

[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

BOSTON UNIVERSITY

Response Counter 10 1

Lecture 3 CH102 A1 (MWF 9:05 am)

Wednesday, January 25, 2017

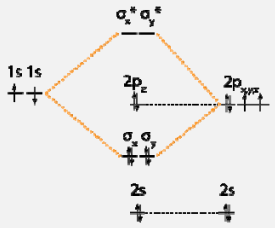
- Water again: Hybrid AO-MO description
- Polyatomic MO recipe: Formaldehyde, H_2CO (localized π bond)

Next: Continue "Hybrid AOs and Polyatomic MOs",
http://goo.gl/6hBD8X: Formic acid, HC(O)OH; formate, $HC(O)O^-$

BOSTON UNIVERSITY

Hybrid AO-MO correlation diagram of HOH

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



BOSTON UNIVERSITY

7

[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

BOSTON UNIVERSITY

Response Counter 10 8

sp^3 hybrid AO-MO correlation diagram of HOH

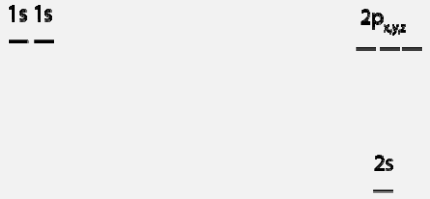
For O AOs, assume the 2p energy −14 eV and 2s energy −18 eV. The energy of each sp^3 hybrid AO will be ...

(3 × (−14 eV) + 1 × (-18 eV)) / 4 = ...

−15 eV

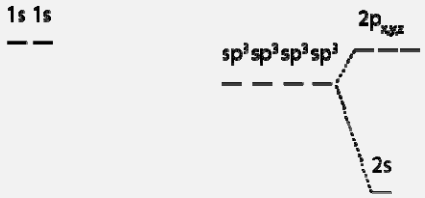
BOSTON UNIVERSITY 9

sp^3 hybrid AO-MO correlation diagram of HOH



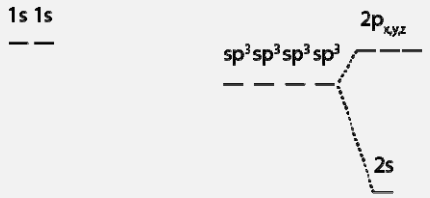
BOSTON UNIVERSITY 10

sp^3 hybrid AO-MO correlation diagram of HOH



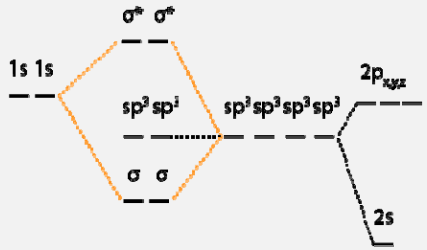
BOSTON UNIVERSITY 11

sp^3 hybrid AO-MO correlation diagram of HOH



BOSTON UNIVERSITY 12

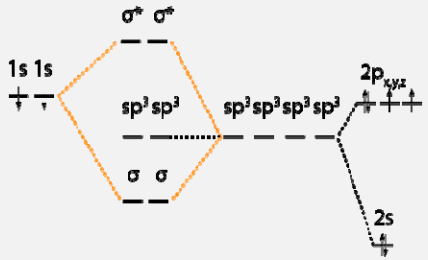
sp^3 hybrid AO-MO correlation diagram of HOH



BOSTON UNIVERSITY

13

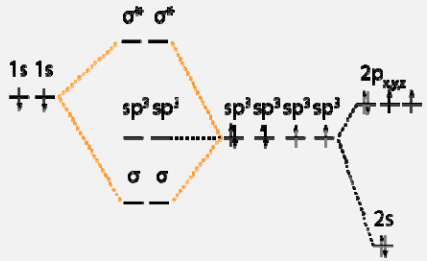
sp^3 hybrid AO-MO correlation diagram of HOH



