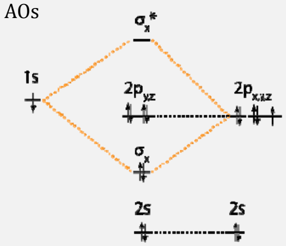


[TP] In the HO^- correlation diagram, the O 2s AO is nonbonding because …

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_{eff} than the O 2p AOs
20% 5. of some other reason



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Lecture 2 CH102 A1 (MWF 9:05 am)

Monday, January 23, 2017

- MO description if 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, H_2CO; formic acid, HC(O)OH; formate acid, $HC(O)O^-$

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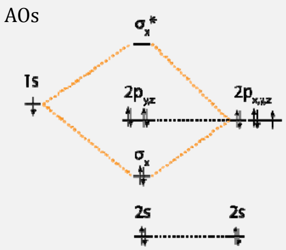
20% 5. of some other reason



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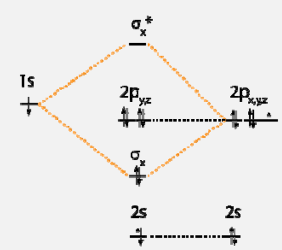
[Quiz] In the HO^- correlation diagram, the two O 2p AOs are nonbonding because …

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_{eff} than the the H 1s AO
25% 4. of some other reason



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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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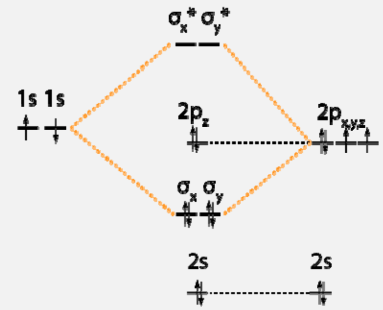
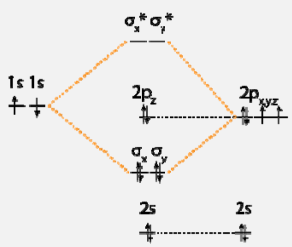


[Group Quiz] Based on the AO-MO correlation diagram of HOH, the H-O-H bond angle must be ...

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



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

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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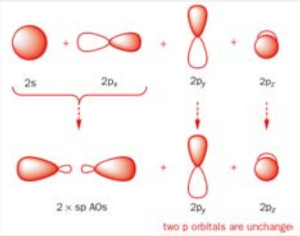

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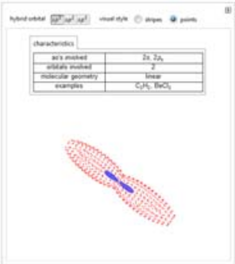

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An s and two p AOs make three sp^2 hybrid AOs

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

120º angle, for SN = 3; trigonal planar geometry

One p AO is unchanged on each atom

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

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120º angle, for SN = 3; trigonal planar geometry

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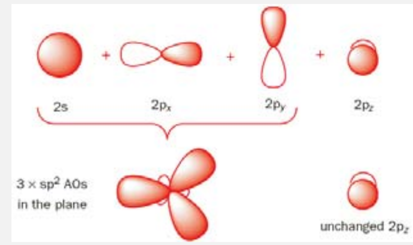

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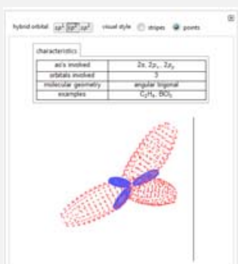
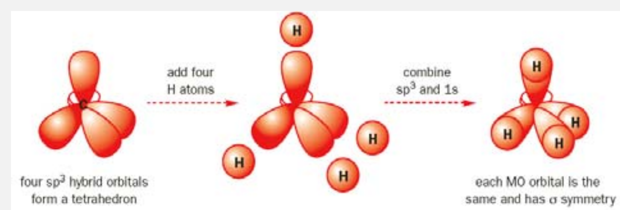


An s and three p AOs make four sp^3 hybrid AOs

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

109º angle, for SN = 4; tetrahedral geometry

All three p AOs are mixed with the s AO



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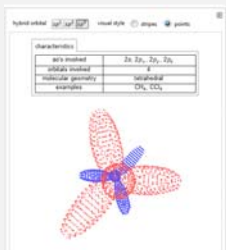

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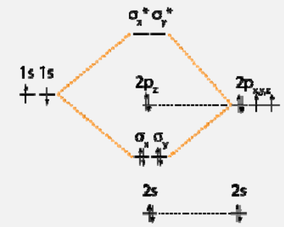
Hybrid AO-MO correlation diagram of HOH

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



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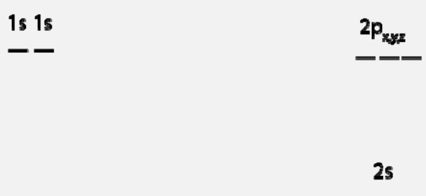
sp^3 hybrid AO-MO correlation diagram of HOH



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