

Connecting Pauling and Mulliken Electronegativities

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Abstract: A conversion formula between Pauling and Mulliken electronegativities is derived from a new analytic treatment of the classic valence bond model for a single bond A–B in terms of Mulliken-Jaffe “a and b” parameters for the atomic valence states. The new formula works better than the traditional linear and half-power empirical formulas. The results are consistent with an absolute Pauling scale in which both electronegativities approach zero simultaneously.

1. Introduction

An unresolved issue in the evolution of modern electronegativity^{1–4} has been the possibility of a practical quantum formula connecting the scales invented by Pauling^{5,6} and Mulliken.^{7,8} Pauling electronegativities from standard heats of formation⁹ are linked to the empirical bond energy formula

$$D(A-B) = \frac{D(A-A) + D(B-B)}{2} + K_P(X_A - X_B)^2 \quad (1)$$

representing nonpolar and polar contributions, respectively, with $K_P = 1.00$ eV. Mulliken electronegativities for atoms in bonds are defined by

$$X = \frac{IE_v + EA_v}{2} \quad (2)$$

with effective ionization energies and electron affinities related to Mulliken-Jaffe “a and b” parameters^{1,2} for common valence states. Although the quantum roots of electronegativity are evident in leading valence bond and molecular orbital approaches^{10,11} and density functional theory^{12–15} this has not identified a clear working formula connecting the Pauling and Mulliken scales. Traditional empirical conversion formulas have assumed a linear relationship. Early formulas based on limited data include Mulliken’s⁸ original formula (1935, 11 atoms)

$$\Delta_P = 0.360\Delta_M \quad (3)$$

for differences $\Delta = |X_A - X_B|$, Skinner and Pritchard’s¹⁶ absolute formula (1953, 15 atoms)

$$X_P = 0.317X_M \quad (4)$$

and Hinze, Whitehead, and Jaffe’s^{17–19} shifted formula (1963, 11 atoms)

$$X_P = 0.336(X_M - 0.615) \quad (5)$$

More recently, Bratsch¹ has proposed an ad hoc half-power formula (1988, 36 atoms)

$$X_P = 1.35X_M^{1/2} - 1.37 \pm 0.14 \quad (6)$$

based on revised and extended electronegativities. While the theoretical basis for these formulas is not clear, Komorowski²⁰ has suggested an interesting possibility for the slope in the linear formula in terms of a constant $(4\pi\epsilon_0/7)^{1/2} = 0.3151$ from a charge-transfer model for Δ_M . Our present theoretical approach identifies new conversion formulas, derived here from an exact nonlinear 2×2 reduction of the classic 3×3 valence bond model. The model simplifies in two different bonding limits. For polar bonds it explains the basis, limitations, and modifications of the traditional linear conversion formula. In the ionic bond limit it yields a nontraditional half-power formula similar to Bratsch’s formula. In both cases the new formulas give more precise fits of empirical electronegativities.

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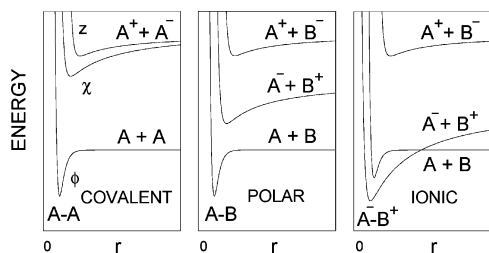


Figure 1. Potential energy curves for covalent and ionic states in simple bonds ($X_A > X_B$). Labels indicate the bonding at the minimum of each ground-state curve.

2. Theoretical Basis

The general strategy first casts the exact bond energy into nonpolar and polar parts

$$D(A-B) = D^n(A-B) + D^p(A-B) \quad (7)$$

and determines Mulliken's Δ_M from a valence bond estimate of the polar term $D^p(A-B)$. The energy separation involves breaking the wave function into orthogonal pieces $\psi = \phi + \chi$ that are symmetric (ϕ) or antisymmetric (χ) when orbitals are switched between the atoms. The nonpolar and polar terms in eq 7 are defined here by the matrix elements $D^n(A-B) = -(\phi|H|\phi)$ and $D^p(A-B) = -(\phi|H|\chi)$ when things are normalized to $(\phi|\phi) = 1$. The connection to Pauling's electronegativity is made directly by setting $D^p(A-B) = K_P(\Delta_P)^2$. One feature of this approach is that it does not depend on Pauling's arithmetic mean approximation. A similar definition of Pauling electronegativities has been made in terms of the charge-transfer affinity²⁰ in the corresponding partial charge model.