BOSTON UNIVERSITY

14

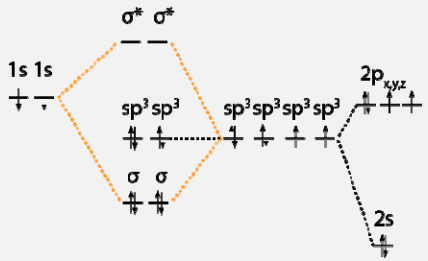
sp^3 hybrid AO-MO correlation diagram of HOH



BOSTON UNIVERSITY

15

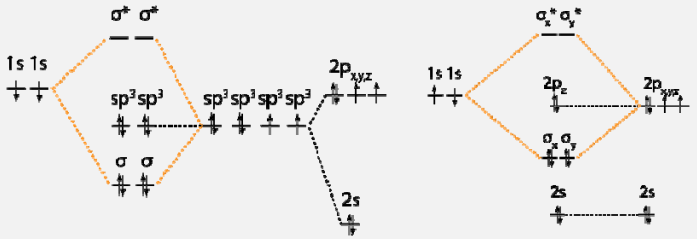
sp^3 hybrid AO-MO correlation diagram of HOH



BOSTON UNIVERSITY

16

Compare AO-MO correlation diagrams of HOH



Polyatomic MO recipe: Formaldehyde, H_2CO

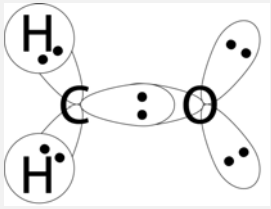
1. Use the Lewis structure to get ...
   - the number of electron pairs
   - make hybrid AO's on each central atom;
     terminal atoms (except H) have same hybrids as central atom

Polyatomic MO recipe: Formaldehyde, H_2CO

1. Use the Lewis structure to get ...
   - the number of electron pairs
   - make hybrid AO's on each atom;
     terminal atoms (except H) have same hybrids as central atom
2. Sketch the σ framework and place pairs ...
   - in each bonding σ MO
   - in each nonbonding hybrid AO

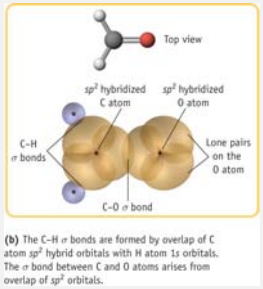
Formaldehyde, H_2CO, σ framework

6 pairs in Lewis structure, 5 pairs in σ framework,
and so 1 pair in (localized) π framework.



H_2CO sp^2 σ framework

6 pairs in Lewis structure, 5 pairs in σ framework,
and so 1 pair in (localized) π framework.



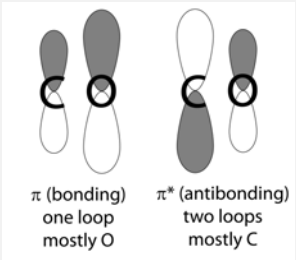
(b) The C–H σ bonds are formed by overlap of C atom sp^2 hybrid orbitals with H atom 1s orbitals. The σ bond between C and O atoms arises from overlap of sp^2 orbitals.

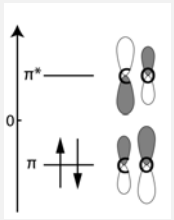
Polyatomic MO recipe: Formaldehyde, H_2CO

1. Use the Lewis structure to get ...
   - the number of electron pairs
   - make hybrid AO's on each atom;
     terminal atoms (except H) have same hybrids as central atom
2. Sketch the σ framework and place pairs ...
   - in each bonding σ MO
   - in each nonbonding hybrid AO
3. Sketch the π framework MO's:
   - mark as bonding, nonbonding, and antibonding
   - place remaining pairs (Auf Bau)
   - get the π bond order

H_2CO π framework

1 pair in (localized) π framework





1 pair in π (bonding); bond order 1

