

Lecture 5 CH102 A2 (MWF 11:15 am) Spring 2018 Copyright © 2018 Dan Dill dan@bu.edu

[TP] In formate, $\text{HC(O)}\text{O}^-$, 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. $5\frac{1}{3}$
20% 3. $5\frac{1}{2}$
20% 4. $5\frac{2}{3}$
20% 5. 6

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Monday, January 29, 2018

- Complete formate, $\text{HC(O)}\text{O}^-$ (delocalized π bonds)
- Postscript on polyatomic MO recipe

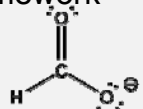
Next: Mahaffy et al., Chapter 11: States of Matter

- Behavior of gases: Macroscopic versus microscopic understanding
- Kinetic molecular theory, PDF: <http://goo.gl/njf3em>

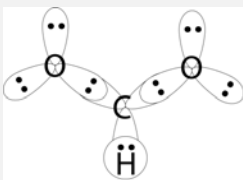
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$\text{HC(O)}\text{O}^-$ sp^2 σ framework



9 pairs in Lewis structure, 7 pairs in σ framework, and so 2 pairs in (delocalized) π framework.

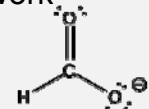


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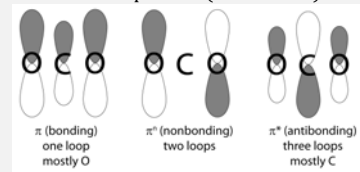
6

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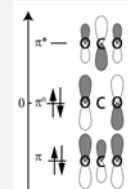
$\text{HC(O)}\text{O}^-$ π framework



2 pairs in (delocalized) π framework



π (bonding) one loop mostly O
 π^* (nonbonding) two loops
 π^* (antibonding) three loops mostly C



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

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20% 1. 5
 20% 2. $5 \frac{1}{3}$
 20% 3. $5 \frac{1}{2}$
 20% 4. $5 \frac{2}{3}$
 20% 5. 6

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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 all π MOs, bonding, non-bonding, and antibonding, and their relative energies.
 The π framework **does not show** the hybrid AO-MO correlation diagram.

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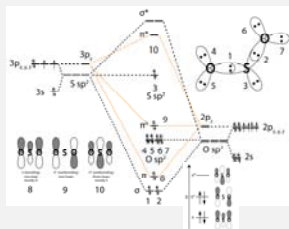
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Postscript on polyatomic MO recipe

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 ...

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

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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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