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On Electron Motion and Resonance in Chemical and Biological Systems

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ABSTRACT

Widely studied molecular resonance forms reflect the fact that electron motion and regional shifts in position are rapid and predictable. Some resonance forms are stable regardless of wide extremes in environmental conditions, while others only exist in certain situations. Transient acetate and stable benzene resonance forms are examined to help characterize the motional behavior of electrons in molecules and the effects such motions have on chemical properties. chemical properties. Resonating electrons are of key importance in metabolism and for light absorption by plant chlorophyl.

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Introduction

It has long been known that chemical reactivity is dependent on the properties and behavior of electrons in molecules. Equilibrium chemistry dictates that equilibrium constants for reactions determine the eventual yield of product. But the speed at which this occurs is the subject matter of kinetics. Ironically any particular chemical reaction may be high yield and yet slow, or low yield and yet fast. All reactions in non-nuclear chemistry involve rearrangements of electrons. Analyzed here are molecules with electrons in distinct states of motion to demonstrate how resonance and structure relate to reactivity.

Methods

Bond energies and lengths, and atomic radii were obtained from [1]. Properties of benzene, acetic acid, acetate, and trifluoroacetic acid were from various sources [1-4].

Results/Discussion

At ambient, nonflammable temperatures, fluorocarbons and benzene are notable examples of extremely stable, nonreactive toxic substances. As for any chemical bond, the C-F bond is formed by electrons that are mobile in a molecular orbital cloud, but localized to allow the partially electron depleted carbon and partially electron rich fluorine nuclei to exist at a close distance. Although the bond is surprisingly relatively nonpolar, the shared electrons involved nevertheless tend to exist at any instant in time enriched over the fluorine atom due to its higher electron affinity than carbon. Moreover, the bond energy is the highest of the carbon halogen bonds at 453 kJ/mole, where C-Cl is 339 kJ/m, C-Br is 276 kJ/m, and C-I is 216 kJ/m. Because the fluorine atom is so tiny at a radius of 72 pm, the bond length is the shortest at 133 pm compared to C-Cl of 177 pm, C-Br of 194 pm and C-I of 213 pm (the radii for the other halogens are Cl at 100 pm, Br at 114, pm, and Iodine at 133 pm). Drugs containing C-F stable, unreactive bonds are not metabolized well by liver enzymes, so that C-F containing drug fragments accumulate long term in bodily lipid regions during chronic consumption.

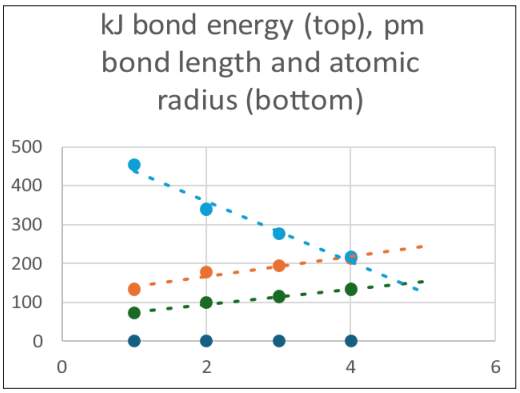

Figure 1: C-F, C-Cl, -C-Br, and C-I bond energies (kJ) are graphed as the top line, bond lengths (pm) are shown by the middle line, and atomic radii (pm) for the F, Cl, Br and I neutral atoms are shown with the bottom line

This demonstrates how electron configuration and density around atoms affects reactivity. The C-F bond is associated with electrons in a cloud region that is short in length and with somewhat more density on the fluorine atom than on carbon. This is based on the finding that C-F bonds in molecules are not readily water soluble and instead are relatively hydrophobic and lipid soluble and of relatively low polarity. This is caused by the facts that fluorine as a neutral atom has a higher electron affinity than carbon but is smaller in diameter (126 pm) than carbon (154 pm). In polar ionic compounds the fluoride anion is very much larger (272 pm) in diameter than in the covalently bonded atom in F_2 or C-F.