2.1. Valence Bond Model. The preceding strategy is applied to the valence bond wave function in terms of covalent and ionic structures (AB) , (A^-B^+) and (A^+B^-) . Figure 1 illustrates the potential energy curves related to the Pauling and Mulliken pictures.

We start with symmetrized wave functions that have the general form

$$\begin{aligned} \phi &= c_1(A_1B_2 + B_1A_2) + c_2(A_1A_2 + B_1B_2) \\ \chi &= c_3(A_1A_2 - B_1B_2) \\ z &= c_4(A_1B_2 + B_1A_2) + c_5(A_1A_2 + B_1B_2) \end{aligned} \quad (8)$$

The covalent bond $A-A$ is 100% ϕ ; the first ionic state above it is 100% χ , and the highest state is 100% z . The polar bond $A-B$ is a blend including mostly ϕ with a weaker admixture of χ . The ionic bond A^-B^+ involves a stronger mix that occurs when the ionic state crosses below the covalent curve. The coefficients c_1 and c_2 for each bond are initially selected to minimize the nonpolar ground-state expectation energy $E_\phi = (\phi|H|\phi)$ with $(\phi|\phi) = 1$. The polar mixing of ϕ and χ then shifts the ground-state energy downward to a new value E described by the 2×2 secular determinant

$$\begin{vmatrix} E_\phi - E & -2^{1/2}c_2\Delta \\ -2^{1/2}c_2\Delta & E_\phi - E + \frac{1}{2}\Sigma \end{vmatrix} = 0 \quad (9)$$

with energy parameters

$$\Delta = \frac{E(A^+B^-) - E(A^-B^+)}{2}$$

$$\Sigma = E(A^+B^-) + E(A^-B^+) - 2E_\phi(AB) \quad (10)$$

consistent with orthonormal orbitals and neglect of differential overlap. The parameter c_2 in the off-diagonal term comes from the coupling between χ and the ionic part of ϕ . The exact ground state is obtained when c_2 is readjusted to minimize E .²¹ This nonlinear approach gives the following optimized formulas:

$$\begin{aligned} E &= E_\phi - \frac{2K\Sigma\delta^2}{1 + \sqrt{1 + 8K\delta^2}} \\ c_3 &= \frac{4c_2\delta}{1 + \sqrt{1 + 8K\delta^2}} \end{aligned} \quad (11)$$

with $K = 4c_2^2$ and $\delta = \Delta/\Sigma$. The polar part of the bond energy is $D^p(A-B) = E_\phi - E$, and the valence bond estimate of the bond partial charge is

$$\delta_{VB} = \frac{4c_2c_3}{1 + 2c_3^2} = \frac{2K\delta}{\sqrt{1 + 8K\delta^2}} \quad (12)$$

Given the simplicity of the model, Pauling's formula, and uncertainties in the empirical electronegativity assignments we focus on the leading order scaling with the valence bond parameters. Perturbation theory gives

$$\begin{aligned} D^p(A-B) &= K\Sigma\delta^2 \\ \delta_{VB} &= 2K\delta \end{aligned} \quad (13)$$

Similar scaling is expected with other wave functions. When overlap (s) between A and B is included in the off-diagonal coupling in eq 9, for example, the Mulliken approximation²² for differential overlap gives

$$\begin{aligned} c_2 &\rightarrow \frac{c_2 + sc_1}{\sqrt{1 - s^2}} \\ K &\rightarrow \frac{1}{1 - s^2} + 2(c_2^2 - c_1^2) \end{aligned} \quad (14)$$

2.2. Electronegativities. Replacing the molecular energies Δ and Σ with equivalent atomic valence energies makes the connection to Mulliken's electronegativity. This gives working valence bond parameters Δ_M , Σ_M , and δ_M defined by

$$\begin{aligned} \Delta_M &= \frac{(IE_v + EA_v)_A - (IE_v + EA_v)_B}{2} \\ \Sigma_M &= (IE_v - EA_v)_A + (IE_v - EA_v)_B \\ \delta_M &= \frac{\Delta_M}{\Sigma_M} \end{aligned} \quad (15)$$

which are related to Mulliken-Jaffe parameters^{1,2} "a" (atom electronegativity) and "b" (atom charge coefficient) by Δ_M

