

[TP] For O AOs, assume the 2p energy −14 eV and 2s energy −18 eV. The energy of each sp^3 hybrid AO will be ...

20% 1. −14 eV
20% 2. −15 eV
20% 3. −16 eV
20% 4. −17 eV
20% 5. −18 eV

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Response Counter 10

Lecture 1 CH102 A1 (MWF 9:05 am)

Wednesday, January 23, 2019

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

Next: Polyatomic MO recipe: Formaldehyde, H_2CO (localized π bond); 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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Sketch the AO-MO correlation diagram of HOH

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

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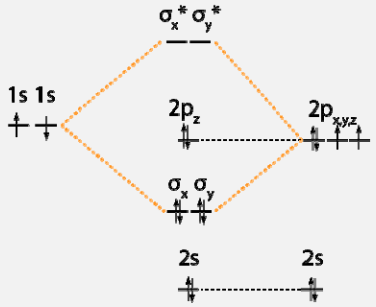
Hint: Represent the second H as an additional 1s AO



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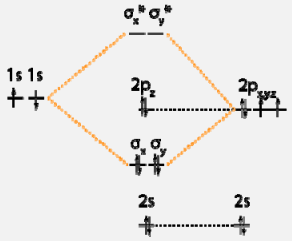
[Group Quiz] Based on the AO-MO correlation diagram of HOH, the H-O-H bond angle must be ...

0% 1. 90°
0% 2. 109°
0% 3. 120°
0% 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 AOs and polyatomic MOs, 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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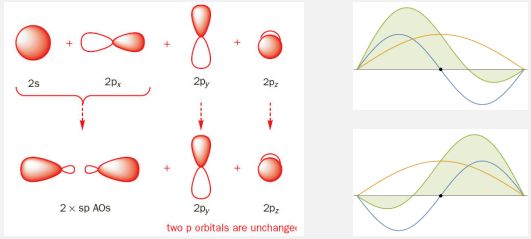

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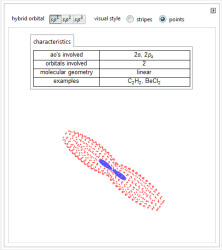

An s and two p AOs make three sp^2 hybrid AOs

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

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

One p AO is unchanged on each atom

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

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

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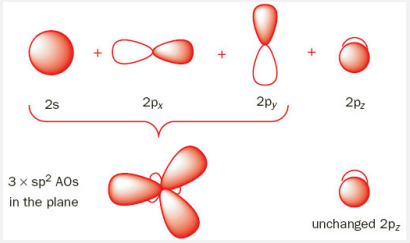

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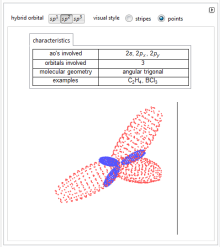

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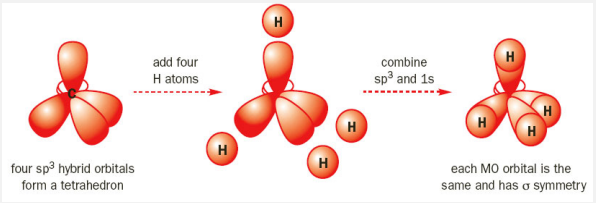
14

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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16

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

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109° angle, for SN = 4; tetrahedral geometry

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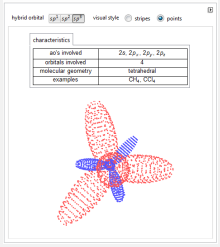

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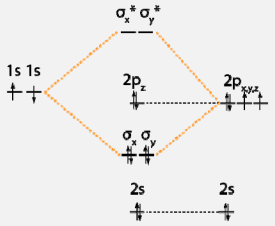
17

Hybrid AO-MO correlation diagram of HOH

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



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19

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0% 4. −17 eV
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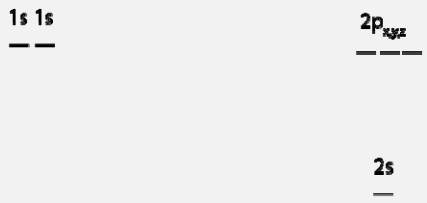
sp^3 hybrid AO-MO correlation diagram of HOH

For O AOs, assume the 2p energy −14 eV and 2s energy −18 eV.

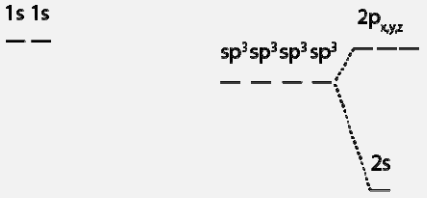
The energy of each sp^3 hybrid AO will be the weighted average of the AO energies,

$$\frac{3 \times (-14\ \text{eV}) + 1 \times (-18\ \text{eV})}{4} = -15\ \text{eV}$$

sp^3 hybrid AO-MO correlation diagram of HOH



sp^3 hybrid AO-MO correlation diagram of HOH



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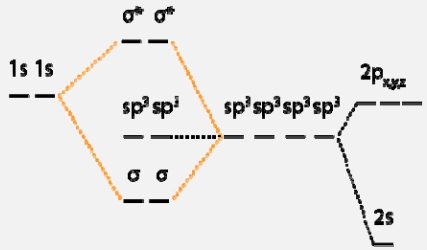

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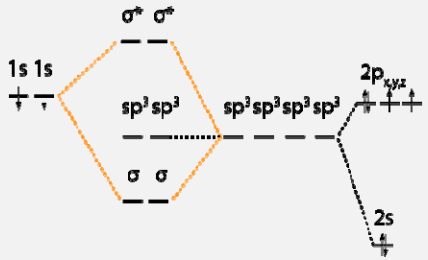
sp^3 hybrid AO-MO correlation diagram of HOH



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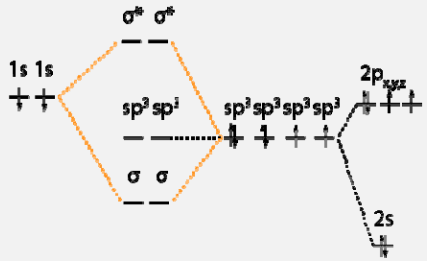
sp^3 hybrid AO-MO correlation diagram of HOH



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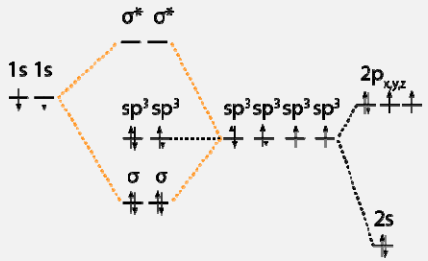
sp^3 hybrid AO-MO correlation diagram of HOH



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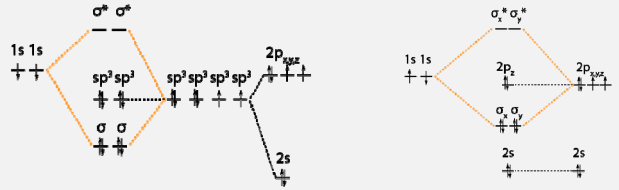
Compare AO-MO correlation diagrams of HOH



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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28