Electronegativities of Pauling and Mulliken in Density Functional Theory

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S *Supporting Information*

ABSTRACT: Electronegativity is a fundamental concept in chemistry that allows one to infer important aspects about the interactions between chemical species. In the present work we make use of the framework provided by the density functional theory of chemical reactivity, to discuss in a unified way the approaches to the concept of electronegativity developed by Pauling and by Mulliken. Our analysis starts by making use of the identification of the electronegativity of Mulliken with the chemical potential of density functional theory, and continues to show that the ionic correction proposed by Pauling can be derived, with certain approximations, from the quadratic smooth interpolation of the energy as a function of the number of electrons in

Electronegativity χ		
Concept		**DFT**
Mulliken	$\chi_M = -\mu$	Chemical potential
$\chi_M = (I + A)/2$	$\mu = (\partial E / \partial N)_{v(r)}$	
Pauling	$\chi_P = \omega$	Electrophilicity
$\Delta^0 = (\chi_P^A - \chi_P^B)^2$	$\omega = \mu^2 / 2\eta$	

terms of the chemical potentials and the hardnesses of the interacting species, from which one can infer the close qualitative relationship between Pauling's electronegativity and the electrophilicity concept.

1. INTRODUCTION

Over the last century, electronegativity (χ) has emerged as a fundamental concept in chemistry. Nevertheless, due to its intuitive nature, it lacks a unique and exact definition to quantify it. In 1930, Pauling[1] introduced the first relative electronegativity scale, based on bond energies of diatomic molecules. Shortly after, Mulliken[2] suggested that the absolute electronegativity may be expressed as $\chi_M = (I + A)/2$ where I and A are the vertical first ionization potential and the electron affinity, respectively.

The electronegativity concept was enunciated by Pauling to justify the asymmetrical distribution of the electronic charge in the boundary region between two atoms. Covalent bonds correspond to the nearly symmetrical distribution case, while in an ionic bond the surrounding electronic cloud is polarized toward one of the atoms. This analysis led Pauling to define later electronegativity as the power of an atom in a molecule to attract electrons to itself.[3] In the original work he defined a normal covalent bond, for the diatomic molecule AB, as one in which the bond energy between atoms A and B, ΔE_{AB}, may be approximated by the average of the bond energies of the homonuclear diatomic molecules AA and BB, ΔE_{AA} and ΔE_{BB}, respectively. The difference between the experimental value for ΔE_{AB} and the average just mentioned was interpreted as an ionic correction term ($\Delta°$) that accounts for the additional stability of the bond, that is

$$\Delta E_{AB} = \frac{1}{2}(\Delta E_{AA} + \Delta E_{BB}) + \Delta° \tag{1}$$

Pauling proposed that this ionic correction term should be proportional to the square of the difference between the electronegativities of atoms A and B,

$$\Delta_P° = (\chi_P^A - \chi_P^B)^2 \tag{2}$$

so that using eqs 1 and 2 with experimental information for the bond energies, he build up a relative scale of electronegativities by assigning a value of 2.1 to the hydrogen atom.

On the other hand, Mulliken established that the energy change associated with the process in which A donates an electron to B, may be approximated by $\Delta E_{A \to B} = I_A - A_B$, while for the case in which A receives an electron from B $\Delta E_{A \leftarrow B} = I_B - A_A$, and suggested that if A and B have equal electronegativities the energy change for both cases should be equal, so that $I_A - A_B = I_B - A_A$, which may be rewritten in the form $I_A + A_A = I_B + A_B$. This analysis led him to propose that the absolute electronegativity of an atom may be defined as $\chi_M = (I + A)/2$.

This definition was generalized by Iczkowski and Margrave[4] to $\chi_M = -(\partial E/\partial N)_{v(r)}$, where E is the electronic energy, N is the number of electrons, and $v(\mathbf{r})$ is the potential generated by

the nuclei. The basis for the generalization comes from the fact that if one performs a smooth quadratic interpolation between the systems with $N_0 - 1$, N_0 and $N_0 + 1$ electrons (N_0 being an integer), the finite differences approximation to the negative of the derivative of E with respect to N evaluated at N_0 leads to Mulliken's expression.

