In the HO⁻ correlation diagram, the O 2s AO is nonbonding because ...

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

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, H₂CO; formic acid, HC(O)OH; formate acid, HC(O)O⁻
Sketch the AO-MO correlation diagram of HOH

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

[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°

Accounting for molecular shape:
Hybrid AO’s account for central atom electron-pair geometry
### Notes for Mahaffy et al., 2e, 10.6 & 10.9

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

---

**Lecture 2 CH102 A1 (MWF 9:05 am) Spring 2017**

---

**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

---

**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

---

**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
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 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
An s and three p AOs make four sp³ hybrid AOs

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

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

Hybrid AO-MO correlation diagram of HOH

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