity scales when plotted on the periodic table coordinates (and *not* that everyone has felt the need to obtain results similar to Pauling or Mulliken). On the other hand, this broad, qualitative similarity is not precise enough to yield a chemically meaningful scale, but we believe that a scale which additionally follows all the guidelines above can greatly extend the periodic table's organizing power.

Application of above Rules to Pauling's χ. Pauling's scale certainly includes all the valence electrons of its atoms and its two highest values belong to atoms (O and F) whose maximum oxidation states are lower than the number of these valence electrons. However, it has $\chi_N < \chi_{Cl}$ and omits the noble gases. Pauling's use of $(\Delta\chi)^2$ instead of $|\Delta\chi|$ thereby forcing χ to have units of $(eV)^{1/2}$ has always confused chemists and seemed an unnecessarily awkward consequence of wanting to better fit a few extra bonds in his original bond energy−bond polarity relationship. It has been entirely ignored in favor of an energy definition by all workers in the field for more than 25 years.

There are three severe flaws in Pauling's electronegativity scale which have strongly influenced chemists' negative attitude toward electronegativity. (a) Many of his transition metal χs grossly violate the Si rule, and chemists have seriously questioned whether electronegativity is realistically applicable to this class of atoms. (b) There has been a major misreading of his χ definition (page 95 of his book[2]) by 15−20% of the texts which discuss his scale: "attraction of a neutral atom in stable molecules for electrons". This has been often interpreted as meaning that electronegativity is an intrinsic, in situ, molecular property, a concept which Pauling effectively denied by affirming Mulliken's free atom + free ion definition in the next sentence of his book. (c) Pauling's definition is not quantum mechanically viable because it is thermodynamically ad hoc and does not build in any of the electronic properties of atoms that result from Schrödinger's equation: quantum numbers, electronic configurations, and energy levels. These electronic features give rise to the stability, identity, and regenerative ability of atomic shell structures. For example, lack of quantum viability leads to an inability to designate χ values for group 18 elements.

TABLE 1: Pauling Electronegativities[6]

atom	χ_P	atom	χ_P	atom	χ_P
H	2.20	Be	1.57	Ge	2.01
Li	0.98	Mg	1.31	Sn	1.96
Na	0.93	Ca	1.00	N	3.04
K	0.82	Sr	0.95	P	2.19
Rb	0.82	B	2.04	As	2.18
F	3.98	Al	1.61	Sb	2.05
Cl	3.16	Ga	1.81	O	3.44
Br	2.96	In	1.78	S	2.58
I	2.66	C	2.55	Se	2.55
		Si	1.90	Te	2.10

TABLE 2: Bond Dissociation Energies[a]

element (A)	D_{A-A}	D_{A-F}	D_{A-Cl}	D_{A-Br}	D_{A-I}
H	436.0	569.4	431.6	366.3	298.4
Li	107.7	579.0	476.3	425.2	357.1
Na	76.8	476.7	410.0	363.1	293.6
K	50.9	494.7	425.0	381.0	321.3
Rb	48.5	491.2	431.7	375.6	322.0
Be	208[b]	638.9	463.5	388.5	300.8
Mg	129[b]	515.5	390.8	336.6	260.1
Ca	105[b]	560.3	446.2	393.5	325.0
Sr	84[b]	544.0	439.9	397.5	326.3
B	290.3[c]	644.4	442.3	366.6	269.8
Al	172.4[c]	592.5	426.1	358.6	281.1
Ga	115.5[c]	476.7	355.8	304.9[d]	243.3[d]
In	105.7[c]	445.7	326.9	287.9[d]	227.9
C	358.3	491.4	325.6	278.5	220.2[d]
Si	225.0	595.1	399.5	328.3	246.9
Ge	187.3	470.1	339.9	280.5	214.7
Sn	150.6	414[b]	314.5	274.2	214.0
N	158.6	280.5[c]	202[f]		
P	201.1	503.8	323.0	266.0	218.3
As	175.6	441.4	309.1	255.8	226.8
Sb	141.8	437.4	313.5	265.0	192.6
O	143.5	191.7[c]	202.0	235[e]	184[e]
S	264.4	365.7	268.6	256.7	
Se	216.0	352.8	255.7	240.0	151[b]
Te	211.7	377.2	283.7	243[b]	192[b]
F	157.8	157.8	250.5	249.3[c]	281.0[c]
Cl	242.6	250.5	242.6	218.6[c]	210.6[c]
Br	192.9	249.3[c]	218.6[c]	192.9	177.8[c]
I	151.0	281.0[c]	210.6[c]	177.8[c]	151.0