This approach found a strong support within the framework provided by density functional theory (DFT), when Parr et al. recognized that the chemical potential (μ) of density functional theory, satisfies the relationships[5]

$$\mu = \frac{\delta E[\rho]}{\delta \rho(\mathbf{r})} = \left(\frac{\partial E}{\partial N}\right)_{v(\mathbf{r})} \qquad (3)$$

where the first equality establishes that the chemical potential is the Lagrange multiplier that comes from the variational procedure of the energy with respect to the electronic density, $\rho(\mathbf{r})$, and the second equality establishes that it is also equal to the derivative of the energy with respect to the number of electrons,[6] at constant external potential. Thus, through the Iczkowski and Margrave expression, Parr et al. were able to identify the electronegativity with the negative of the chemical potential of DFT

$$\chi_M = -\mu = -\left(\frac{\partial E}{\partial N}\right)_{v(\mathbf{r})} \qquad (4)$$

where through the subindex M it is emphasized that this identification corresponds to Mulliken's approach to electronegativity.

Together with the chemical potential, eq 4, Parr and Pearson[7] identified the intuitive concept of hardness, previously developed by Pearson[8,9] to establish the hard and soft acids and bases principle, with the second derivative of the energy with respect to the number of electrons at constant external potential

$$\eta = \left(\frac{\partial^2 E}{\partial N^2}\right)_{v(\mathbf{r})} \qquad (5)$$

It is important to note that the evaluation of electronegativity and hardness through eqs 4 and 5 implies that one needs to know the behavior of the energy for a fractional number of electrons. In order to determine this behavior, one needs to make use of the theoretical framework provided by the grand canonical ensemble,[10] in which one deals with an open quantum system that may exchange electrons with the reservoir. The fractional numbers appear because since the number of electrons varies, one must consider the average of the ensemble, $\langle N \rangle$, and this quantity can be an integer or a real number. Also, for the energy, one must consider the average of the ensemble, $\langle E \rangle$. In this context,[11,12] the electronic chemical potential and the electronic chemical hardness are given by $\mu_e = (\partial \langle E \rangle / \partial \langle N \rangle)_{v(\mathbf{r})}$ and $\eta_e = (\partial^2 \langle E \rangle / \partial \langle N \rangle^2)_{v(\mathbf{r})}$.

Thus, for a chemical species with an integer number of electrons, N_0, Perdew, Parr, Levy, and Balduz[10] made use of the grand canonical ensemble composed by the systems with $N_0 - 1$, N_0, and $N_0 + 1$ electrons in their ground state, to show that, in the zero temperature limit, the behavior of $\langle E \rangle$ as a function of $\langle N \rangle$ is given by a series of straight lines connecting the integer values of $\langle N \rangle$. It is important to mention that the same result was found, later, from properties of the universal density functional.[13,14]

Now, since it has been proven that the three ground-sates ensemble model is adequate for temperatures of chemical interest,[15] one can use it to derive[11,12] the temperature dependent expressions for $\langle N \rangle$ and $\langle E \rangle$. Through this procedure, one can show[11] that the average energy for $T \neq 0$ is a smooth function of $\langle N \rangle$, so that the derivatives of $\langle E \rangle$ with respect to $\langle N \rangle$ of all orders exist and can be evaluated analytically. This result is important because it gives a formal support to reactivity indicators like the ones expressed in eqs 4 and 5, and others. A relevant aspect is related to the fact that the effects of temperature in the values of these derivatives is negligible, in practically all cases, for temperatures of chemical interest, a situation that indicates that one can evaluate them with the approximate expression usually used in the zero temperature limit. However, conceptually one may consider that these values are valid for real situations where the temperature is not zero, and therefore when the derivatives are well-defined.

