

Polarity of a dative bond. Donor and acceptor electronegativities

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Abstract

The polarity of a dative bond between identical atoms can not be explained based on the usual electronegativities. If we assume identical electronegativities for both bonded atoms, the atom charges (using the absolute value of the electron charge as unity) will be the formal charges, i.e. -1 for the acceptor atom and $+1$ for the donor atom. This involves an abnormally high polarity for a covalent bond. A procedure to calculate donor and acceptor electronegativities to obtain a more realistic description for the charge transfer in a dative bond is proposed, where donor electronegativities are greater than acceptor electronegativities. Then, even in the case of a dative bond between identical atoms, the shared electron pair is "closer" to the donor atom. These new electronegativities can be used to calculate partial charges by a procedure suitable for undergraduate chemistry courses.

Resumen (Polaridad de un enlace dativo. Electronegatividades dadoras y receptoras)

La polaridad de un enlace dativo entre átomos idénticos no puede ser explicada con base en las electronegatividades usuales. Si suponemos que ambos átomos tienen la misma electronegatividad, las cargas atómicas serán (tomando como unidad el valor absoluto de la carga del electrón) las cargas formales; esto es: -1 para el átomo receptor y $+1$ para el átomo dador. Esto implica una polaridad anormalmente alta para un enlace covalente. En este trabajo se

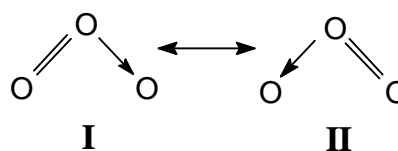
propone un cálculo de electronegatividades dadoras y receptoras que nos permite obtener una descripción más realista de la transferencia de carga en un enlace dativo, donde las electronegatividades dadoras son mayores que las receptoras, de manera que, incluso en el caso de un enlace dativo formado por átomos del mismo elemento, el par electrónico compartido está más "cerca" del átomo dador. Estas nuevas electronegatividades pueden ser usadas para calcular cargas atómicas parciales mediante un procedimiento apropiado para cursos de Química de pregrado.

Introduction

In a dative bond between two atoms the shared electron pair is contributed by one of the bonded atoms. The later is named as donor atom and the former as the acceptor atom.

Dative bonds can be involved in the description of one or more bonds in a molecule and, sometimes, as in the case of coordination compounds (Haaland, 1989), they can represent the main contribution for a bond.

The polarity of a dative bond between identical atoms can not be explained based on the usual electronegativities. If we assume the same electronegativity for the bonded atoms, the atom charges (using the absolute value of the electron charge as unity) will be the formal charges, i.e. -1 for the acceptor atom and $+1$ for the donor atom. This involves an abnormally high polarity for a covalent bond. For example, the valence bond theory describes the ozone molecule (O_3), as a resonance hybrid between, mainly, the following contributing structures



Each structure **I** and **II** has the same contribution and involves a double bond and a dative bond, the last

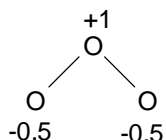
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depicted as an arrow with the tip directed to the acceptor atom (also, a common representation is $O(\text{donor})^+ - O(\text{acceptor})^-$, in which the formal charges are denoted). If equal electronegativities for all oxygen atoms is assumed, the atom charges of O_3 molecule, averaged by resonance, will be



which involve (taking $d_{O-O} = 1.278 \text{ \AA}$ and $O-\hat{O}-O = 116.8^\circ$ [Lide, 1996-97] a dipole moment of 3.21 D, much greater than the observed dipole moment (0.534 D [Lide, 1996-97]).

In a dative bond between atoms of the same element, although its polarity is qualitatively indicated by formal charges, the electron pair can not be equally shared. In general, schemes of partial charges calculation ignore this feature. On the other hand, an specific observation on this subject was made by Smith (1990), who proposes to replace a dative bond by an “ordinary” covalent bond (i.e. when the electron pair is formed by the contribution of one electron per atom) and then replace acceptor and donor atoms with more electronegative and less electronegative atoms, respectively, for charges calculation. However, this correction should be not necessary if the following hypothesis is true:

“through a dative bond between atoms of the same element, donor atom has greater electronegativity than acceptor atom”

The aim of this work is to obtain a foundation to support this hypothesis and analyze its consequences.

