[TP] In formate, $HC(O)O^-$, some valence electrons are shared between atoms and some valence electrons are localized on atoms. There are the same number of valence electrons localized on each O of formate. The number of valence electrons localized on one O atom is …

20% 1. 5
20% 2. 5 1/3
20% 3. 5 1/2
20% 4. 5 2/3
20% 5. 6

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Response Counter 10

Lecture 3 CH102 A1 (MWF 9:05 am)

Monday, January 28, 2019

- π framework and resonance Lewis structures
- Localized versus delocalized π bonds
- Postscript on polyatomic MO recipe

Begin Mahaffy et al., Chapter 11: States of Matter

- Behavior of gases: Macroscopic versus microscopic understanding

Next: Kinetic molecular theory, PDF: http://goo.gl/njf3em

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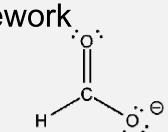
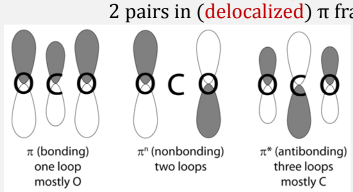
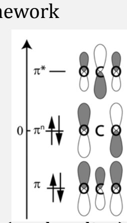
$HC(O)O^-$ π framework



2 pairs in (delocalized) π framework





1 pair in π (bonding) and 1 pair in π^n (nonbonding); bond order 1

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$HC(O)O^-$ π framework

The π framework subsumes the need for resonance Lewis structures.

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Localized and delocalized π orbitals

Localized π orbitals are those MOs built from only two AOs, each AO on adjacent atoms. As a result, localized π orbitals extend over only two adjacent atoms.

Delocalized π orbitals are those MOs built from more than two AOs, on more than two adjacent atoms. As a result, delocalized π orbitals extend over more than two adjacent atoms.

Localized and delocalized electrons

A localized electron is in an orbital that has zero density between adjacent atoms.

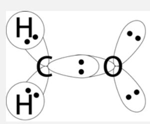
A delocalized electron is in an orbital that has non-zero density between adjacent atoms.

Localized and delocalized electrons

An electron is localized on an atom if it is …

in a σ framework non-bonding orbital,

For example, each of the lone-pair electrons on the O of formaldehyde is localized on the O atom

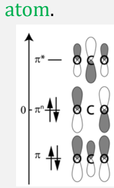


Localized and delocalized electrons

An electron is localized on an atom if it is …

in a π framework orbital that has a nodal plane (or 0 amplitude) between adjacent atoms

For example, the electrons in the π^n orbital of formate, $HC(O)O^-$, are localized on the O atoms, one-half of each electron on each O atom.



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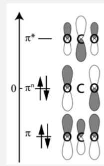
Localized and delocalized electrons

An electron is localized on an atom if it is …

in a π framework orbital that has a nodal plane (or 0 amplitude) between adjacent atoms

Note that the π (bonding) orbital does not have a nodal plane, and so the two electrons it contains are spread among O-C-O atoms, rather than being localized on each atom.



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[TP] In formate, HC(O)O⁻, some electrons are shared between atoms and some electrons are localized on atoms. There are the same number of electrons localized on each O of formate. The number of electrons localized on one O atom is …

20% 1. 5
20% 2. 5 1/3
20% 3. 5 1/2
20% 4. 5 2/3
20% 5. 6

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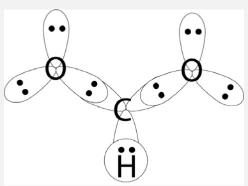
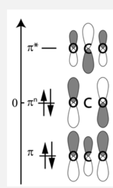
Localized and delocalized electrons

Therefore in formate, HC(O)O⁻, there are a total of 5 electrons (4 in the σ framework + 1 in the π framework)) localized on each O atom.





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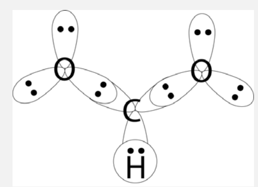
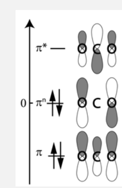
[Quiz] The total number of electrons localized on C in formate, HC(O)O⁻ is …

20% 1. 0
20% 2. 1/3
20% 3. 2/3
20% 4. 1
20% 5. 2





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Postscript on polyatomic MO recipe

The σ framework is a visual representation of the bonding σ MOs.

The antibonding σ MOs are not shown, since they are never needed.

The σ framework does not show the hybrid AO-MO correlation diagram.

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Postscript on polyatomic MO recipe

The π framework is a visual representation of the all of the π MOs (bonding, non-bonding, and antibonding, since they may be needed to accommodate electrons not accommodated in the σ framework.

The π framework shows the relative energies of the π MOs .

The π framework does not show the hybrid AO-MO correlation diagram.

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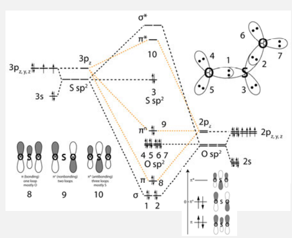
Postscript on polyatomic MO recipe

It is possible to show the σ and π correlation diagrams, and an example is that for SO_2, shown in slide 30 of http://goo.gl/6hBD8X.

However, we will not ask that you do this and so you are not responsible for knowing how to do so.



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Behavior of gases

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[TP] A container of volume V is filled with a gas at 20 °C. If V is decreased (while keeping T constant), pressure P exerted by the gas on the walls of the container must ...

25% 1. go down
25% 2. stay the same
25% 3. go up
25% 4. Further information needed

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Macroscopic behavior

Very likely you know and have a lot of experience working with the ideal gas equation relating P, T, V and n, ...

$PV = nRT$

In term of the gas constant ...

$R = 8.314 \text{ J /(K mol)}$

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Macroscopic behavior

Using $PV = nRT$ we know algebraically that if V is decreased (while keeping T constant), the pressure P exerted by the gas on the walls of the container must go up, since the right-hand side of the equation is unchanged.

This is an example of macroscopic understanding.

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Microscopic behavior

Our goal is to understand this kind of behavior at a microscopic level.

That is, at the level of the individual particles of the gas.

Our method is called the kinetic molecular theory of gases.

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