Taking into account the preceding discussion, one should recall that noninteger populations of atoms in molecules are commonly used in chemistry to describe charge transfer processes. In this context, if one considers the approximation for the description of the energy as a function of the number of electrons, provided by the smooth quadratic interpolation between the energy of the systems with $N_0 - 1$, N_0, and $N_0 + 1$ electrons, that is

$$\Delta E = \mu \Delta N + \frac{1}{2}\eta(\Delta N)^2 \qquad (6)$$

where $\Delta N = N - N_0$, one finds that the derivatives of eqs 4 and 5, evaluated at the reference point N_0, are given by $\mu = -\chi_M = -(I + A)/2$ and $\eta = I - A$. This result provides a strong support to the identification of μ (i.e., $-\chi$) and η as the first and second derivatives of the energy with respect to the number of electrons, because if one makes use of the experimental values of I and A, one finds that the values for the chemical potential (minus the Mulliken electronegativity) and the hardness follow approximately the same trends of the qualitative scales established for these properties.

Equation 6 allows one to quantify the amount of charge transferred between two species, A and B, and the energy change associated with it, when one neglects the effects produced by the changes in the external potential,[7] and because of its simplicity and at the same time clear chemical meaning, it has been used to describe a wide variety of aspects involved in charge transfer processes.[7,16−47] In particular, from this expression Parr, Von Szentpaly, and Liu[20] determined the maximum amount of charge that a chemical species can accept when it is immersed in an idealized zero-temperature free electron sea of zero chemical potential, $\Delta N_{max} = -\mu/\eta > 0$, for which the energy change becomes $\Delta E = -\mu^2/2\eta < 0$. This analysis led them to define the electrophilicity index as

$$\omega = \mu^2/2\eta \qquad (7)$$

It is important to mention that in the temperature dependent situation, it has been found[48,49] that the Helmholtz free energy, at high temperatures, shows a nearly parabolic behavior that exhibits a minimum at noninteger positive values of the fractional charge.

Recently,[50,51] several important aspects concerning the electronegativity of chemical species have been reviewed leading to new proposals. In this work we have adopted a different perspective, by performing an analysis of the ionic

correction term introduced originally by Pauling in the framework provided by conceptual density functional theory, to show that the electronegativity of Pauling is closely related with the electrophilicity concept,[20] a result that complements the identification of the electronegativity of Mulliken with the chemical potential.[5]

2. THEORETICAL DEVELOPMENT

Let us write the total energy for the species AB, E_{AB}, in the form $E_{AB} = E_A + E_B - \Delta E_{AB}$, where as mentioned before ΔE_{AB} represents the bond energy between A and B, whereas E_A and E_B are the total energies of A and B when they are isolated from each other. Similarly, the total energy for the species AA and BB is given by $E_{AA} = 2E_A - \Delta E_{AA}$ and $E_{BB} = 2E_B - \Delta E_{BB}$, respectively. For stable molecules ΔE_{AB}, ΔE_{AA}, and ΔE_{BB} are positive definite quantities. Combining the three equations in this paragraph one finds that

$$\Delta E_{AB} = \frac{1}{2}(\Delta E_{AA} + \Delta E_{BB}) + \frac{1}{2}(E_{AA} + E_{BB} - 2E_{AB}) \quad (8)$$

The comparison of this expression with eq 1 implies that

$$\Delta^\circ = \frac{1}{2}(E_{AA} + E_{BB} - 2E_{AB}) \quad (9)$$

Since the first term in the right-hand side of eq 8 represents the contribution to the bond energy coming from the normal covalent bond, while the second term corresponds, following the arguments of Pauling, to the ionic correction Δ°, this one may be interpreted as arising exclusively from the charge transfer process between A and B. Thus, one may consider the reaction $A + B \rightarrow AB$, for which the energy change associated exclusively with the charge transferred may be expressed as $\Delta E_{AB}^{CT} = E_{AB} - E_A - E_B$, so that combining it with the corresponding expressions for the cases of AA and BB, that is, $\Delta E_{AA}^{CT} = E_{AA} - 2E_A$ and $\Delta E_{BB}^{CT} = E_{BB} - 2E_B$, respectively, one finds that eq 9 becomes equal to $\Delta_{CT}^\circ = (\Delta E_{AA}^{CT} + \Delta E_{BB}^{CT} - 2\Delta E_{AB}^{CT})/2$, where we have explicitly indicated that in this case Δ° will be obtained from a charge transfer model. Now, assuming that $\Delta E_{AB}^{CT} = \Delta E_A^{CT} + \Delta E_B^{CT}$, and that these energy changes may be estimated through eq 6, one can show that $\Delta E_{AB}^{CT} = -(\mu_A - \mu_B)^2/2(\eta_A + \eta_B)$. Through the same arguments one sees that $\Delta E_{AA}^{CT} = 0$ and $\Delta E_{BB}^{CT} = 0$, and therefore