Benzene is a stable unreactive system for a very different reason, and that is the phenomenon referred to as resonance and aromaticity. The ring of carbon atoms consists of electron pairs forming single bonds between the atoms, as also exist in cyclohexane, with additional electrons that are delocalized in π bond clouds argued to form a ring current. The fact that the

polarity of benzene is zero suggests that these ring currents may resonate in opposite directions on opposite sides of the ring plane. It is important to note that the system at non-igniting temperatures exists in perpetuity with extreme stability because so much energy is required to withdraw resonating electrons, much like the difficulty of corralling an uncaged wild animal. Resonance forms such as this are insensitive to and unaffected by the environment, such as extremes in temperature, polarity, ionic strength, and acidity/basicity because of such electron freedom. Benzene is a dangerous substance with an LD_{50} of 3.8 ml/kg (density 0.8787 g/ml) and is a known certain carcinogen from chronic exposure [3]. Unfortunately, the flat planar ring structure inserts into the alpha helical coils of DNA. Although electrons being of the same negative charge exhibit repulsion among them, nevertheless the delocalized electron arrangement in benzene is known as an electron withdrawing group, where electrons from neighboring atoms shift toward the ring, compared to the more restricted electron arrangement in cyclohexane.

In contrast to the stable benzene ring, resonance in the carboxylic acids for example only exists when the group is de-protonated as the anionic carboxylate form. This only occurs in neutral or basic solutions. In acidic solutions, the conjugate intact acid form has no resonance delocalization and instead electrons travel in regional clouds enriched on the oxygen atoms, as discussed for the C-F example. The resonance again ensures stability of the anion, but at neutral pH only about 1% of the molecules are anions while 99% are intact acetic acid in spite of this resonance stability. This is an example of resonance that is determined by the environment, rather than the very stable resonance in benzene.

The benzene aromatic ring is so unreactive and stable that even at extremely harsh conditions, 1500 psi pressure (100 atm) and a high 150^{o} C temperature with a metal catalyst, the strongest oxidizing agent known, fluorine gas generated in a laboratory, forms only the substitution reaction product hexafluorobenzene, where the aromatic ring remains intact. The industrial process of hydrogenation under the above harsh conditions with finely divided metal catalysts can saturate the ring to form cyclohexane.

These examples demonstrate that electrons in molecules are very mobile in molecular orbital clouds, but are also regionally localized. It is not certain if electrons can exchange between localized regions, but electron motional speed is rapid in molecular orbital clouds. An earlier study reported that the average velocity of the single ground state electron in the hydrogen atom is estimated from the Bohr model at about 2.19×10^6 m/s or about 0.73% of the speed of light which compares favorably with the most probable velocity determined from quantum mechanics considerations [5]. In molecular orbital cloud regions, it is widely presumed that orbital lobes contain electron pairs that are relatively isolated from each other. For example, in methane the central carbon sp^3 hybridized lobes form a tetrahedral shape where each sp^3 lobe binds with hydrogen 1s lobes to form sigma single bonds. Whether or not these bonding electrons can interchange with each other is unclear but certainly possible. For resonating forms, electrons are less localized and are motional over wider domains among atoms.

It is usually argued that electrons forming bonds, whether resonating or not, do not exchange with each other between localized regions. For example, valence shell electron pair repulsion models of covalent molecules predict bond angles well and rely on the fact that electron pairs repel each other and are thus thought to remain within bonding or nonbonding domains. Evidence against such exchange is that the benzene ring is impervious to reduction under conditions where the hydrogen substitution reaction takes place, as though the resonating electrons only exist as a distinct system from those electrons in the sigma C-H bonds. In orbital hybridization theory it is assumed that electrons first in atomic orbitals that are well characterized become re-localized into hybridized bonding regions between two atoms. Protected nitroxide R-N-O molecules with a single unpaired electron in a p orbital exhibit electron spin resonance in an applied magnetic field during absorption of microwave radiation, where these states of little difference in energy are electrons that remain in the same molecular orbital. This is a 'micro-transition' compared to a transition of electrons between atomic energy levels. So, it is logical to assume that inner orbital electrons do not exchange with valence electrons on atomic or molecular surfaces under ambient environmental conditions. And that in molecules the bonding electrons should not interchange between bonds even among bonds having the same energy.

However, evidence for exchanging of electrons among bonding orbitals of similar energy in general are the facts that 1) quantum mechanics considerations indicate that there is a finite probability for an electron in an infinite potential energy well to exist outside that well, and of course 2) it is generally accepted that metal surfaces exist in what is considered a sea of valence electrons. Quantum mechanics probability calculations for the electron in atomic hydrogen are in agreement with this since the 1*s* orbital probability function overlaps to some degree with the 2*s* and 2*p* orbital functions while having of course distinct separate average energies. In a hydrogen molecule however, electron density spreads over the molecule where electrons have finite probability to be outside the H-H interatomic region. It is of interest that transition metal elements for example have color because even ambient visible light wavelengths are continuously absorbed that energize electrons into orbitals with more energy, causing a stable color [6].