[a] All energies in kJ mol^{-1}; calculated from data in ref 17 unless otherwise noted. [b] Reference 18. [c] Calculated from data in ref 19. [d] Calculated from data in ref 20. [e] Reference 21. [f] Calculated from data in ref 22.

Pauling's Bond Energy−Bond Polarity Relationships

The Pauling electronegativity values were derived from his extra ionic energy (EIE) relationships, first formulated[2] as

$$D_{AB} = {}^{1}/_{2}(D_{AA} + D_{AB}) + 23(\Delta\chi)^2$$

with D values in kcal mol^{-1} and 23 a conversion factor which suggests that the units of χ are $(eV)^{1/2}$. From this equation, EIE

TABLE 3: Evaluation of Bond Energy−Bond Polarity Relationship for Diatomic Halides[a]

	line of best fit				
	through origin ($C = 0$)		unrestricted		
equation	k	r	k	c	r
$D_{AA} - (D_{AA}\,D_{BB})^{1/2} = k\,(\Delta\chi)^2 + c$	50.0	0.881	40.2	+60.8	0.927
$D_{AA} - {}^1/_2(D_{AA} + D_{BB}) = k(\Delta\chi)^2 + c$	48.4	0.904	39.9	+52.7	0.940
$D_{AA} - (D_{AA}\,D_{BB})^{1/2} = k\lvert\Delta\chi\rvert + c$	127.3	0.960	146.7	−42.2	0.971
$D_{AA} - {}^1/_2(D_{AA} + D_{BB}) = k\lvert\Delta\chi\rvert + c$	122.7	0.965	145.0	−48.4	0.980

Pauling Equations

$D_{AA} - (D_{AA}\,D_{BB})^{1/2} = 125(\Delta\chi)^2$

$D_{AA} - {}^1/_2(D_{AA} + D_{BB}) = 96.5(\Delta\chi)^2$

[a] All bond energies in kJ mol^{-1}. r = least-squares correlation coefficient.

is defined as $D_{AB} - {}^1/_2(D_{AA} + D_{BB})$. The more familiar equation

$$D_{AB} = (D_{AA}D_{BB})^{1/2} + 30(\Delta\chi)^2$$

was devised to allow the alkali metal hydrides to have positive values for their EIE's (however, it still produces negative values for the C−I and Se−I bonds). Clearly, the equation using the arithmetic mean is conceptually superior since bond energies (like other energies) combine additively in their contribution to heats of reaction. One of us (A.L.A.) used the arithmetic mean in his 1961 revision of the Pauling scale (Table 1) noting that "the postulate of the geometric mean is difficult to apply".[6]

Both of Pauling's equations state that the extra ionic energy of a A−B bond is proportional to the square of the electronegativity difference, $(\Delta\chi)^2$, between A and B. As noted above, a consensus has developed that energy per electron is the appropriate dimension for electronegativity,[7] suggesting that electronegativity should enter the D_{AB} expressions as $|\Delta\chi|$.

The validity of the bond energy−bond polarity relationship was assessed by comparing EIE values with Pauling electronegativity differences for a variety of bonds. The element−halogen bonds of the main group elements were selected as the primary database since reliable dissociation energies (Table 2) could be obtained for nearly all of them from highly accurate heats of formation of binary compounds. The 103 halides employed cover a wide range of electronegativity differences and include most of the compounds used in previous studies.