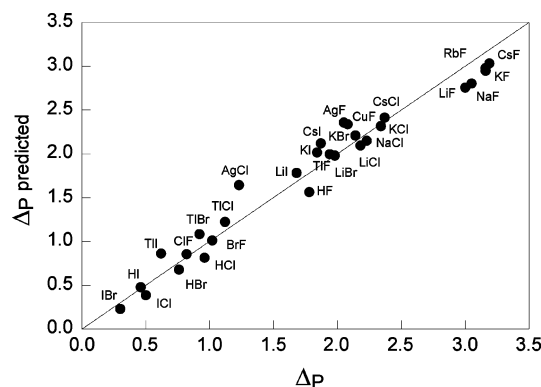


Figure 2. Correlation of predicted electronegativity Δ_P (eq 17, $\alpha = 1.065$) with Pauling's Δ_P . Line is predicted $\Delta_P = \Delta_P$.

$\leftrightarrow a_A - a_B, \Sigma_M \leftrightarrow b_A + b_B$ and $\delta_M \leftrightarrow \delta_{MJ}$ (partial ionic charge parameter). The important point here is that eq 13 connects Pauling and Mulliken electronegativities through the formula

$$K_P(\Delta_P)^2 = K_M \Sigma_M \delta_M^2 \quad (16)$$

where K_M is treated initially as an empirical constant.

3. Theoretical Analysis

3.1. Conversion Formulas. Two alternative forms of eq 16 are the conversion formula

$$\Delta_P = \alpha \frac{\Delta_M}{\sqrt{\Sigma_M}} \quad (17)$$

with $\alpha = (K_M/K_P)^{1/2}$ and the partial charge formula

$$\delta_M = \beta \frac{\Delta_P}{\sqrt{\Sigma_M}} \quad (18)$$

with $\beta = (K_P/K_M)^{1/2}$. Note that interpretations with these formulas will depend on the weight factor $1/(\Sigma_M)^{1/2}$ in addition to electronegativities in the conjugate scaling variables $\Delta_M/(\Sigma_M)^{1/2}$ and $\Delta_P/(\Sigma_M)^{1/2}$. In particular, eq 17 predicts the traditional linear scaling law $\Delta_P \propto \Delta_M$ only to the extent that Σ_M is constant. Figure 2 shows the empirical correlation between eq 17 and Pauling's Δ_P for a sample of 29 diatomic bonds. All electronegativity data were taken from Bratsch's tables.¹ The standard deviation of the fit is 23% lower than that for the conventional linear fit $\Delta_P \propto \Delta_M$. According to eq 17 this improvement reflects a greater uncertainty in the linear fit due to the distribution of values of Σ_M (13–31, $\text{avg} = 20 \pm 5$) over the sample. Figure 3 shows the related correlation of the same data between eq 18 and the Mulliken-Jaffe partial charge. Figure 4 shows a similar, but weaker correlation between eq 18 and the historical degree of ionization^{10,11} $\delta_d = \mu/r_e$ from experimental dipole moments and bond lengths.²³ Although it is well known that the empirical values of δ_d do not represent a simple dipole charge^{10,11} the correlation with the current formula for δ_M is nonetheless interesting.

3.2. Dependence of K on Partial Ionic Charge. Additional improvements can be made by taking into account variations of the valence bond coefficient $K = 4c_2^2$ with bond

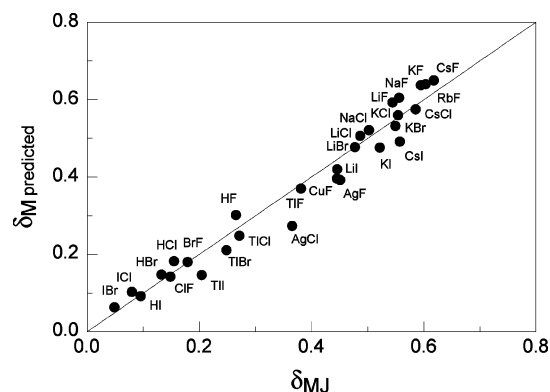


Figure 3. Correlation of predicted partial ionic charge δ_M (eq 18, $\beta = 0.939$) with Mulliken-Jaffe partial ionic charge δ_{MJ} . Line is $\delta_M = \delta_{MJ}$.