Discussion

The hypothesis stated here also involves the possibility for a bonded atom to have different electronegativities for each bond. This is related with the concept of orbital electronegativity (Hinze and Jafé; 1962; Hinze et al., 1963). In the case of O_3 , the central oxygen in, for example, contributing structure **I**, is bonded to the left oxygen by one sigma bond and one pi bond, and to the right oxygen, by one sigma dative bond. Then, in structure **I**, left oxygen has associated two different electronegativities (sigma and pi), central oxygen has associated three different electronegativities (sigma, pi, and sigma-donor), and

right oxygen is involved with only one electronegativity (sigma-acceptor). In general, considering only the participation of s and p orbitals, all possible electronegativities will be, sigma: X^σ , sigma-donor: $X^{\sigma d}$, sigma-acceptor: $X^{\sigma a}$, pi: X^π , pi-donor: $X^{\pi d}$, pi-acceptor: $X^{\pi a}$.

The advanced treatment (Hinze and Jafé; 1962; Hinze et al., 1963; Bergmann y Hinze, 1987; Bergmann y Hinze, 1996), based on the definition of electronegativity as an electrical potential (Bergmann y Hinze, 1987), allows to set out orbital electronegativity as a function of orbital charge, $X(q)$. Three values are of interest: for an orbital with one electron ($q = -1$), for an empty orbital ($q = 0$) and for a fully occupied orbital ($q = -2$). Values given for $X(q = -1)$ are well correlated with the values of electronegativity, such as Pauling and Mulliken scales (in particular, $X(q = -1)$ is identical with Mulliken definition; eq 2 below). As stated in Bergmann y Hinze (1996), $X(0)$ is the potential of an empty orbital to attract electrons and $X(-2)$ is the potential to withhold electrons. In this sense, $X(q = 0)$ and $X(q = -2)$ should be equivalent to X^a and X^d , respectively. However, calculations performed from the respective formulations (Hinze et al., 1963; Bergmann y Hinze, 1987; Bergmann y Hinze, 1996), show that for an orbital of one element $X(q = -2)$ is lower than $X(0)$, which is against the hypothesis proposed here. Therefore, donor and acceptor electronegativities in the context of the present work must be calculated by an alternative procedure.

Calculation of X^a and X^d

From Pauling's definition (Pauling, 1960), electronegativity is the power of one atom (an orbital in the present case) in a molecule to attract electrons to itself. For non-dative bonds this attraction is exerted on the electron pair formed by contribution of both bonded atoms. For dative bonds, *donor electronegativity (X^d) must measure the attraction by the donor atom on its initially lone electron pair, and acceptor electronegativity (X^a) must measure the attraction by the acceptor atom on the initially lone electron pair of donor atom*. Then, it could be suggested, for an atom in the appropriate valence states, the following relationships holds

$$X^{\sigma d} > X^\sigma > X^{\sigma a}$$

and/or

$$X^{\pi d} > X^\pi > X^{\pi a}$$

(1)

Inequalities 1, if right, should validate the stated

hypothesis because $X^{\sigma d} > X^{\sigma a}$ (or $X^{\pi} > X^{\pi a}$). From this last qualitative vision, a formulation to calculate acceptor and donor electronegativities can be made. As a starting point, the conceptual base given by the Mulliken formulation will be considered. Mulliken electronegativity, X_M is given by (Bergmann y Hinze, 1987).

$$X_M = (I + EA)/2 \quad (2)$$

where I and EA are the ionization energy and electron affinity (in eV), respectively, with the signs convention shown in fig. 1.

Eq 2 allows the calculation of orbital electronegativities for different valence states. In the case of a non-dative bond, Eq 2 measures the average attraction of a singly occupied orbitals towards one electron. The application of Eq 2 to orbitals involved in a dative bond, is possible for a donor atom as single-positive ion and for an acceptor atom, as a single-negative ion, because for both cases the orbitals are singly occupied. This choice of valence states for donor and acceptor orbitals not only allows the application of Eq 2, but is also reasonable: the polarity of a non dative bond $A-B$ could be associated to a charge transference from a starting state in which the electron pair is equally shared. This involve both A and B atom as initially neutral species and their electronegativities will control the charge transference. For a dative bond $A \rightarrow B$, the starting state of equally shared electron pair involve A^+ and B^- species. Then the charge transference will depend on the electronegativity of each ion.

