

Lecture 2 CH102 A1 (MWF 9:05 am) Spring 2017 Copyright © 2017 Dan Dill dan@bu.edu

[TP] In the  $\text{HO}^-$  correlation diagram, the O 2s AO is nonbonding because ...

20% 1. it has no net overlap with the H 1s AO  
 20% 2. It has the wrong symmetry  
 20% 3. it has a lower ionization energy than the O 2p AOs  
 20% 4. it has a larger  $Z_{\text{eff}}$  than the O 2p AOs  
 20% 5. of some other reason

The diagram shows the energy levels for H 1s, O 2s, and O 2p orbitals. The H 1s orbital is at a higher energy than the O 2s orbital. The O 2p orbitals are at a higher energy than the O 2s orbital. The resulting MOs are  $\sigma_x^*$  and  $\sigma_x$ . The  $\sigma_x$  orbital is nonbonding and has the same energy as the O 2s orbital. The  $\sigma_x^*$  orbital is bonding and has a lower energy than the O 2p orbitals.

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 Monday, January 23, 2017

- MO description of water
- Accounting for molecular shape: Hybrid AOs
- Water again: Hybrid AO-MO description

Next: Continue "Hybrid AOs and Polyatomic MOs",  
<http://goo.gl/6hBD8X>: Water again: Hybrid AO-MO description;  
 Formaldehyde,  $\text{H}_2\text{CO}$ ; formic acid,  $\text{HC(O)OH}$ ; formate acid,  $\text{HC(O)O}^-$

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 20% 5. of some other reason

The diagram shows the energy levels for H 1s, O 2s, and O 2p orbitals. The H 1s orbital is at a higher energy than the O 2s orbital. The O 2p orbitals are at a higher energy than the O 2s orbital. The resulting MOs are  $\sigma_x^*$  and  $\sigma_x$ . The  $\sigma_x$  orbital is nonbonding and has the same energy as the O 2s orbital. The  $\sigma_x^*$  orbital is bonding and has a lower energy than the O 2p orbitals.

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[Quiz] In the  $\text{HO}^-$  correlation diagram, the two O 2p AOs are nonbonding because ...

25% 1. they have no net overlap with the H 1s AO  
 25% 2. they have a higher ionization energy than the H 1s AO  
 25% 3. they have a larger  $Z_{\text{eff}}$  than the H 1s AO  
 25% 4. of some other reason

The diagram shows the energy levels for H 1s, O 2s, and O 2p orbitals. The H 1s orbital is at a higher energy than the O 2s orbital. The O 2p orbitals are at a higher energy than the O 2s orbital. The resulting MOs are  $\sigma_x^*$  and  $\sigma_x$ . The  $\sigma_x$  orbital is nonbonding and has the same energy as the O 2s orbital. The  $\sigma_x^*$  orbital is bonding and has a lower energy than the O 2p orbitals.

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### Sketch the AO-MO correlation diagram of HOH

Hint: Represent the second H as an additional 1s AO

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### Sketch the AO-MO correlation diagram of HOH

Hint: Represent the second H as an additional 1s AO

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**[Group Quiz]** Based on the AO-MO correlation diagram of HOH, the H-O-H bond angle must be ...

25% 1. 90°  
25% 2. 109°  
25% 3. 120°  
25% 4. 180°

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Accounting for molecular shape:  
Hybrid AO's account for central atom electron-pair geometry

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## Notes for Mahaffy et al., 2e, 10.6 & 10.9

Hybrid AO's and polyatomic MO's, PDF, 39 pages  
<http://goo.gl/6hBD8X>

Supporting pages of Mahaffy et al., 2e, are  
 pp 386 (middle)--397 (middle)  
 pp 406 (middle)--407

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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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2s 2p<sub>x</sub> 2p<sub>y</sub> 2p<sub>z</sub>

2 × sp AOs 2p<sub>y</sub> 2p<sub>z</sub>

two p orbitals are unchanged

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

characteristics	
orbital hybrid	2s, 2p <sub>x</sub>
hybrid orbital	2
molecular geometry	linear
examples	C <sub>2</sub> H <sub>2</sub> , BeCl <sub>2</sub>

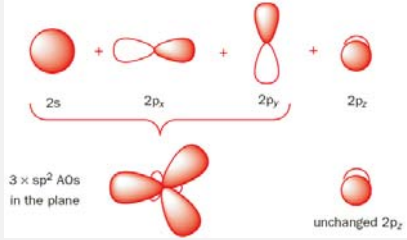
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### An s and two p AOs make three $sp^2$ hybrid AOs

<http://demonstrations.wolfram.com/HybridOrbitalsInOrganicChemistry/>  
 120° angle, for SN = 3; **trigonal planar** geometry  
 One p AO is unchanged on each atom

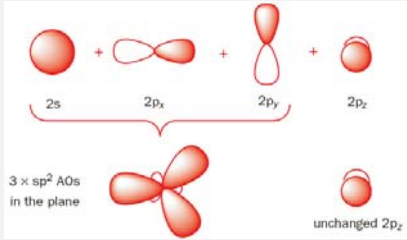


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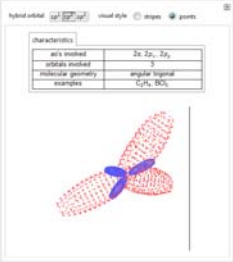


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 180° angle, for SN = 2; **linear** geometry  
 Two p AOs are unchanged on each atom

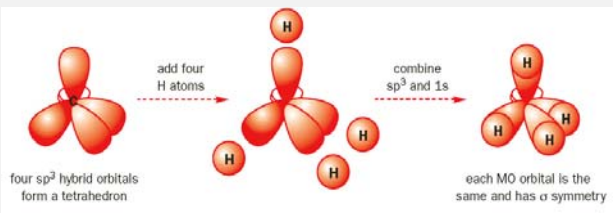


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### An s and three p AOs make four $sp^3$ hybrid AOs

<http://demonstrations.wolfram.com/HybridOrbitalsInOrganicChemistry/>  
 109° angle, for SN = 4; **tetrahedral** geometry  
 All three p AOs are mixed with the s AO

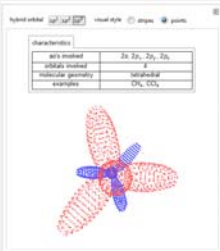


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## An s and three p AOs make four $sp^3$ hybrid AOs

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 109° angle, for SN = 4; **tetrahedral** geometry  
 All three p AOs are mixed with the s AO



Characteristics	
sp orbital	2s, 2p, 3s,
hybrid orbital	4
molecular geometry	tetrahedral
examples	CH <sub>4</sub> , SiCl <sub>4</sub>

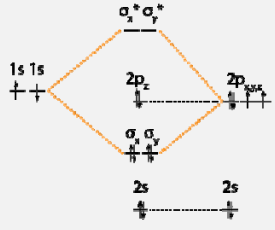
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## Hybrid AO-MO correlation diagram of HOH

What changes are needed to our earlier AO-MO diagram, below?

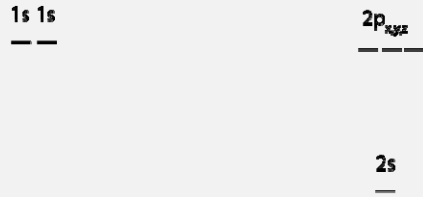


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## $sp^3$ hybrid AO-MO correlation diagram of HOH



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