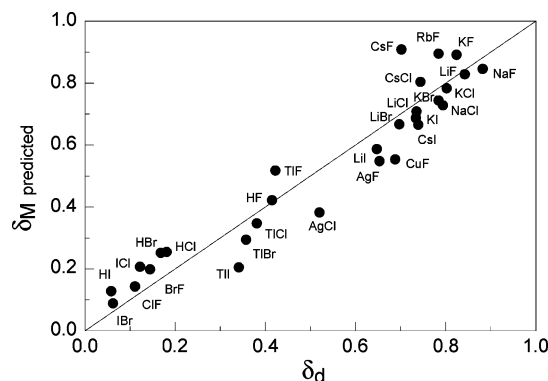


Figure 4. Correlation of predicted partial ionic charge δ_M (eq 18, $\beta = 1.31$) with empirical "dipole charge" $\delta_d = \mu/r_e$. Line is $\delta_M = \delta_d$.

polarity. Minimizing E in eq 9 tends to shift K to higher values due to a negative slope $dE/dc_2 < 0$ at the initial minimum for E_ϕ . As a simple model, the polar molecular orbital wave function $\lambda_1\lambda_2$ with

$$\lambda = \sqrt{\frac{1+\delta}{2}}A + \sqrt{\frac{1-\delta}{2}}B \quad (19)$$

gives $K = 2/(2 - \delta^2)$, which increases between $K = 1$ for a nonpolar bond ($\delta = 0$) and $K = 2$ for an ionic bond ($\delta = 1$). A model more consistent with the current valence bond approach is obtained from

$$\begin{bmatrix} -E & 2\beta & 0 \\ 2\beta & \frac{1}{2}\Sigma_0 - E & -\Delta \\ 0 & -\Delta & \frac{1}{2}\Sigma_0 - E \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = 0 \quad (20)$$

in terms of effective resonance and average excitation energy parameters β and Σ_0 . Matching this to the energies E_ϕ and Σ in eq 9 when $\delta = 0$ gives the relationship $\Sigma_0 = \Sigma(1 - \gamma^2)$ with the reduced resonance parameter $\gamma = 4\beta/\Sigma$. Figure 5 illustrates general behavior of the mixing coefficients between the covalent and ionic regions when γ is constant.

A formula for K as a function of δ is derived from an exact representation of eq 20 with a nonlinear 2×2 matrix for ϕ in which the coupling with χ is folded in as an effective potential $H_{\phi\chi}(E - H_{\chi\chi})^{-1}H_{\chi\phi}$. In terms of reduced energies ϵ

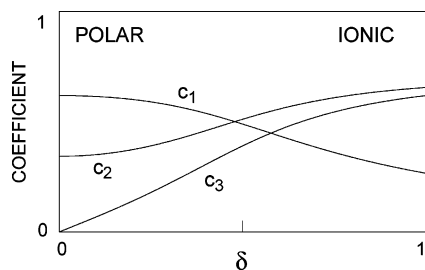


Figure 5. Dependence of ground-state valence bond coefficients ($\gamma^2 < 1$) on the partial charge parameter δ . This illustrates a smooth increase of c_2 and hence of K . According to eq 14 the coefficient K satisfies $K > 1$ on the ionic side of the crossing point $c_1 = c_2$. At high δ the coefficients approach $c_1 = 0$ and $c_2 = c_3 = 1/2^{1/2}$ with $K = 2$ for the ionic limit A^-B^+ . When $\gamma^2 > 1$, the order of the coefficients c_1 and c_2 at $\delta = 0$ switches to $c_2 > c_1$ with $K > 1$.