In molecular systems, electrons are in a dynamic state of repulsion between each other, avoiding each other with changing electric force magnitude in time, while also continuously being attracted to the opposite charged nuclei with electrical attractive forces that continuously change in time as well. Two electrons can occupy the same spatial molecular coordinate but only at different times, while both electrons act together in any instant in time to form the bond. It should be emphasized that electron orbitals for example described well for the hydrogen atom, only exist if an electron is present in them. For a transition from the 1s to 2p orbital or vice versa, the orbital forms when the electron is present to form it, and the orbital the electron had existed in no longer exists after the transition. So high energy orbitals in atoms are able to be formed only if an electron is present to form them.

In fluoroacetate, the resonating electrons are shifted toward the high electron affinity fluorine atom, technically causing further delocalization. This results in fluoroacetic acid being a stronger acid ($pK_a = 2.6$) than acetic acid having a K_a of 1.8×10^{-5} Trifluoroacetic acid may be considered a strong acid ($pK_a = 0.3$ [3]). This indicates the relativity of electron delocalization which is modulated by the atomic structure around which the electrons travel. Fluoroacetic acid is the extremely toxic citric acid cycle blocking poison known as gifblaar with a lethal dose of about 2 mg/kg, found naturally South Africa in dichapetalum cymosium, one of the most poisonous plants [3].

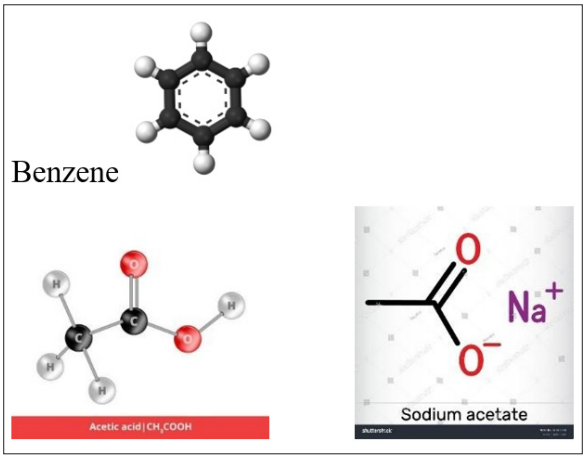

Figure 2: Models of the Molecular Structures for Benzene, Acetic Acid, and Acetate are Shown

Quantum mechanics principles dictate that electrons in atomic orbital regions are not only quantized but also reside in definable probability distributions. Although most of an atom is empty vacuum of space at any instant in time between the outer electron and the nucleus, the fast-moving electron can exist at any instant in time anywhere within that space cloud volume. When near the positive nucleus, its speed is fastest, and at the farthest regions of the cloud its speed is slowest. The force of attraction between the nucleus and the electron counter the centrifugal force due to its motion at all times, as the electron travels through the region in wave like states of motion. In a two-atom bond, the computations are much more difficult but it is held that electron pairs shield the repelling force between nuclei having the same positive charge while being attracted at the same time to those nuclei and also repelling each other having the same negative charge. The complex system involves constantly vibrating nuclei that generate infrared radiation while the electrons roam in mutually allowed spatial regions to maintain molecular stability. Three atom molecules are even more complex, where it is not clear if electron pairs between atoms forming a bond interchange or not with electrons forming the adjacent bond. If so, this would mean the electrons are already technically delocalized to some degree within the molecule. The difference between this state, and a molecule having resonance, may be the extent or speed with which this electron delocalization occurs.

The likelihood that electrons do interchange among atomic orbitals in a structure is supported by the quantum mechanics argument that electrons in infinite potential energy wells nevertheless have a nonzero probability of being outside the well. This should not be surprising since an infinitely impenetrable barrier cannot extend to an infinite distance in space. The question also remains whether covalent shared electrons among atoms can exchange with electrons in what are considered nonbonding orbitals. Two electron pairs in water form not only two O-H bonds but there are also two presumed nonbonding regions for two pairs as well. These likely have different energies, so an energy barrier exists to prevent or minimize exchange, but the idea that some exchange might exist is not overruled for the reasons just mentioned. In a molecule such as methane, CH_4, where all the sigma bonds between presumably hybridized carbon sp^3 lobes and 1s orbitals of the H atoms, any inter-bond exchange is not hindered in this way because each of the bonds have equal energy. On the other hand, the Pauli exclusion principle indicates that electrons can form bonds in pairs in a shared spatial domain only if spins are oriented oppositely, otherwise too much magnetic energy would be present. Also, electrons themselves repel each other, so these effects would combine to tend to minimize inter-bond exchange.