Therefore, the electronegativities for both donor and acceptor orbitals, that involve a valence state singly occupied, will be given by¹

$$X_M^d = (I^+ + EA^+)/2 = (I^+ + I^0)/2 \quad (3)$$

$$X_M^a = (I^- + EA^-)/2 = (EA^0 + EA^-)/2 \quad (4)$$

where superscripts 0, + and -, refer to neutral, single-positive and single-negative atoms, respectively. (In eqs 3 and 4 the equalities $EA^+ = I^0$, $I^- = EA^0$ were also used.) Figure 2 represents each of quantities involved in eqs 3 and 4.

The calculation of each quantity contained in

¹ Donor and acceptor electronegativities should be symbolized $X_M^{d(+1)}$ and $X_M^{a(-1)}$ to denote the charges of involved species. However, to simplify the notation, this feature will be not included in symbols for electronegativity.

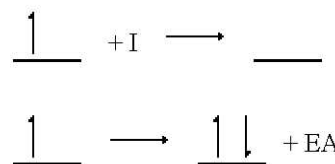


Figure 1. Definition of ionization potential and electron affinity through the usual representation of orbital electronic configuration.

eqs 3 and 4 (see Appendix) can be performed, for several valence states, from tabulated data of ground ionization potentials and electron affinities (I_g and EA_g) and the appropriate promotion energies (Hinze et al., 1963; Bergmann y Hinze, 1987; Bergmann y Hinze, 1996). However, data of EA_g^- for most of elements is not available. Moreover, the electron affinity of a single-negative ion can correspond to an endothermic process and with an absolute value greater than the electron affinity for neutral atom. As expressed by Eq 4, for these cases, acceptor electronegativity would be negative. In order to overcome this problem, and taking into account that electron affinity of a single-negative ion could be affected by an important error, preferably should be considered $EA^- = 0$ for all valence states.

In Table 1, computed values of donor and acceptor electronegativities are presented along with traditional electronegativities, X^{σ} , and π electronegativities, X^{π} (averaged values after Bergmann y Hinze, 1987). Hereinafter Pauling units are used. From Table 1 it can be seen that all values are in

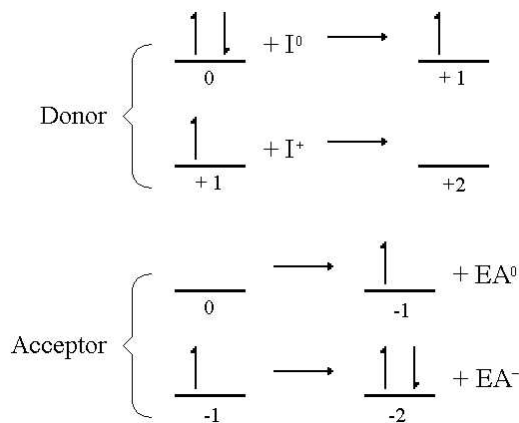


Figure 2. Definition of ionization potentials and electron affinities involved in eqs 3 and 4 (for each configuration the atom charges are also indicated).

Table 1. All kinds of electronegativities for some elements.

| | | | | | | | | |
|--|--|--|--|--|--|--|--|--|
| $\begin{matrix} X^{\sigma d} & X^{\sigma} & X^{\sigma a} \\ X^{\pi d} & X^{\pi} & X^{\pi a} \end{matrix}$ | | | $\begin{matrix} & & H^+ \\ - & - & 2.20 \\ - & - & - \end{matrix}$ | | | $\begin{matrix} & & H \\ - & 2.20 & - \\ - & - & - \end{matrix}$ | | |
| $\begin{matrix} & B & & & C & & & N & & & O & & & F \\ - & 2.04 & 0.51 & - & 2.55 & - & 7.70 & 3.04 & 1.28 & 9.22 & 3.44 & 1.52 & 11.3 & 3.98 & - \\ - & - & - & - & 1.81 & 0.19 & 6.17 & 2.60 & 0.50 & 7.49 & 3.15 & - & 8.75 & - & - \end{matrix}$ | | | $\begin{matrix} & & P & & S & & & Cl \\ - & 1.61 & 0.53 & - & 5.84 & 2.19 & 0.61 & 6.42 & 2.58 & 0.99 & 7.17 & 3.16 & - \\ - & - & - & - & 4.77 & 2.35 & 0.38 & 5.36 & 2.37 & - & 5.92 & - & - \end{matrix}$ | | | | | |

agreement with inequalities 1, then *starting hypothesis*, $X^d > X^a$, is verified for both, σ and π orbitals.