First, it was necessary to establish the most appropriate form of the relationship. This was done by applying the four equations

$$D_{AB} - {}^1/_2(D_{AA} + D_{BB}) = k(\Delta\chi)^2$$

$$D_{AB} - (D_{AA}D_{BB})^{1/2} = k(\Delta\chi)^2$$

$$D_{AB} - {}^1/_2(D_{AA} + D_{BB}) = k|\Delta\chi|$$

$$D_{AB} - (D_{AA}D_{BB})^{1/2} = k|\Delta\chi|$$

to the 26 diatomic halides (16 alkali metal halides, 4 hydrogen halides, and 6 interhalogens) and comparing the correlation coefficients obtained for the least squares regression lines. The results, summarized in Table 3, show that (a) much higher correlation coefficients are observed when $|\Delta\chi|$ is used as the function of χ, and somewhat higher ones when arithmetic rather than geometric mean is used to calculate EIE; (b) the proportionality constants (gradients of the lines of best fit) are much lower than those proposed by Pauling; (c) none of the lines of best fit intercept the EIE axis at the origin. The inescapable conclusion is that the optimum relationship between bond energy and $\Delta\chi$ is of the type $D_{AB} - {}^1/_2(D_{AA} + D_{BB}) = k|\Delta\chi|\ ]+ c$, and this is the one which was examined for all of the binary main group halides of formula type AX_x ($x = 1-4$). When EIE is plotted against $|\Delta\chi|$ for the 103 A−X bonds (X = halogen), the regression line is $D_{AB} - {}^1/_2(D_{AA} + D_{BB}) = 157.3\,|\Delta\chi| - 47.5$ kJ mol^{-1}. Although the overall correlation coefficient for this line is high (0.953), the intercept of −47.5 kJ mol^{-1} is a substantial fraction of most bond energies, which confirms that EIE as defined by Pauling is not directly proportional to $\Delta\chi$. When the 103 molecules are examined in various subsets—halides of elements in the same group or in the same period, or compounds of the same halogen—the regression lines have slopes ranging from 110 to 207, intercepts from −22 to −99 kJ mol^{-1}, and correlation coefficients from 0.869 to 0.998, The data are available in Table S1 of Supporting Information.

TABLE 4: Additional Bond Dissociation Energies[a]

element (A)	D_{A-H}	D_{A-O}	D_{A-C}	element (A)	D_{A-H}	D_{A-O}	D_{A-C}
H	436.0	463.5	415.9	Ge	288.9		213^{b}
Li	288.2	376		Sn	252.6		226^{b}
Na	201.0	273		N	390.9	201^{b}	304.6^{b}
K	184.0	267		P	321.6	335^{b}	264^{b}
Rb	167			As	296.5	301^{b}	
Be	317.3^{c}			Sb	257.8		
Mg	240^{f}			O	463.5	143.5	357.7^{b}
Ca	225^{d}			S	366.8		272^{b}
Sr	210^{f}			Se	321.1		
B	388.0^{c}	536^{b}	372^{b}	Te	274.1		
Al	288^{c}		255^{b}	F	569.4	191.7^{c}	491.4
Ga	269^{e}			Cl	431.6	202.0	325.6
In	245^{e}			Br	366.3	235^{e}	278.5
C	415.9	357.7^{b}	358.3	I	298.4	184^{e}	220.2^{d}
Si	321.9	452^{b}	318^{b}				

[a] All energies in kJ mol^{-1}; calculated from data in ref 17 unless otherwise noted. [b] Reference 18. [c] Calculated from data in ref 19. [d] Calculated from data in ref 20. [e] Reference 21. [f] Calculated from data in ref 22.