$= 2E/\Sigma$ and $\sigma = \Sigma_o/\Sigma = 1 - \gamma^2$, this projection gives

$$\begin{bmatrix} -\epsilon & \gamma \\ \gamma & \sigma - \epsilon - \omega \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0 \quad (21)$$

with the effective ionic interaction

$$\omega = \frac{4\delta^2}{\sigma - \epsilon} \quad (22)$$

ground-state energies from

$$\epsilon = \frac{1}{2}(\sigma - \omega) - \sqrt{\frac{1}{4}(\sigma - \omega)^2 + \gamma^2} \quad (23)$$

and

$$K = \frac{2}{1 + (\gamma/\epsilon)^2} \quad (24)$$

The curves for K as a function of δ have a positive curvature at $\delta = 0$, and they approach the limit $K = 2$ at high δ . At $\delta = 0$ eq 24 reduces to

$$K = \frac{2\gamma^2}{1 + \gamma^2} \quad (25)$$

which gives a range of values $K = 0-1$ when $\gamma^2 < 1$ (mostly covalent nonpolar bond), $K = 1$ when $\gamma^2 = 1$ (50% covalent and 50% ionic nonpolar bond), and $K = 1-2$ when $\gamma^2 > 1$ (mostly ionic nonpolar bond). The value $\gamma^2 = 1/3$ is special because it makes the leading valence bond partial charge in eq 13 equal to the Mulliken-Jaffe partial charge, $\delta_{VB} = \delta_M$. The crossover value $\gamma^2 = 1$ gives an exact solution $\omega = 4\delta^2/(1 + 4\delta^2)^{1/2}$ with $K = (1 + 4\delta^2)/(1 + 2\delta^2)$. At $\delta = 0$ this reduces to the molecular orbital model in eq 18. For other values of γ^2 , we found that using the empirical function $\omega = 4\delta^2/(1 + 3\delta^2)^{1/2}$ directly in eq 23 gives surprisingly good estimates of K over $\delta = 0-1$.

3.3. Empirical Values of K_M . Figure 6 compares the models for K to empirical values of K_M from eq 16. The previous fits in Figures 2 and 3 correspond here to a constant value $K_M = 1.13$. Curve A shows the gradual rise of K predicted by the molecular orbital model. Curve B shows K

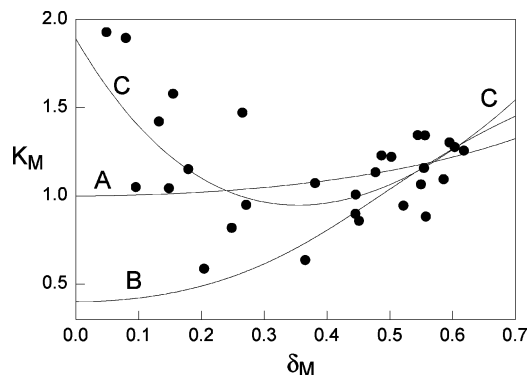


Figure 6. Dependence of empirical values of $K_M = K_P \Sigma_M (\Delta_P / \Delta_M)^2$ on partial charge $\delta_M = \Delta_M / \Sigma_M$. Curves: A) molecular orbital model; B) valence bond model; C) fit in eq 26.

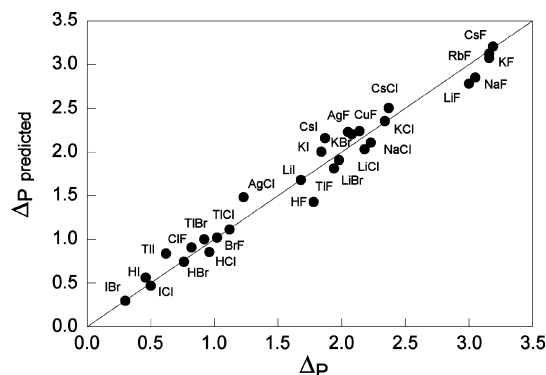


Figure 7. Improved correlation of predicted electronegativity Δ_P (eq 17 using K from eq 26) with Pauling's Δ_P . Line is predicted $\Delta_P = \Delta_P$.

from the valence bond model with fixed parameters $\Sigma = 16$ eV and $\beta = -2$ eV selected to represent the lower covalent region. Further improvements with these data for K_M are found with functions that have a minimum near $\delta = 0.3-0.4$. Curve C shows one empirical function

$$K_M = 1.89e^{-3.23\delta} + 2.75\delta^2 \quad (26)$$

which describes a minimum at $\delta = 0.35$. The comparison to Pauling's Δ_P is shown in Figure 7, which includes noticeable improvements over Figure 2. The standard deviation of the fit is 31% lower than that for the linear fit $\Delta_P \propto \Delta_M$. This improves to 35% when the function in eq 26 is optimized in terms of the scaling variable $\Delta_M/(\Sigma_M)^{1/2}$ instead of δ_M .