$$\Delta_{CT}^\circ = -\Delta E_{AB}^{CT} = \frac{1}{2}\frac{(\mu_A - \mu_B)^2}{\eta_A + \eta_B} \quad (10)$$

In this expression, one can identify that the numerator corresponds to the square of a chemical potential difference, which through the use of eq 4 would correspond to the square of the difference of what we have called Mulliken's electronegativity. Thus, one can see that this relationship, although not exactly equal, resembles Pauling's proposal, expressed in eq 2. However, from our viewpoint, it is more tempting to first analyze eq 10 from the perspective that since the charge transferred associated with it is given by

$$\Delta N_A^{CT} = -\Delta N_B^{CT} = \frac{\mu_B - \mu_A}{\eta_A + \eta_B} \quad (11)$$

the chemical potential difference, indicates the direction of the flow of charge, and eq 10 represents the stabilization energy associated with this amount of charge transferred. Thus, through this procedure we have derived an expression to approximately determine the ionic contribution to the bond

energy of a system AB, in terms of the chemical potential and the hardness of the isolated species A and B. It is important to note that eq 2 is a proposal done precisely to introduce the concept of electronegativity, while eq 10 is a derivation based on the assumption that this term corresponds exclusively to the charge transferred, and the approximations used to determine it, namely that the contributions to this term from the changes in the external potential are neglected, and that the energy change is determined from the smooth quadratic interpolation indicated in eq 6. Even though the expression for ΔE_{AB}^{CT} was first introduced by Parr and Pearson, and as already mentioned it has been used since then to describe different charge transfer processes,[7,16−47] in the present work it is found that it also corresponds to the ionic contribution associated with the normal covalent bond energy defined by Pauling (first term in the right-hand side of eq 1).