Few other heteronuclear single bonds have dissociation energies which are accurately known; values for the 28 A−H, 14 A−O, and 14 A−C bonds (Table 4) correlate poorly with $|\Delta\chi|$, as shown in the Supporting Information, Table S1 (r values are 0.328 for A−H, 0.676 for A−O, and 0.778 for A−C). Only 41 of these bonds are not already in the A−X database; the line of best fit for the combined set of 144 bonds:

$$D_{AB} - {}^1/_2(D_{AA} + D_{BB}) = 148.0|\Delta\chi| - 51.3 \text{ kJ mol}^{-1}$$

has a correlation coefficient of only 0.882 (a significant drop from the $r = 0.953$ for the 103 A−X, X = halogen database) and with $c = -51.3$ kJ mol^{-1} represents an even higher fraction of a typical bond energy.

Our analysis shows the intrinsically weak correlation between bond energy and bond polarity, as measured by $\Delta\chi$. Electronegativity is a one-electron energy parameter, while bond energy

TABLE 5: Correlation of "Extra Ionic Energy" with Electronegativity Difference[a]

data set	equation[b]	r[c]
10 elements		
(H, C, N, P, O, S, F, Cl, Br, I)	$D_{AB} - {}^1/_2(D_{AA} + D_{BB}) = 96.3(\Delta\chi)^2$	0.959
38 A−B bonds		
29 elements	$D_{AB} - {}^1/_2(D_{AA} + D_{BB}) = 56.0(\Delta\chi)^2$	0.856
103 A−halogen bonds	$D_{AB} - {}^1/_2(D_{AA} + D_{BB}) = 157.3\lvert\Delta\chi\rvert - 47.5$	0.953
29 elements	$D_{AB} - {}^1/_2(D_{AA} + D_{BB}) = 54.1(\Delta\chi)^2$	0.835
144 A−B bonds	$D_{AB} - {}^1/_2(D_{AA} + D_{BB}) = 148.0\lvert\Delta\chi\rvert - 51.3$	0.882
(B = halogen, H, C, O)		

[a] All energies in kJ mol^{-1}. [b] Line of best fit. [c] Correlation coefficient.

is a two-electron energy that requires a sophisticated electron−electron correlation energy treatment (which is a principal goal of today's most advanced electronic structure research). Chemically, this is manifesting itself in polarizability, lone pair−lone pair repulsion, lone pair−vacant orbital interactions, and steric effects.

Pauling's original equation gave self-consistent results for the low-polarity bonds formed among 10 nonmetallic elements (the halogens, O, S, N, P, C, and H), using 38 bond energies. The data in Table 5 show that inclusion of more elements and more bonds greatly changes the proportionality constant between EIE and $(\Delta\chi)^2$ and significantly lowers the correlation coefficient.

The widespread early popularity of Pauling's χ led many quantum mechanicians to try and derive his equation in the period between 1935 and 1978.[8−15] These efforts generally employed simple molecular orbital constructs, but were far short of adequate formulations for bond energies. Given the research advances of the last 20 years, these efforts do not merit detailed analysis. The problem also lies with the inherent inadequacy of Pauling bond energy−bond polarity equation itself. It may be that Nelson,[15] in the most recent paper on derivation attempts, will conclude this unsuccessful research by his comment, "The physical basis of Pauling's equation cannot be uniquely specified... that the same equation should hold for different families of atoms is highly coincidental."

There have also been some direct experimental tests of Pauling's bond energy−bond polarity relationships, the most significant of which was carried out by Pearson[16] on gas phase reactions involving halogen exchange. He reports a number of such reactions for which the sign of the ΔH value is found to be negative but from the Pauling equation is calculated as positive.

Summary and Conclusions

1. The Pauling scale satisfies only rules 4 and 5 of the criteria for an acceptable scale of electronegativities. Major shortcomings of Pauling's scale have led chemists to accept only a few of his χ values (groups 1 and 17, and the second and third rows of the p-block) and otherwise to seriously question χ as an important chemical parameter. The erratic and largely unrealistic values for transition metals have been a significant factor in leading to this conclusion.

