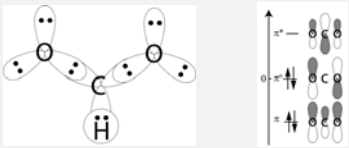


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[TP] How many **pairs of electrons are shared** by each O and the C of formate,  $\text{HC(O)}\text{O}^-$

20% 1. 1 pair (2 electrons)  
 20% 2. 1 ½ pair (3 electrons)  
 20% 3. 2 pair (4 electrons)  
 20% 4. Something else  
 20% 5. The answer is different for the two O-C bonds



The Lewis structure shows a central carbon atom bonded to a hydrogen atom and two oxygen atoms. One oxygen is double-bonded to the carbon, and the other is single-bonded and carries a negative charge. The molecular orbital diagram shows the energy levels of the atoms and the resulting molecular orbitals for the C-O bonds.

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### Lecture 5 CH102 A1 (MWF 9:05 am) Monday, January 30, 2017

- Complete: Polyatomic MO recipe: Formate,  $\text{HC(O)}\text{O}^-$  (**delocalized**  $\pi$  bonds)

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

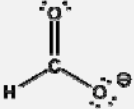
- Behavior of gases: Macroscopic versus microscopic understanding
- Kinetic molecular theory, PDF: <http://goo.gl/njf3em>

Next: Continue ch11: Molecular speeds and their distribution; real gases (attraction and size)

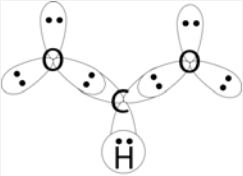
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### $\text{HC(O)}\text{O}^-$ $\text{sp}^2$ $\sigma$ framework



9 pairs in Lewis structure, 7 pairs in  $\sigma$  framework, and so 2 pairs in (**delocalized**)  $\pi$  framework.



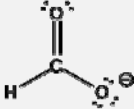
The diagram shows the  $\text{sp}^2$  hybrid orbitals on the carbon and oxygen atoms, forming the  $\sigma$  framework of the molecule.

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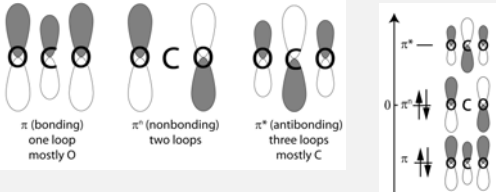
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### $\text{HC(O)}\text{O}^-$ $\pi$ framework



2 pairs in (**delocalized**)  $\pi$  framework



The diagram shows the  $\pi$  orbitals formed by the overlap of p orbitals on the carbon and oxygen atoms. It identifies the bonding  $\pi$  orbital (one loop, mostly on oxygen), the nonbonding  $\pi^n$  orbital (two loops), and the antibonding  $\pi^*$  orbital (three loops, mostly on carbon).

1 pair in  $\pi$  (bonding) and 1 pair in  $\pi^n$  (nonbonding);  
bond order 1

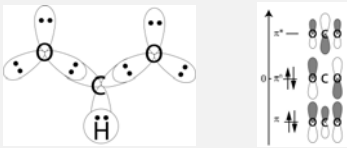
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**[TP]** How many **pairs of electrons are shared** by each O and the C of formate,  $\text{HC}(\text{O})\text{O}^-$

20% 1. 1 pair (2 electrons)  
 20% 2. 1 ½ pair (3 electrons)  
 20% 3. 2 pair (4 electrons)  
 20% 4. Something else  
 20% 5. The answer is different for the two O-C bonds



The Lewis structure shows a central carbon atom bonded to a hydrogen atom and two oxygen atoms. One oxygen atom has a negative charge. The orbital diagram shows the carbon atom with three sp<sup>2</sup> hybrid orbitals forming sigma bonds with the hydrogen and two oxygen atoms, and one unhybridized p orbital. The oxygen atoms have two sp<sup>2</sup> hybrid orbitals each, one forming a sigma bond with carbon and the other containing a lone pair. The unhybridized p orbitals on carbon and oxygen overlap to form pi bonds.