Thus, a first aspect to consider is related with the degree of precision that eq 10 has to predict the experimental values of Δ°, which correspond to the ones obtained from the experimental bond energies ΔE_{AA}, ΔE_{BB}. and ΔE_{AB}, since from eq 1 $\Delta^\circ = \Delta E_{AB} - {}^1/_2(\Delta E_{AA} + \Delta E_{BB})$. In order to test this precision, we computed Δ_{CT}° and Δ_P° for a total of 56 heteronuclear diatomic molecules using the atomic data given in Table S1 (in which the values corresponding to Pauling's electronegativity are those refined by Allred,[52] who fixed the value for hydrogen at 2.2), to calculate the values given in Table S3 (both tables form part of the Supporting Information). For the experimental values, Δ°, we found accurate values for 43 molecules of the 56 considered (see Table S2, Supporting Information). In Figure 1 we present a plot of Δ_P°(eq 2) and of Δ_{CT}° (eq 10) as a function of Δ°. In order to analyze this plots it is important to note that in the case of Δ_P°, one determines first the electronegativity difference, for a set of diatomic molecules, with the experimental information, using eq 2 with Δ_P° replaced by Δ°, so that $|\chi_P^A - \chi_P^B| = (\Delta^\circ)^{1/2}$, and then one fixes the value for the hydrogen atom at 2.2, to calculate the electronegativity of all the other atoms. Thus, using the electronegativities from the relative scale one determines the electronegativity difference to calculate Δ_P° through eq 2. This procedure implies that there will be differences between Δ° and Δ_P° because the values of $|\chi_P^A - \chi_P^B|$ determined with the relative scale are different from the values obtained with the experimental information. The correlation between Δ° and Δ_P°, $R^2 = 0.875$, obtained in this case provides a measure of the quality achieved with the relative scale of electronegativities. On the other hand, in the case of Δ_{CT}°, one determines the values in terms of the square of the chemical potential difference (Mulliken's electronegativity difference) of the two interacting species divided by the sum of their hardnesses. Since the electronegativities and hardnesses are determined through the expressions $\mu = -\chi_M = -(I + A)/2$ and $\eta = I - A$, respectively, they make use of the experimental values of I and A of the atoms that form the diatomic molecule. This situation indicates that Δ_{CT}° is determined from atomic values that introduce the information about the interacting partner through the simple charge transfer model expressed by eq 10, while Δ_P° is determined, although indirectly, from molecular values that do have direct information about the interacting partner. Thus, the fact that the correlation between Δ° and Δ_{CT}°, $R^2 = 0.865$, is very close to the value obtained for the correlation between Δ° and Δ_P°, and that the plot of Δ_{CT}° as a function of Δ_P° (Figure 2) shows a rather good correlation, $R^2 = 0.950$, indicates that the simple
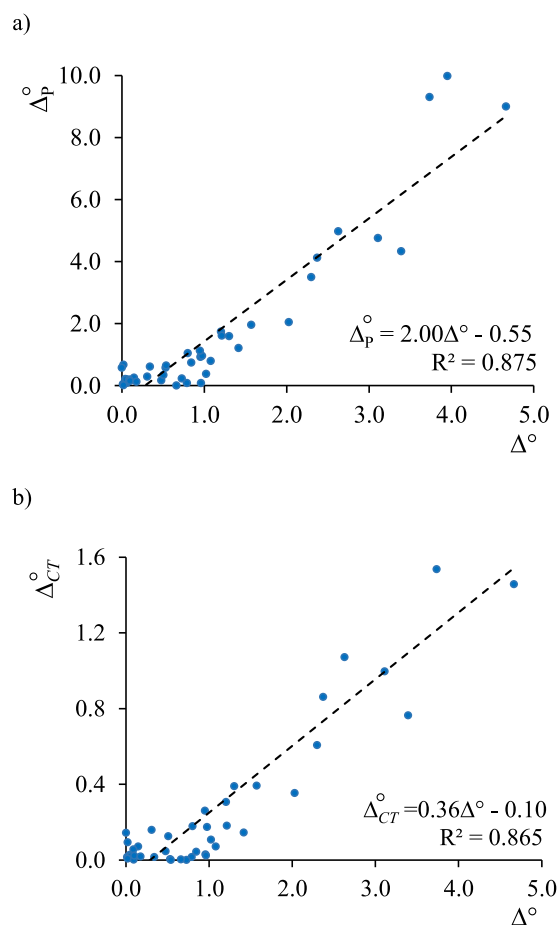
a)

b)

Figure 1. (a) Plot of the Pauling expression for the ionic correction term (Δ_P°) given by eq 2 versus the experimental value (Δ°). (b) Plot of the simple charge transfer model expression for the ionic correction term (Δ_{CT}°) given by eq 10 versus the experimental value (Δ°).
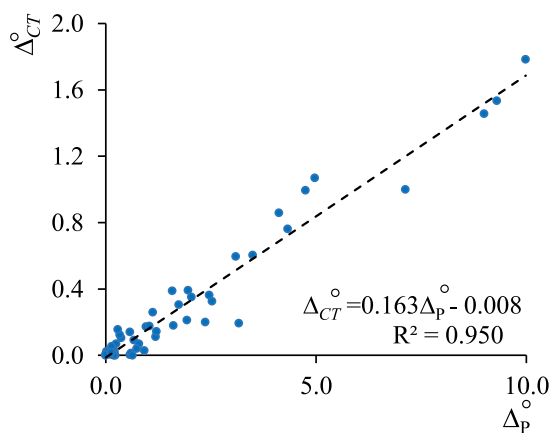

Figure 2. Plot of the simple charge transfer model expression for the ionic correction term (Δ_{CT}°) given by eq 10 versus the Pauling expression for the ionic correction term (Δ_P°) given by eq 2.

charge transfer model describes indeed, approximately, the ionic contribution to the bond energy of a heteronuclear diatomic molecule proposed by Pauling.