Confusion over whether χ is to be thought of as an in situ, in-the-molecule quantity, or an independent atomic property (as so listed in all tables) and Pauling's failure to further elucidate this problem have also contributed to chemical uncertainty.

The most important defect in Pauling's χ is its lack of quantum mechanical viability. This shows up directly in its inability to satisfy the Si rule for transition metals or to assign χ values to group 18 elements (likewise, as noted in the Appendix, chemists' frequent use of different Pauling χs for different oxidation states of the same main group element to rationalize changes in molecular behavior is in conflict with the quantum related energy level spacings of these atoms).

2. Pauling electronegativities were derived from an equation that is valid for only a small number of bonds with low polarities.

3. Of the possible Pauling-type relationships for EIE and $\Delta\chi$, the one which correlates best for diatomic halides is

$$D_{AB} = {}^1/_2(D_{AA} + D_{BB}) + k\lvert\Delta\chi\rvert + c$$

where c is about −50 kmol^{-1}, an appreciable fraction of most bond energies and larger than one-third of the EIE values.

4. Very poor correlations between EIE and $\lvert\Delta\chi\rvert$]are observed when bonds other than A−X bonds are considered, showing the impossibility of deriving a generally applicable relationship between the two.

Appendix: The Quantum Atom

Every student in freshman chemistry hears about wave−particle duality, the Heisenberg uncertainty principle, quantum numbers, and the periodic table buildup scheme, but there are a number of less familiar quantum aspects needed for understanding atoms and especially their electronegativity. A good deal of this elucidation comes from recognition of the sharp differences in the intuitive and linguistically familiar classical mechanics of planetary motion versus the quantum mechanics of atoms (even though both follow the same inverse square law of attraction). Because their motion is governed by initial conditions at their formation, a set of planets plus a sun with identical masses to our solar system (which we may discover some day) will show many differences in their orbits from ours. On the other hand, gold atoms mined in South Africa or Alaska are identical and completely independent of their prior history. If an earth-like planet passed through our solar system, it would drastically change the orbits of our planets and might well destroy the whole pattern, but if we compare a free nitrogen atom with one taken out of NH_3 or an amino acid, the N atom is found to regenerate itself exactly. Likewise, an atom retains most of its identity when bound into a molecule because of the large spacing of its occupied energy levels and its HOMO−LUMO separation. Atomic energy level spacings are always greater than those of molecules made from a collection of similar atoms. Binding energies, and energy changes following oxidation state changes, are also smaller, illustrating the remarkable stability of atoms. Electronegativity is an atomic property which must reflect this high stability and a very common mistake among chemists is to imagine a classical mechanics-like continuous deformation of an atom such that its electronegativity parallels its oxidation state (higher OS associated with higher χ). This error has been especially prevalent among the users of Pauling χ, and it has reduced confidence in the quantification of χ and in the utility of χ itself.

It is also worth noting that the indivisibility and wholeness of atoms means that electronegativity is essentially restricted to atoms themselves and a few molecular entities which act like large atoms. For example, group χ, a string of atoms and/or small molecular fragments bound to a "lead atom". The π electrons of organic rings that are the ligands in metallocenes can also be assigned a χ value as can the properly oriented small molecules that often act as ligands in transition metal complexes.

The atomic physics outlined above originated from two eloquent and pedagogically superb, non-mathematical, essays written some years ago by the eminent (now retired) MIT physics professor Victor F. Weisskopf.[23]

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Supporting Information Available: A table listing slopes, intercepts, and correlation coefficients of the extra ionic energy−$\Delta\chi$ equation for various subsets of element halogen and other heteronuclear bonds. This material is available free of charge on the Internet at http://pubs.acs.org.

References and Notes

(1) As described in the Appendix and ref 23, the quantum revolution of the 1920s and early 1930s (which was started by Bohr's assignment of electron configurations to atoms in 1922) demonstrate the remarkable stability and integrity of atoms as they are bound into molecules.

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