Noble gases

In agreement with the exposed, the only electronegativity that can be defined for noble gases is a donor electronegativity. Although these values were not used in the present work, is interesting to mention that Eq 3 is exactly the same expression proposed by Mee k (1995) for the calculation of electronegativities, in Mulliken Scale, for single charged cations of noble gases.

Ozone revisited

In the light of the obtained results we can again analyze the ozone molecule. The working hypothesis was elaborated from the requirement that, in a dative bond, donor atom must exert a resistance to the electronic transfer to the acceptor atom that results in a lower polarity than predicted considering donor and acceptor electronegativities as equal. This must be reflected in atom charges. Therefore Oxygen electronegativities X^d and X^a can be used in any appropriate scheme of partial charges calculation that accounts for each bond. For instance, Allen (1989) has proposed a simple formula suitable for this goal which is expressed as

where Q_A is the partial charge on atom A, that has

$$Q_A = (VE)_A - (LPE)_A - 2 \sum_i \frac{X_A}{X_A + X_i} \quad (5)$$

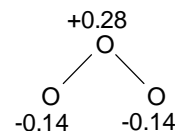
$(VE)_A$ valence electrons and $(LPE)_A$ lone pair electrons in the molecule, X_A is the electronegativity of A and X_i is the electronegativity of the atom bonded to A through the i th bond. The application of Eq 5 to, for example, the contributing hybrid I of ozone, gives for the partial charges on left (Q_{OL}), central (Q_{OC}) and right (Q_{OR}) oxygens, the following values

$$Q_{OL} = 6 - 4 - 2 \left(\frac{X_{OL}^{\sigma}}{X_{OL}^{\sigma} + X_{OC}^{\sigma}} + \frac{X_{OL}^{\pi}}{X_{OL}^{\pi} + X_{OC}^{\pi}} \right) = 6 - 4 - 2 \left(\frac{3.44}{3.44 + 3.44} + \frac{3.15}{3.15 + 3.15} \right) = 0$$

$$Q_{OC} = 6 - 2 - 2 \left(\frac{X_{OC}^{\sigma}}{X_{OC}^{\sigma} + X_{OL}^{\sigma}} + \frac{X_{OC}^{\pi}}{X_{OC}^{\pi} + X_{OL}^{\pi}} + \frac{X_{OC}^{\sigma a}}{X_{OC}^{\sigma a} + X_{OL}^{\sigma a}} \right) = 6 - 4 - 2 \left(\frac{3.44}{3.44 + 3.44} + \frac{3.15}{3.15 + 3.15} + \frac{9.22}{9.22 + 1.52} \right) = +0.283$$

$$Q_{OR} = 6 - 6 - 2 \left(\frac{X_{OR}^{\sigma a}}{X_{OR}^{\sigma a} + X_{OC}^{\sigma d}} \right) = 6 - 6 - 2 \left(\frac{1.52}{1.52 + 9.22} \right) = -0.283$$

The oxygen charges averaged by resonance between contributing structures I and II will be



which involve a dipole moment of 0.90 D. This calculation using donor and acceptor electronegativities allows the estimation of dipole moment for ozone which does not exaggerate its polarity, as should be using usual electronegativities. In this calculation the contribution of free electron pairs was not took into account, because there is no available data to incorporate it as a correction (a dipole associated to free electron pairs of the order of 1/2 Debye should be required to obtain the correct value for dipole moment of ozone).

