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[TP] In formic acid, HC(O)OH, the hybridization on the O **single-bonded** to the C is (use the Lewis structure) ...

25% 1. none
25% 2. sp
25% 3. sp²
25% 4. sp³

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Friday, January 26, 2018

- Hybrid review
- Water review
- Polyatomic MO recipe: Formaldehyde, H₂CO (localized π bond)

Next: Formic acid, HC(O)OH (localized π bonds); Formate, HC(O)O⁻ (delocalized π bonds)

"Hybrid AOs and Polyatomic MOs," <http://goo.gl/6hBD8X>

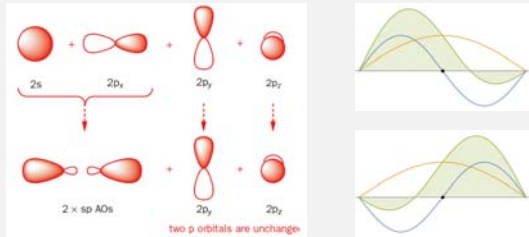
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An s and a p AO make two **sp hybrid AOs**

<http://demonstrations.wolfram.com/HybridOrbitalsInOrganicChemistry/>

180° angle, for SN = 2; **linear** geometry
Two p AOs are unchanged on each atom

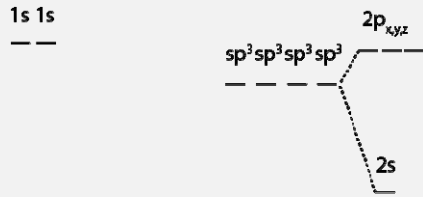


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5

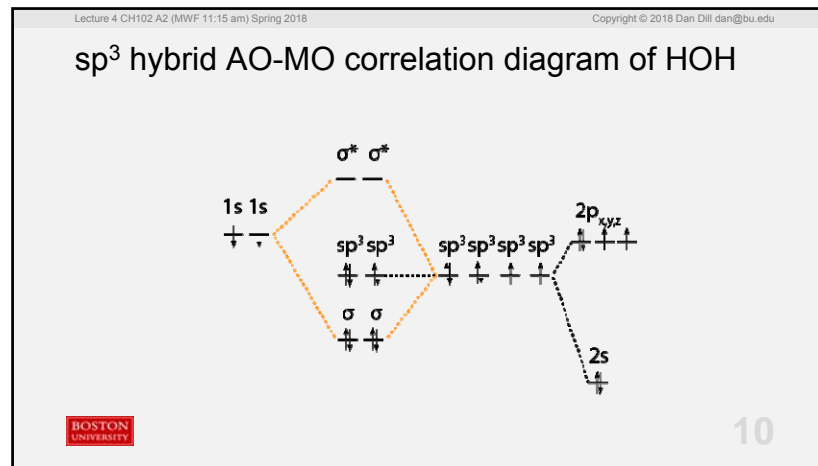
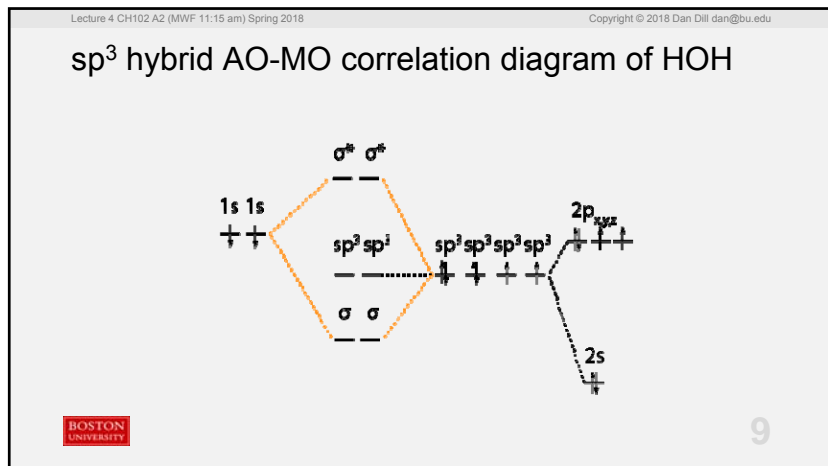
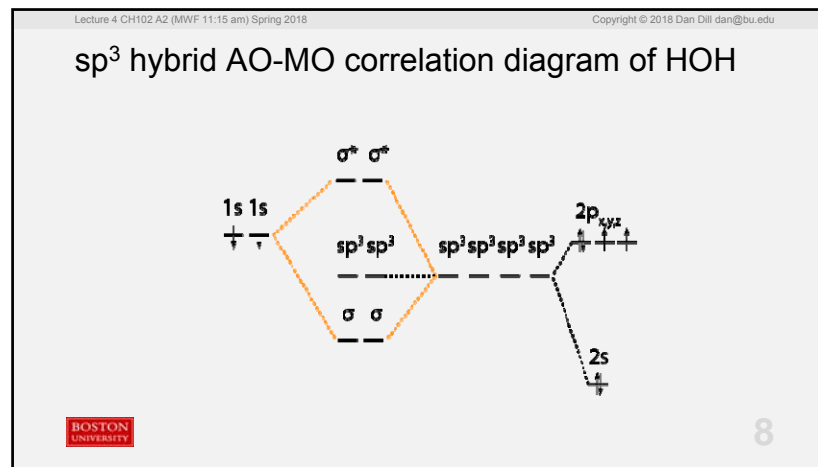
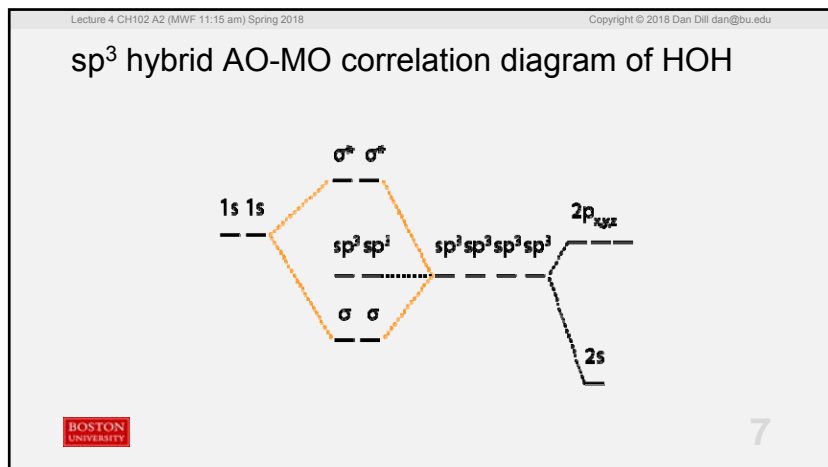
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sp³ hybrid AO-MO correlation diagram of HOH