Resonance states involve systems with three or more atomic centers. Lewis dot structures readily predict which systems have resonance due to the fact that atomic arrangements are preferred by atoms according to the chemical family in which they belong. Ozone O_3 for example is a small resonating system.

For a typical four atom arrangement, the usual representation of resonance in acetate for example involves two canonical forms with electron motion diagrammed as follows. Here the two forms interconvert as shown by the arrows for electron pairs that shift from nonbonding to bonding orbital positions, indicating the electron resonance is quickly reversible between these states.

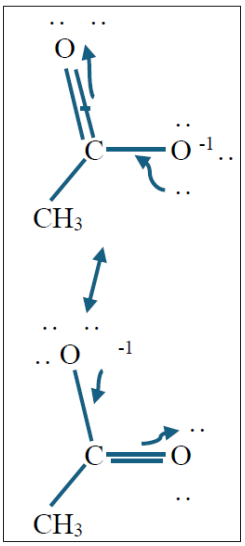

Figure 3: Traditional Resonance forms for the acetate anion are drawn with arrows representing next movements of electron pairs. Nonbonding electrons (shown as dots) drift into bonding regions on one oxygen while the reverse occurs on the other oxygen.

The formal charge on one oxygen atom is 6 - 2(2) - 2 = 0 and the other is 6 - 3(2) -1 = -1. Since both atoms are in reality equivalent, this representation incorrectly implies that a charge magnitude exists that is not actually real.

An improved representation of resonance in acetate might be as shown below where the rapidity with which electron motion occurs makes the bonds to both oxygens equivalent, in essence a bond and a half, with the negative partial charges also being equal on the oxygen atoms at any instant.

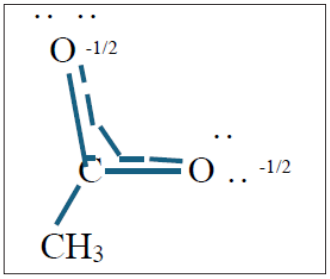

Figure 4: A proposed representation of the resonating electrons in the acetate anion is shown. Both oxygen atoms are effectively equivalent at any instant in time

Among the O-C-O region there are 6 + 6 + 3 electrons involved in bonding since one of four carbon electrons is shared with the other carbon. Formal charges for the equivalent oxygen atoms in this form are realistic and both the same, where six atomic electrons minus two lone pairs minus one bonding pair leaves, with an average overall charge of -1/2, a remaining -3/2 term (6 - 2(2) - 1 - 3/2 = -1/2). This suggests that the 3 remaining electrons in the system distribute equally among the O-C-O regional atoms forming effectively a one and a half C-O bond for both. This representation reflects that the three electrons are simply distributed so quickly that, being shared, each has an effective charge of -1/2 around each O atom so that 6 – 4 – 1 - 3(-1/2) = -1/2. So, studies with labeled oxygen should show that protonation of acetate with one labeled and one unlabeled oxygen should show equal protonation of both.

For the fluoroacetate anion in aqueous solution, which is the conjugate base of the strong acid, its reneutralization with a proton is difficult. This is represented by resonance forms being shifted so that electron concentration near the oxygen to be protonated is diluted, with a formal charge much less than either -1 shown in the first diagram or -1/2 in the improved version form. The entire system has the single overall negative charge distributed more equally along the entire molecule because of the electron withdrawing power of the fluorine atoms so that protonation of the anion is not favorable. This effect can only be represented with arrows indicating the relative drift of electrons so that unequal sharing occurs where electron density is withdrawn from carbon by the high electron affinity fluorine atoms that is partially replaced by electron density withdrawn from the oxygen atoms (Figure 5). For normal acetate, the electron density is largest around the oxygen atoms. In trifluoroacetate the electron density is still largest around the oxygen atoms that are attached to carbon directly, but is more diluted and less dense than before, where electrons have shifted toward the carbon atom since the fluorine atoms also cause electron density to be larger on the fluorine atoms than on hydrogen atoms. The resonating electrons still are still delocalized, but in a cloud shape skewed toward carbon more than for normal acetate.