A relevant aspect is related to the fact that eqs 2 and 10 imply that the ionic contribution to the dissociation energy depends simultaneously on the properties of the two interacting species, and in both cases because of the presence

of the square of a difference one can not separate the right-hand side into the sum of a term that only depends on the properties of A and a term that only depends on the properties of B, so that the individual terms for A and for B could be identified with the definition of an absolute electronegativity. This situation indicates that, through the present approach, one can only build up a scale of electronegativities relative to a given reference system, as Pauling did.

Therefore, if one were to establish a scale of electronegativities based on eq 10, one could select the same reference system B for every system A. An immediate choice for such reference system could be an ideal bath for which the chemical potential is equal to zero and the hardness is also equal to zero, leading to

$$\Delta_{CTIdeal}^{\circ} = -\Delta E_A^{CTIdeal} = \frac{\mu_A^2}{2\eta_A} = \omega_A \qquad (12)$$

where in the last equality we are using eq 7 to indicate that this relationship corresponds to the definition given by Parr, Von Szentpaly, and Liu[20] of electrophilicity. That is, through the present analysis we are identifying the intuitive concept of electronegativity with the electrophilicity index, when one makes use of a reference system that corresponds to an ideal bath. In this case, if one makes use of the smooth quadratic interpolation in which $\mu = -\chi_M = -(I + A)/2$ and $\eta = I - A$, one finds that $\omega = (I + A)^2/8(I - A)$. If one makes use of the experimental values of I and A for atoms, one finds that, qualitatively, ω follows the same trends that χ_M and χ_P. However, beyond the quantification of electronegativity through the electrophilicity values, the latter concept in itself has been very important to describe and understand many aspects of charge transfer processes.[27,29,34,53−65] Thus, the relationship established in this work through the derivation of the ionic contribution in terms of the simple charge transfer model provides new insights into the close relationship that conceptually one could expect between electronegativity and electrophilicity.

It is important to mention that Noorizadeh and Shaker-zadeh[66] arguing from the perspective that since electrophilicity measures the energy lowering of a species arising from the maximum number of electrons accepted from the bath, it provides a measure of the capacity of a species to attract electrons to itself, an interpretation that is in line with the concept of electronegativity proposed by Pauling. In this context, they showed that if the first (chemical potential) and second (hardness) derivatives of the energy with respect to the number of electrons are determined starting from a Morse like function for the energy in terms of the number of electrons, one obtains values for the electrophilicity that show a rather good correlation with the scale of Pauling, $R^2 = 0.979$. They also showed that their new scale based on electrophilicity, shows a rather good correlation for calculating bond dissociation energies.[67]

An interesting aspect of this identification comes from the fact that if one makes use of the expressions derived by Chattaraj and Ayers[25] for the values of the chemical potential and the chemical hardness of the species AB, once the charge transfer between A and B given by eq 11 has occurred, namely

$$\mu_{AB} = \frac{\mu_A \eta_B + \mu_B \eta_A}{\eta_A + \eta_B} \qquad (13)$$

and

$$\eta_{AB} = \frac{\eta_A \eta_B}{\eta_A + \eta_B} \tag{14}$$

one finds that the electrophilicity of the product AB is given by[68]

$$\omega_{AB} = \frac{\mu_{AB}^2}{2\eta_{AB}} = \frac{(\mu_A \eta_B + \mu_B \eta_A)^2}{2\eta_A \eta_B (\eta_A + \eta_B)} \tag{15}$$

With this expression one can calculate the electrophilicity change associated with the formation of AB, that is[69]

$$\Delta\omega = \omega_{AB} - \omega_A - \omega_B = \frac{\mu_{AB}^2}{2\eta_{AB}} - \frac{\mu_A^2}{2\eta_A} - \frac{\mu_B^2}{2\eta_B}$$
$$= -\frac{1}{2}\frac{(\mu_A - \mu_B)^2}{\eta_A + \eta_B} \tag{16}$$

where eq 15 has been used. Comparing eq 16 with eq 10 one has that $\Delta_{CT}^\circ = -\Delta\omega$, which means that the ionic contribution to the bond energy, when approximated through the charge transfer model, is given by the total electrophilicty change associated with the formation of AB, from A and B. This fact also supports, partially, the identification of electrophilicity with electronegativity, because since electrophilicity is associated with an energy change that results from a charge transfer process, one can infer from eq 16 that the amount of charge transferred from one species to the other will be the one that minimizes the electrophilicity change, since eq 10 corresponds to the minimum energy change that results from the charge transferred, given by eq 11.