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Compare AO-MO correlation diagrams of HOH

Non-hybrid AO result: 90° bond angle and lone pairs of different energies.

Hybrid AO result: 109° bond angle and lone pairs of the same energy.

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Polyatomic MO recipe: Formaldehyde, H_2CO

- Use the Lewis structure to get ...
 - the number of electron pairs
 - make hybrid AO's on each central atom; terminal atoms (except H) have same hybrids as central atom

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Polyatomic MO recipe: Formaldehyde, H_2CO

- Use the Lewis structure to get ...
 - the number of electron pairs
 - make hybrid AO's on each atom; terminal atoms (except H) have same hybrids as central atom
- Sketch the σ (MO) framework and place pairs ...
 - in each bonding σ MO
 - in each nonbonding hybrid AO

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Formaldehyde, H_2CO , σ framework

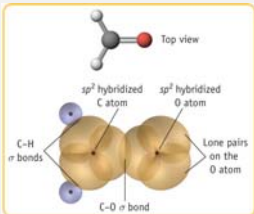
6 pairs in Lewis structure, 5 pairs in σ framework, and so 1 pair in (localized) π framework.

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H₂CO sp² σ framework

6 pairs in Lewis structure, 5 pairs in σ framework,
and so 1 pair in (localized) π framework.



(b) The C-H σ bonds are formed by overlap of C atom sp² hybrid orbitals with H atom 1s orbitals. The σ bond between C and O atoms arises from overlap of sp² orbitals.

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Polyatomic MO recipe: Formaldehyde, H₂CO

- Use the Lewis structure to get ...
 - the number of electron pairs
 - make hybrid AO's on each atom; terminal atoms (except H) have same hybrids as central atom
- Sketch the σ framework and place pairs ...
 - in each bonding σ MO
 - in each nonbonding hybrid AO
- Sketch the π framework MO's:
 - mark as **bonding, nonbonding, and antibonding**
 - place **remaining pairs** (Auf Bau)
 - get the **π bond order**

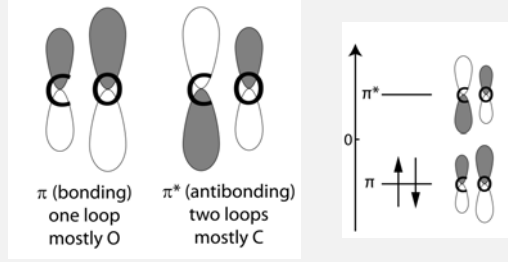
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H₂CO π framework

1 pair in (localized) π framework



π (bonding) one loop mostly O

π* (antibonding) two loops mostly C

1 pair in π (bonding); **bond order 1**

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Formic acid, HC(O)OH

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[TP] In formic acid, HC(O)OH, the hybridization on the O **single-bonded** to the C is (use the Lewis structure) ...

25% 1. none
 25% 2. sp
 25% 3. sp²
 25% 4. sp³

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[Quiz] In formic acid, HC(O)OH, the hybridization on the O **double-bonded** to the C is (use the Lewis structure) ...

25% 1. none
 25% 2. sp
 25% 3. sp²
 25% 4. sp³

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HC(O)OH σ framework

- Hybridization of **terminal atoms** the **same as their central atom**
- Terminal H **never hybridized**
- One pair in each hybrid AO **σ bonding MO**
- One pair in each **non-bonded hybrid AO**

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π framework

- mark as **bonding, nonbonding, antibonding**
- place **remaining pairs** (Auf Bau)
- get the **π bond order**

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HC(O)OH π framework

1 pair in (localized) π framework

π (bonding)
one loop
mostly O

π^* (antibonding)
two loops
mostly C

1 pair in π (bonding); bond order 1

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Formate, HC(O) O^-

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[TP] Formic acid, HC(O)OH, and its conjugate base formate, HC(O) O^- , each have 9 pairs of electrons. How many pairs of electrons are in the σ framework of formate?

20% 1. 3 pairs
20% 2. 5 pairs
20% 3. 7 pairs
20% 4. 8 pairs
20% 5. 9 pairs

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HC(O) 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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[TP] How many pairs of electrons are in the π framework of formate?

25% 1. 0 pairs
 25% 2. 1 pairs
 25% 3. 2 pairs
 25% 4. 3 pairs

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HC(O)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^n (nonbonding);
bond order 1

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31