Other examples

Partial charges calculation through Eq 5 will be performed for two molecules with dative bonds: the coordination compound $\text{H}_3\text{N} \rightarrow \text{BH}_3$ and N_2O .



$$Q_{\text{H}(\text{bonded to N})} = 1 - 0 - 2 \left[\frac{X_{\text{H}}^{\sigma}}{X_{\text{H}}^{\sigma} + X_{\text{N}}^{\sigma}} \right] = +0.160$$

$$Q_{\text{H}(\text{bonded to B})} = 1 - 0 - 2 \left[\frac{X_{\text{H}}^{\sigma}}{X_{\text{H}}^{\sigma} + X_{\text{B}}^{\sigma}} \right] = -0.038$$

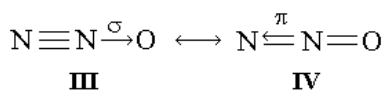
$$Q_{\text{N}} = 5 - 0 - 2 \left[\frac{X_{\text{N}}^{\sigma}}{X_{\text{N}}^{\sigma} + X_{\text{H}}^{\sigma}} + \frac{X_{\text{N}}^{\sigma}}{X_{\text{N}}^{\sigma} + X_{\text{H}}^{\sigma}} + \frac{X_{\text{N}}^{\sigma}}{X_{\text{N}}^{\sigma} + X_{\text{H}}^{\sigma}} + \frac{X_{\text{N}}^{\sigma\text{d}}}{X_{\text{N}}^{\sigma\text{d}} + X_{\text{B}}^{\sigma\text{a}}} \right] = -0.357$$

$$Q_{\text{B}} = 3 - 0 - 2 \left[\frac{X_{\text{B}}^{\sigma}}{X_{\text{B}}^{\sigma} + X_{\text{H}}^{\sigma}} + \frac{X_{\text{B}}^{\sigma}}{X_{\text{B}}^{\sigma} + X_{\text{H}}^{\sigma}} + \frac{X_{\text{B}}^{\sigma}}{X_{\text{B}}^{\sigma} + X_{\text{H}}^{\sigma}} + \frac{X_{\text{B}}^{\sigma\text{a}}}{X_{\text{B}}^{\sigma\text{a}} + X_{\text{N}}^{\sigma\text{d}}} \right] = -0.011$$

The calculated charges involve a transfer of $0.12e^-$ from N to B, about half the value predicted by quantum mechanics calculation (Haaland, 1989) ($0.20e^-$), but better than the calculated value with Eq 5 ($0.80e^-$) considering, for N and B and for all bonds, their conventional electronegativities.



Nitrous oxide is one of the molecules used by Allen (1989) to test his formulation for atom charge calculation (Eq 5). N_2O molecule is depicted as the resonance hybrid



with III weighted twice IV (Allen, 1989). Then σ and π -dative bonds will contribute to the real N_2O structure. It is interesting to compare Allen (1989) results ($\text{N}^{-0.33} \text{N}^{+1.10} \text{O}^{-0.77}$) with the calculation through Eq 5, including the corresponding donor and acceptor electronegativities ($\text{N}^{-0.05} \text{N}^{+0.32} \text{O}^{-0.27}$). The latter calculation avoid the overestimation of charges

on O and central N associated to an excessive charge transfer from donor N to acceptor atoms.

Conclusion

The definitions of donor and acceptor electronegativities (eqs 3 and 4) give values (Table 1) that allow generalize the following observation: *donor orbital electronegativities are greater than acceptor orbital electronegativities, even in the case of orbitals of the same element.* Donor and acceptor electronegativities could be used in any appropriate schemes for partial charges calculation. In particular, the introduction of these electronegativities in Allen formulation (Eq 5) allows to obtain reasonable partial charges in molecules with dative bonds by a procedure suitable for instruction at undergraduate chemistry courses.

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APPENDIX

Ionization energies and electron affinity calculations

For an atom valence state, "v", the ionization energy (I_v) and the electron affinity (EA_v) are given by

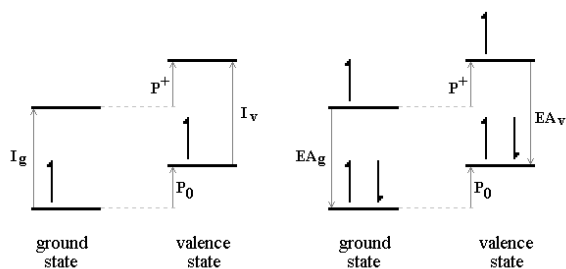


Figure A1. Electronic transitions corresponding to eqs A1 and A2.