That is, according to eq 1, the additional stability of the bond between atoms A and B comes from the charge transferred between them. From it, Pauling proposed, through eq 2, that the charge will be transferred from the less electronegative atom to the more electronegative atom, and that the stabilization energy resulting from this charge transfer could be approximated by the square of the difference of electronegativities of A and B. Later, Sanderson[70,71] complemented the electronegativity concept by postulating that the equilibrium is reached when the electronegativities of A and B are equal to each other, and equal to the electronegativity of the molecule AB.

However, one could also think directly in terms of the energy change, because Δ° has energy units. In this context, one could consider that the maximum additional stability should correspond to the case when Δ° reaches a maximum. Since electrophilicity has energy units, that measure the stabilization associated with the maximum amount of charge that a given species can accept, one can expect, first, that the charge will be transferred from the less electrophilic atom to the more electrophilic atom, because the second one has greater capacity to accept charge, and, second, that according to eq 16, the maximum stabilization occurs when the electrophilicity change reaches a minimum. This last result is in agreement with the minimum electrophilicity princi-ple,[27,55–57,59,60,62] which states that atoms and molecules tend to reduce their electrophilicity during a chemical process. On the other hand, from the perspective of Mulliken's electronegativity, the amount of charge transferred is the one that equalizes the chemical potentials of A and B.

3. CONCLUDING REMARKS

In the present work, it has been established that the framework provided by the density functional theory of chemical reactivity, allows one to discuss in a unified way the approaches to the concept of electronegativity developed by Pauling and by Mulliken.

Thus, we have seen that since the original definitions, the Pauling approach is based on the ionic contribution to the bond energy, while the Mulliken approach is centered more on the capacity of a given species to accept or to donate charge. That is, in the first case the concept is associated with an energy difference between two interacting species, while in the second case it is associated with a response function of an isolated species (the derivative of the energy with respect to the number of electrons). In fact, through the generalization of the original idea of Mulliken expressed in eq 4, the chemical potential (minus the electronegativity) may be taken to be a measure of the intrinsic strength of a Lewis acid or base.[26]

An important aspect that arises from these two definitions is related with the absolute nature of χ_M, because it refers to an intrinsic property of the isolated species, and the relative nature of χ_P, because it refers to a property that involves two species, so that if one is going to make a comparison among a large group of systems, one needs to fix all the values in relation to a reference system. It is in this context that the derivation in this work of eq 10, strongly suggests that the reference system could be an ideal bath, which leads to the association of χ_P with the electrophilicity index. However, the relative nature of χ_P is highly significant from the chemical viewpoint and should always be considered, because the behavior of a given species A is going to be influenced by the nature of the interacting partner B, a situation that is recognized in eq 10.

In summary, when one analyzes the ionic contribution to the bond energy in the framework provided by the simple charge transfer model expressed in eq 6, which stands on two fundamental concepts, μ and η, one is led to eq 10 and to eq 12, which reflect that the concept of electronegativity originally expressed by Pauling could be considered as a property that depends on the chemical potential and the hardness and that it is closely related to the electrophilicity index. Meanwhile, the definition of electronegativity proposed by Mulliken only depends on the chemical potential.

■ ASSOCIATED CONTENT

ⓢ Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jpca.9b07468.

> Values of Pauling's electronegativity, chemical potential, and chemical hardness for the atoms involved in the diatomic molecules considered, plus values of the experimental dissociation energy of the species in Figure 1, and a table of the values of the quantities involved in Figures 1 and 2 (PDF)

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