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[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 1

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 Wednesday, January 24, 2018

- 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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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 ...

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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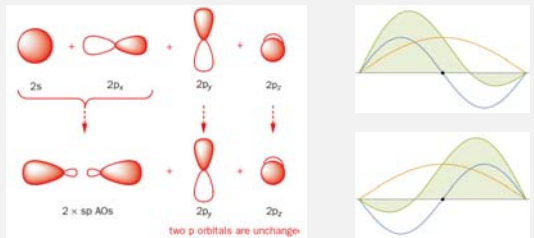
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2s + 2p_x + 2p_y + 2p_z

2 × sp AOs 2p_z 2p_z

two p orbitals are unchanged

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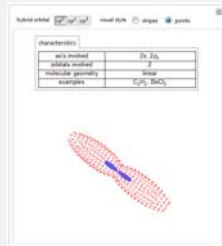
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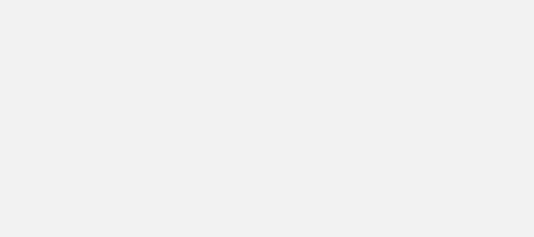
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An s and two p AOs make three **sp² hybrid AOs**

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

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

One p AO is unchanged on each atom



2s + 2p_x + 2p_y + 2p_z

3 × sp² AOs in the plane unchanged 2p_z

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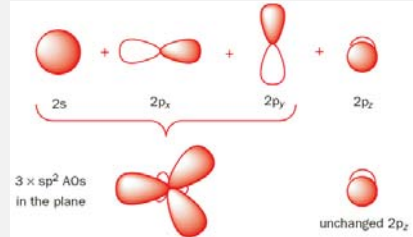
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3 × sp² AOs in the plane unchanged 2p_z

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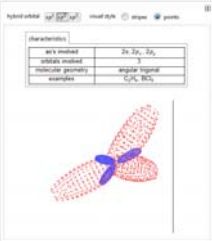
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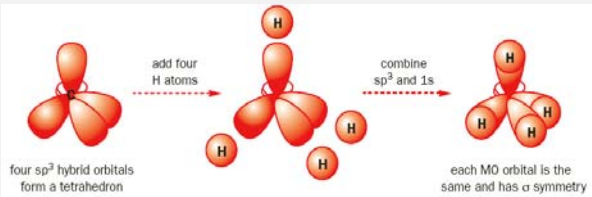
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An s and three p AOs make four sp^3 hybrid AOs

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

109° angle, for SN = 4; **tetrahedral** geometry

All three p AOs are mixed with the s AO



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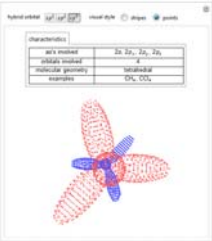
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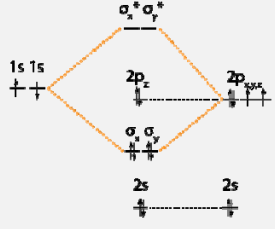
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Hybrid AO-MO correlation diagram of HOH

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



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sp^3 hybrid AO-MO correlation diagram of HOH

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,

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



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sp^3 hybrid AO-MO correlation diagram of HOH

1s 1s

2p_{xyz}

2s
 -



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sp^3 hybrid AO-MO correlation diagram of HOH

1s 1s

sp³sp³sp³sp³ 2p_{xyz}

2s
 -



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