$$I_v = I_g + P^+ - P_0 \quad (A1)$$

$$EA_v = EA_g + P_0 - P^- \quad (A2)$$

Where subscript “g” refers to the ground state, and P_0 , P^+ and P^- are the promotion energies of neutral atom, single-positive ion and single-negative ion, respectively. Values for I_g and EA_g are currently tabulated on textbooks. Figure A1 schematizes the electronic transitions that explain eqs A1 and A2. Values for promotion energies are tabulated in Hinze and Jafé (1962).

As expressed in the main text, in order to calculate donor and acceptor electronegativities, only I_v^0 , I_v^+ and EA^0 must be known. The expression to calculate I_v^+ , is (by analogy with Eq A1)

$$I_v^+ = I_g^+ + P^{++} - P^+ \quad (A3)$$

Nomenclature for a given valence state

Abbreviations di, tr and te, represent sp , sp^2 and sp^3 hybrids, respectively. Also, p_σ , and s orbitals are denominated σ and p_π orbitals are named as π . Then the valence state for nitrogen in NH_3 , HNO_3 , $N \equiv CH$, are, $te^2tetete$, $tr^{2trtr\pi}$ y $di^2di\pi\pi$, respectively

Main valence state for nonmetallic elements

Electronic affinities and ionization energies can be calculated for a wide number of valence states. Therefore, it will be useful to obtain representative values for σ and π orbitals. That estimation can be made averaging on values corresponding to the main valence states. Table A1 summarizes the relevant valence states and shows a representative molecule for each state.

Table A2 shows the calculated donor and acceptor and electronegativities for the valence states consigned in table A1. Table A3 shows the average electronegativities values.

Table A1. Representative valence states.

| Element | Valence state | Example molecule | Element | Valence state | Example molecule |
|----------------|-------------------|------------------|---------|--------------------|------------------|
| H ⁺ | \underline{s}^0 | | N (P) | $trtrtr\pi^2$ | |
| B (Al) | $tetetete^0$ | | O (S) | $te^2te^2te^2te^0$ | |
| C | $di^2di\pi\pi^0$ | | O (S) | $tr^2tr^2t\pi$ | |
| C | tr^2trtr^0 | | O (S) | te^2te^2tete | |
| N (P) | $te^2te^2tete^0$ | | O (S) | $di^2di\pi\pi^2$ | |
| N (P) | $tr^2tr^2tr\pi^0$ | | O (S) | $tr^2trtr\pi^2$ | |
| N (P) | $di^2di\pi\pi$ | | F (Cl) | $tr^2tr^2tr^2\pi$ | |
| N (P) | $te^2tetete$ | | F (Cl) | $te^2te^2te^2te$ | |
| N (P) | $di^2tr\pi^2$ | | F (Cl) | $s^2p^2p^2p$ | |

Table A2. Calculated donor and acceptor electronegativities (Mulliken scale)