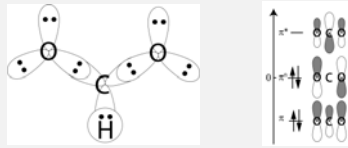
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**[Group quiz]** How many **lone pairs of electrons** are on each O of formate,  $\text{HC}(\text{O})\text{O}^-$

14% 1. 1 pair (2 electrons)  
 14% 2. 1 ½ pair (3 electrons)  
 14% 3. 2 pair (4 electrons)  
 14% 4. 2 ½ pair (5 electrons)  
 14% 5. 3 pair (6 electrons)  
 14% 6. Something else  
 14% 7. The answer is different for the two O atoms



The Lewis structure shows a central carbon atom bonded to a hydrogen atom and two oxygen atoms. One oxygen atom has a negative charge. The orbital diagram shows the carbon atom with three sp<sup>2</sup> hybrid orbitals forming sigma bonds with the hydrogen and two oxygen atoms, and one unhybridized p orbital. The oxygen atoms have two sp<sup>2</sup> hybrid orbitals each, one forming a sigma bond with carbon and the other containing a lone pair. The unhybridized p orbitals on carbon and oxygen overlap to form pi bonds.

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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  $n$ , ...

$$PV = RnT$$

The constant of proportionality is the gas constant ...

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

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## Macroscopic behavior

From

$$PV = RnT$$


we know 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 left-hand side of the equation is **unchanged**.

This is an example of **macroscopic** understanding.

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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## 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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## Kinetic-molecular theory of gases

**Goal:** Get microscopic expression for pressure  $P$

**Key idea 1:** Pressure is due to force exerted by particles during collisions with the container walls

**Key idea 2:** Force is due to momentum change in collision with the container walls.

**Note:** Here **upper-case**  $P$  is used for pressure and **lower-case**  $p$  is used for momentum.

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### Kinetic-molecular theory of gases

$$P = \frac{F}{A} = \frac{\text{force}}{\text{area}} = \frac{\text{force}}{L^2}$$

$$\text{force} = \frac{\text{change in momentum}}{\text{time}} = \frac{\Delta p}{\Delta t}$$

$$\Delta p = p_2 - p_1, \quad p_2 = m \cdot u_2, \quad p_1 = m \cdot u_1$$

$$\Delta p_{\text{particle}} = (-72 \text{ kg} \cdot \text{m/s}) - (72 \text{ kg} \cdot \text{m/s}) = -144 \text{ kg} \cdot \text{m/s}$$

$$\Delta p_{\text{wall}} = +144 \text{ kg} \cdot \text{m/s}$$

$$\Delta p_{\text{wall}} = 2 \cdot m \cdot u$$

$$\Delta p_{\text{particle}} + \Delta p_{\text{wall}} = 0$$
 elastic collision  

$$\Delta p_{\text{particle}} = -\Delta p_{\text{wall}}$$

$$\text{volume} = L^3$$
  

$$\text{area} = L^2$$

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### Kinetic-molecular theory of gases

$$\text{force} = \frac{\Delta p_{\text{wall}}}{\Delta t_{\text{collision}}} = \frac{2mu}{\Delta t_{\text{collision}}}$$

$$\Delta t_{\text{collision}} = \frac{2L}{u} = \frac{2 \cdot 10 \text{ m}}{1 \text{ m/s}} = 20 \text{ s}$$

$$\text{force} = \frac{2mu}{2L/u} = mu^2/L$$

$$\text{pressure} = \frac{\text{force}}{\text{area}} = \frac{mu^2/L}{L^2}$$

$$P = \frac{mu^2}{L^3} = \frac{mu^2}{V}$$

$$PV = mu^2 \sim nRT = PV$$

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### Kinetic-molecular theory of gases

① we have not one particle, but a lot  
 ② particles move at different speeds

$$P_{\text{due to one particle}} = \frac{mu^2}{V}$$

$$P_1 = \frac{mu_1^2}{V} = 1$$

$$P_2 = \frac{mu_2^2}{V}$$

$$\vdots$$

$$P_N = \frac{mu_N^2}{V}$$

$$P = \frac{m}{V} (u_1^2 + u_2^2 + \dots + u_N^2)$$

$$= \frac{m}{V} N \left( \frac{u_1^2 + u_2^2 + \dots + u_N^2}{N} \right) = \frac{m}{V} N u_{\text{avg}}^2$$

$$PV = (mN) u_{\text{avg}}^2 \quad \text{total mass} = mN$$

$$N = 10^{29}$$

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