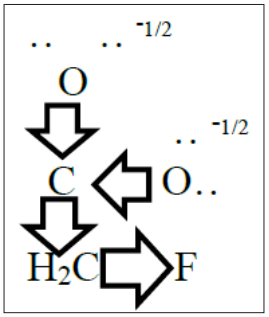

Figure 5: The fluoroacetate anion is represented as having electrons that are shifted toward the fluorine atoms. The electron density on the oxygen atoms is lessened by the shift of all electrons in the molecule spatially toward the fluorine atom. The overall negative charge remains negative one, equally distributed between the two identical oxygen atoms, but is in a skewed spatial region compared to that in normal acetate.

The bond energy of hydrogen gas, H-H, is 436 kJ/m (7.2 x 10^{-19} J per molecule), only somewhat less than its ionization energy at 1,312 kJ/m (21.6 x 10^{-19} J per electron) and is comparable to the electronic transition from the innermost n = 1 orbital to the n = 2 orbital, at 10.9 x 10^{-19} J per electron.

The oxidation of water to supply replacement electrons on chlorophyll has a potential of =-1.23 volts, for $2H_2O$ to $4H^+ + O_2 + 4e^-$. This is the same voltage for the electrolysis of water to hydrogen and oxygen gas.

The relation of free energy and voltage produces G = -nFE = 4(96485)(1.23) = 4.74 x 10^5 kJ/m which is 7.88 x 10^{-16} J per 4 electrons, or 1.97 x 10^{-19} J per electron. This compares favorably with the energy required to oxidize chlorophyll.

The energetics of photosystem II in plant photosynthesis suggest the light sensitive pathway that replenishes electrons for photosystem I may function as a biological photoelectric effect. The energy of a light photon of 680 nm wavelength is 2.93 x 10^{-19} J. The kinetic energy range computed for ejected electrons compares to the water oxidation energy. The precise electron that is removed from chlorophyll by light absorption is not known. Normally resonating electrons are most stable which would suggest the bonding electrons with higher energy would be released. However, light energy that is absorbed by an electron having the proper specific energy to cause light absorption could be even a resonating electron in this complex system.

The chloroplast is a miraculous system where red light has not only the proper energy required to eject chlorophyll electrons into the membrane transport chain, but also has a particular EM frequency $f = c/l$ = [3 x 10^8 m/s]/680 nm = 4.4 x 10^{14} Hz. This compares to the computed oscillation frequency for electrons in the chlorophyll planar ring system having a circumference C = 4.5 nm, where $f = 1/t = 0.0073c/C$ = 4.8 x 10^{14} Hz. These matching frequencies could explain why higher energy photons do not eject electrons from the ring, unlike the photoelectric effect where electrons are ejected by light at any frequency above a minimum threshold. Plants are known to be green because of the absorption of red light. Perhaps red is the color absorbed because of both these energy and frequency requirements.

Resonance can be pH dependent. So, the extent of resonance in amino acids, fatty acids, phospholipids, nucleic acids, and adenosine phosphates and other phosphates can differ between the highly alkaline intestines and slightly alkaline bloodstream versus the acidic stomach and cell cytoplasm. Amino acid carboxylic acid groups have pKa's ranging from 1.77 to 2.58 and are essentially fully dissociated at physiologic pH except in the acidic stomach at about pH 2-3. Fatty acid carboxylic groups and phospholipid phosphates are negative charged resonating systems, R-COO- and R-O-PO_3^{-2}, at physiologic pH. The inner surface of membrane bilayers is rich in phosphatidylserine making the inner layer more negatively charged with -2 charged phosphate and -1 charged serine carboxylate, while the outer layer is rich in phosphatidylcholine with only -1 charged phosphate.

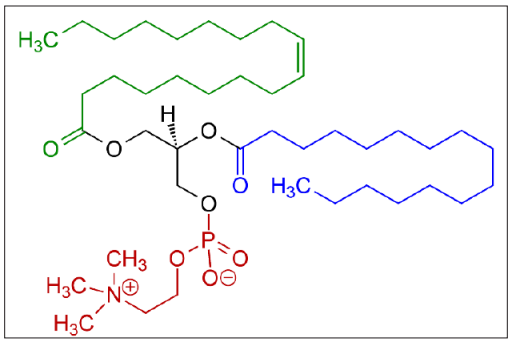

Figure 6: Molecular structure of phosphatidylcholine with one resonating negative charged phosphate group that is enriched in the outer leaflets of biologic cell bilayer membranes [3].