The apparent rise of the empirical values of K_M near $\delta_M = 0$ in Figure 6 corresponds to a higher slope in eq 17 for the bonds IBr , ICl , HBr , HCl and HF , possibly due in part to systematic deviations between Δ_P and Δ_M . Higher values of K for weakly polar bonds would also be consistent with shifts of the parameter γ^2 to higher values with $\gamma^2 > 1$. Because of these possibilities it is not clear to what extent the empirical behavior of K_M might reflect higher order contributions from the exact valence bond energy in eq 11. This would have K_M approach zero at high δ and give a negative curvature at $\delta = 0$ when $\gamma^2 > 1$.

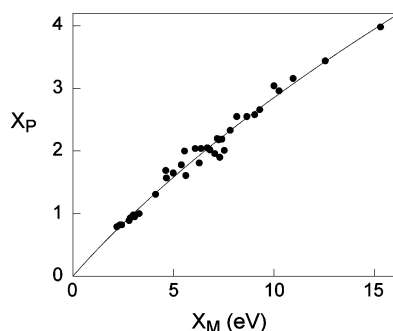


Figure 8. Correspondence between Pauling and Mulliken electronegativities from ref 1. Curve is the ionic bond half-power formula in eq 29 which gives a zero intercept at $X_M = 0$. Comparable curve is described by the polar bond half-power formula in eq 30.

4. Half-Power Scaling

The valence bond formulas also suggest a partial basis for Bratsch's empirical half-power formula in eq 6. For comparison we first fitted the same data for 36 atoms with eq 17 relative to fluorine. This gave a better fit

$$X_P = 3.98 + \alpha \frac{X_M - 15.30}{\sqrt{b_{MJ} + 17.81}} \pm 0.11 \quad (27)$$

with a single adjustable parameter $\alpha = 1.137$. While this improvement over eq 6 suggests half powers may not be necessary, it is interesting that the valence bond model does in fact predict half-power scaling under certain conditions.

One approach involves the ionic bond limit of the exact solution of the secular determinant

$$K_P(\Delta_P)^2 \propto \frac{2K\Sigma\delta^2}{1 + \sqrt{1 + 8K\delta^2}} \quad (28)$$

For small δ this reduces to the polar bond formula in eq 16. At high values of δ it gives the half-power formula $\Delta_P \propto (\Delta_M)^{1/2}$, including Bratsch's formula as a special case when the reference state in Δ_M is assumed to have $X_M = 0$. Relaxing this condition gives a better global fit

$$X_P = 1.934\sqrt{X_M + 7.02} - 5.12 \pm 0.12 \quad (29)$$

which is shown in Figure 8.

In a second approach, we note that the polar bond formula eq 27 predicts a half-power directly for low values of δ when the charge coefficient b_{MJ} is a linear function of X_M . This is not a bad approximation,¹ and a direct fit with $b_{MJ} = cX_M + d$ gives $c = 1.04 \pm 0.08$ and $d = 0.93 \pm 0.57$. Refitting eq 27 with a similar linear function gives the half-power formula

$$X_P = 3.98 + 1.154 \frac{X_M - 15.30}{\sqrt{X_M + 19.68}} \pm 0.12 \quad (30)$$

which gives results similar to eq 29. It also reduces to a simple half-power formula at high X_M .

An interesting feature of the independent half-power fits in eqs 29 and 30 is that both functions extrapolate to a zero

intercept $X_P = 0.00$ at $X_M = 0$. This empirical result supports a possible absolute Pauling scale as a nonlinear generalization of the Skinner and Pritchard formula in eq 4. Both eqs 29 and 30 give the same linear formula $X_P = 0.36X_M$ near the intercept, including a slope consistent with Mulliken's original empirical formula in eq 3.

5. Conclusion

A method for polar contributions to the bond energy described herein was applied to the valence bond wave function to derive formulas and results which appear to clarify and improve the connection between Pauling and Mulliken electronegativities. In effect the relationship in eq 17 (and its application such as eq 27) defines a semiempirical Pauling scale for valence states consistent with Mulliken-Jaffe parameters. And eq 18 defines a semiempirical partial charge consistent with Pauling's electronegativity. These conjugate formulas provide a self-consistent basis for further studies and possible refinements of the electronegativity scales.

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