| Element | Valence state* | I ^o /eV | I ⁺ /eV | EA ^o /eV | X _M ^d /eV (eq 3) | X _M ^a /eV (eq 4)** |
|------------------|--|--------------------|--------------------|---------------------|--|--|
| H ⁺ § | <u>s</u> ^o | 13.6 | – | 0.75 | – | 7.18 |
| B | <u>tetete</u> ^o | – | – | 3.37 | – | 1.68 |
| Al | <u>tetete</u> ^o | – | – | 3.48 | – | 1.74 |
| C | <u>di²diππ</u> ^o | – | – | 1.22 | – | 0.61 |
| C | <u>tr²trtr</u> ^o | – | – | 1.28 | – | 0.64 |
| N | <u>te²te²te</u> ^o | – | – | 8.49 | – | 4.24 |
| N | <u>tr²tr²tr</u> ^o | – | – | 3.31 | – | 1.66 |
| N | <u>di²diππ</u> | 17.24 | 37.02 | – | 27.13 | – |
| N | <u>te²te²te</u> | 14.14 | 33.31 | – | 23.72 | – |
| N | <u>di²diππ²</u> | 12.06 | 28.72 | – | 20.39 | – |
| N | <u>trtrtr</u> ² | 11.96 | 28.72 | – | 20.34 | – |
| P | <u>te²te²te</u> ^o | – | – | 4.01 | – | 2.00 |
| P | <u>tr²tr²tr</u> ^o | – | – | 2.47 | – | 1.24 |
| P | <u>di²diππ</u> | 14.04 | 26.94 | – | 20.49 | – |
| P | <u>te²te²te</u> | 12.09 | 24.03 | – | 18.06 | – |
| P | <u>di²diππ²</u> | 10.95 | 20.62 | – | 15.78 | – |
| P | <u>trtrtr</u> ² | 10.76 | 20.61 | – | 15.68 | – |
| O | <u>te²te²te²te</u> ^o | – | – | 10.07 | – | 5.04 |
| O | <u>tr²tr²trπ</u> | 20.15 | 42.53 | – | 31.34 | – |
| O | <u>te²te²te</u> | 18.70 | 40.35 | – | 29.52 | – |
| O | <u>di²diππ²</u> | 15.24 | 34.22 | – | 24.73 | – |
| O | <u>tr²trtr</u> ² | 15.30 | 34.12 | – | 24.71 | – |
| S | <u>te²te²te²te</u> ^o | – | – | 6.55 | – | 3.28 |
| S | <u>tr²tr²trπ</u> | 14.38 | 29.06 | – | 21.72 | – |
| S | <u>te²te²te</u> | 13.64 | 27.73 | – | 20.68 | – |
| S | <u>di²diππ²</u> | 11.51 | 23.77 | – | 17.64 | – |
| S | <u>tr²trtr</u> ² | 11.64 | 23.82 | – | 17.73 | – |
| F | <u>tr²tr²tr²π</u> ## | 28.75 | 51.19 | – | 39.97 | – |
| F | <u>te²te²te²te</u> # | 23.43 | 45.41 | – | 34.42 | – |
| F | <u>s²p²p²p</u> | 18.11 | 39.64 | – | 28.88 | – |
| Cl | <u>tr²tr²tr²π</u> ## | 19.28 | 30.77 | – | 25.02 | – |
| Cl | <u>te²te²te²te</u> # | 16.31 | 28.26 | – | 22.28 | – |
| Cl | <u>s²p²p²p</u> | 13.34 | 25.75 | – | 19.54 | – |

The involved orbital is underlined. **Assuming EA⁻ = 0 (see text). # Calculated as $[I(s) + 3I(p)]/4$. ## Calculated as $[I(s) + 2I(p)]/3$.

§ For H⁺, eq 4 must be replaced by $X_M^a = (I^0 + EA^0)/2$, which agree with current H electronegativity.

Table A3. Averaged (sigma and pi) donor and acceptor electronegativities.

| Element | Orbital | X _M ^d /X ^{d*} | X _M ^a /X ^a | Element | orbital | X _M ^d /X ^d | X _M ^a /X ^a |
|----------------|---------|--|---|---------|---------|---|---|
| H ⁺ | σ | – | 7.18/2.20 | P | π | 15.73/4.77 | – |
| B | σ | – | 1.68/0.51 | O | σ | – | 5.04/1.52 |
| Al | σ | – | 1.74/0.53 | O | σ | 30.43/9.22 | – |
| C | π | – | 0.62/0.19 | O | π | 24.72/7.49 | – |
| N | σ | – | 4.24/1.28 | S | σ | – | 3.28/0.99 |
| N | π | – | 1.66/0.50 | S | σ | 21.20/6.42 | – |
| N | σ | 25.42/7.70 | – | S | π | 17.68/5.36 | – |
| N | π | 20.36/6.17 | – | F | σ | 37.20/11.27 | – |
| P | σ | – | 2.00/0.61 | F | π | 28.88/8.75 | – |
| P | π | – | 1.24/0.38 | Cl | σ | 23.65/7.17 | – |
| P | σ | 19.28/5.84 | – | Cl | π | 19.54/5.92 | – |

X_M: Mulliken scale. X: Pauling scale ($X = 0.303X_M$ (Bergmann y Hinze, 1996)).