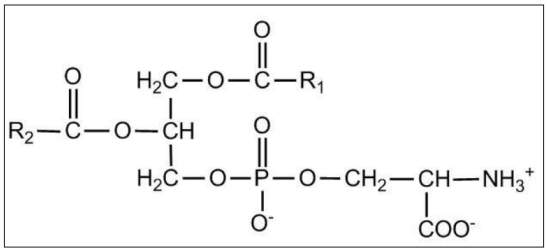

Figure 7: Molecular structure of phosphatidylserine with two resonating systems, the phosphate and carboxylate negative charged groups that is enriched in the inner membrane leaflets of biological cell membranes [3].

Calcium ion concentrations outside cells is in the 1 mM range, while intracellular levels are maintained at an extremely low micromolar range due to action of calcium ATPase pumps to prevent neutralizing inner membrane charges which decrease the fluidity of the lipid bilayer and can cause cell death. Magnesium ion concentrations are approximately 1 mM on both sides of the membrane in mammalian cells, but the affinity for phosphate is 10,000 times stronger for calcium than for magnesium, where the K_{sp} for Ca_3PO_4 is 2 x 10^{-29} and for Mg_3PO_4 is 2 x 10^{-25} [7,8]. These stable resonating systems are essential for proper membrane function.

Biologically, the most important resonating system is the phosphate produced from ATP hydrolysis that drives otherwise unfavorable coupled reactions to proceed. Adenosine triphosphate hydrolysis produces energy required for virtually all biologic systems to function. Here, ATP → ADP + Pi + 69 kJ/mole energy or 1.1 x 10^{-19} J per molecule. This is comparable to the energy in a photon of infrared light. Most of the ATP utilized in any given day is used to drive cell membrane protein ATPase pump enzymes to maintain proper gradients, for Na^+ and Ca^{2+} ions to remain largely outside cells and K^+ ion inside to support normal membrane functions. Although the reaction is entropy driven, energetically favored, and enzyme catalyzed to proceed at rapid rates, resonance stability is the driving factor for this. Not only is entropy increased due to the production of more product molecules in number, which is a more chaotic state, but the extent of resonance in the product phosphate is largely increased. Two shared electrons continuously resonate rapidly among four P-O bonds, usually described with Lewis structures as shown in Figure 8.

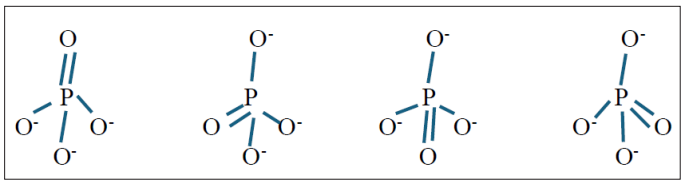

Figure 8: Canonical resonance depictions for inorganic phosphate PO_4^{-3}. The true structure is an averaged arrangement where all four P-O bonds are equivalent. All oxygens also have two nonbonding lone pairs not shown. All five valence electrons from P are bonding.

Transmission electron microscopy of molecules reveals their overall shape in a manner unlike X-ray diffraction that relies on EM radiation. Pictures of carbon dioxide and also fatty acid molecules suggest that electrons are not isolated in distinctly separated regions, but rather that electrons appear to span over interatomic areas [9]. Since electrons repel each other while protons absorb electrons, the reflected images indicate that electron density exists not only between bonds but over atomic nuclei in the molecule as well. So all electron motion in multi-atom molecules may be compared to resonance, while resonating systems may simply involve more rapid and extensive, less geometrically constrained motion. Electron density can vary between regions of a molecule and resonating systems have a different density than a non-resonating bonding region. The ring current in benzene has a different electron density than the electrons forming the C-C sigma bonds for example. Further, the resonating carboxylate anion has more electron density than when the system is acidified and not resonating. Here the bonding O-H electrons are released into the resonating form.

A more detailed version of this paper is available online at SSRN: https://ssrn.com/abstract=5903003 or http://dx.doi.org/10.2139/ssrn.5903003.

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