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CONFERENCIA DE QUÍMICA

Teatro Heredia, Santiago de Cuba, Cuba, 7-9 de diciembre 2005

El departamento de Química de la Universidad de Oriente se complace en invitar a esta Conferencia. El programa científico incluye conferencias magistrales, conferencias plenarias, exhibición de carteles, mesas redondas y talleres.

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ENVÍO DE RESÚMENES Y TRABAJOS

Las comunicaciones cortas, así como los trabajos completos (estos últimos si se desea que sean publicados en las memorias electrónicas del Congreso), **deberán enviarse a la dirección electrónica de los secretarios de cada temática, el 15 DE MAYO** si se trata de una comunicación corta y **el 30 DE SEPTIEMBRE** si es un trabajo completo, indicando en el asunto la sesión a la que corresponde el trabajo.

El Comité Científico hará la selección de resúmenes y trabajos y enviará la aceptación hasta el **20 DE JULIO del 2005**.

El formato para enviar la comunicación corta se expone a continuación:

Una página (hoja carta 8.5 x 11")
Espaciado sencillo

Título (Mayúscula)
Autor (es)
Institución (es)
Dirección
Palabras clave
(Todo lo anterior escrito en:
Times New Roman 12)

Introducción
Reactivos, equipamiento y métodos empleados
Discusión de Resultados
Conclusiones
Bibliografía
(Todo lo anterior escrito en:
Times New Roman 10, y en dos columnas)

El formato para el trabajo completo se expone a continuación:

1. Todo el trabajo (revisión, artículo o comunicación corta) se deberá presentar en hojas tipo carta (8.5 x 11"), numeradas de forma consecutiva, a dos espacios. Las tablas, gráficos, notas al pie, etc. deberán presentarse por separado y se señalará en el texto el lugar de ubicación entre paréntesis.

2. El título lo más corto posible; la(s) inicial(es) de los nombres de los autores seguidas de punto y los apellidos, separados por comas, incluyendo su dirección de correo electrónico, de ser posible. El resumen del trabajo y cinco palabras claves que identifiquen el contenido del trabajo.

3. El texto del trabajo debe seguir la siguiente estructura: introducción, métodos experimentales (o metodología para los trabajos teóricos), resultados y discusión, y referencias. Los trabajos no deberán exceder de 15 cuartillas.

4. Las tablas y gráficos deberán presentarse con la herramienta Excel (Windows), y se numerarán de forma consecutiva con números arábigos (1, 2, 3) junto con el pie de figura.

5. Las reglas de nomenclatura de la Unión Internacional de Química Pura y Aplicada (IUPAC) deberán ser aplicadas en todos los trabajos. Cuando se mencione por primera vez en el texto un nombre trivial, se deberá mencionar entre paréntesis el nombre IUPAC.

6. Las referencias deben citarse en el texto con un superíndice con menor puntaje y se numerarán de acuerdo con el orden de aparición. La bibliografía al final del trabajo deberá seguir el estilo siguiente: número de referencia, punto, apellidos, inicial(es) del nombre, seguidas de punto. En caso de más de cuatro autores, se pondrán hasta cuatro seguidos de *et al.*, título del artículo (en el idioma original y entre comillas), abreviatura de la revista (según nomenclatura de revistas internacionalmente aceptadas), volumen, raya de quebrado (*slash*), número, dos puntos, página inicial, guión, página final y año (entre paréntesis).

7. Ejemplo:

1. J.C. Elliot, G.R. Davis, P. Anderson, *et al.* "Application of laboratory microphotography to the study of mineralised tissues" *Anal. Química* 93/1:877-882 (1997).

FECHAS IMPORTANTES

Mayo 15, 2005

Solicitud de inscripción y envío de comunicaciones cortas

Julio 20, 2005

Aceptación de trabajos y comunicación a los autores

Septiembre 30, 2005

Envío de los trabajos completos

COSTOS DE INSCRIPCIÓN

Hasta el 30 de Septiembre / Después de 30 de Septiembre
Delegados \$200.00 \$250.00
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- Actividad final
- Materiales del evento

Costos de alojamiento (4 noches) en Santiago de Cuba

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- Alojamiento, desayuno y cena.
- Transportación de llegada y salida en Santiago de Cuba, y a las actividades del evento.

Para mayor información

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