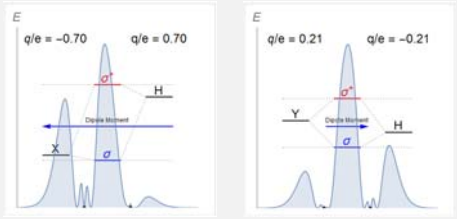
[TP] Which molecule has stronger covalent bonding?

33% 1. XH
33% 2. YH
33% 3. They are equal



BOSTON UNIVERSITY

Lecture 2 CH102 A2 (MWF 11:15 am)

Monday, January 22, 2018

- Covalent versus ionic character
- MO description of hydroxide, OH^-
- MO description of water

Next: Accounting for molecular shape: Hybrid AOs; Water again: Hybrid AO-MO description; Polyatomic MO recipe: Formaldehyde, H_2CO (localized π bond)

"Hybrid AOs and Polyatomic MOs," http://goo.gl/6hBD8X ;

BOSTON UNIVERSITY

Practice

Questions on Symmetry, Overlap, Energy
http://goo.gl/oYEf3b

BOSTON UNIVERSITY

[Quiz] Atom X has $IE_1 = 17$ eV and atom Y has $IE_1 = 12$ eV. Compared to molecule X:H, ...

0% 1. molecule Y:H has a greater dipole moment
0% 2. molecule Y:H has the same dipole moment
0% 3. molecule Y:H has a smaller dipole moment
0% 4. Neither molecule is polar
0% 5. Cannot know relative polarity without knowing the electronegativities of atoms H, X, and Y.

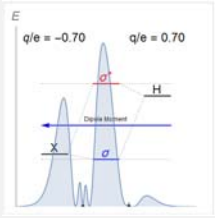
BOSTON UNIVERSITY

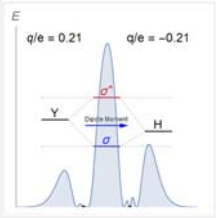
Covalent versus ionic character

Atom X has $IE_1 = 17$ eV, atom Y has $IE_1 = 12$ eV , and H has $IE_1 = 13.6$ eV.

Since the ionization energies of X:H differ more than those of Y:H, ...

X:H has a larger dipole moment than Y:H.

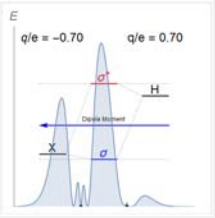


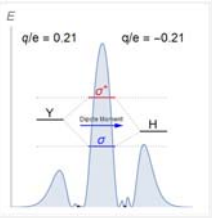


BOSTON UNIVERSITY

[TP] Which molecule has a stronger covalent bonding?

33% 1. XH
33% 2. YH
33% 3. They are equal

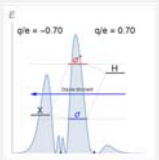


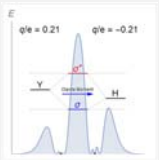


BOSTON UNIVERSITY

Covalent versus ionic character

The charge shift results in the contribution $\frac{\delta^- e \times \delta^+ e}{4\pi\epsilon_0 R_e}$ to the bond strength.

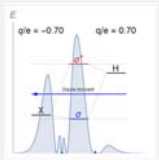


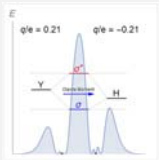


BOSTON UNIVERSITY

Covalent versus ionic character

The charge shift results in the contribution $\frac{\delta^- e \times \delta^+ e}{4\pi\epsilon_0 R_e}$ to the bond strength.





While XH has smaller covalent bond effect, its larger charge shift means it has a larger ionic contribution to the bonding,

$$\left|\frac{\delta^- e \times \delta^+ e}{4\pi\epsilon_0 R_e}\right| = \left|-\frac{0.70^2 e^2}{4\pi\epsilon_0 R_e}\right| > \left|-\frac{0.21^2 e^2}{4\pi\epsilon_0 R_e}\right|$$

For this reason, we say XH has more ionic character than YH

BOSTON UNIVERSITY

MO description of water

BOSTON UNIVERSITY

13

Sketch the AO-MO correlation diagram of HO^-

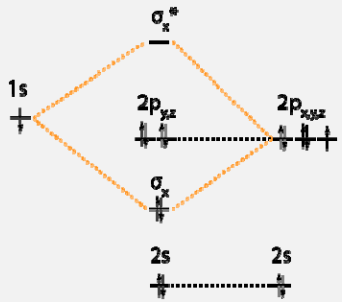
Note: $IE_O > IE_H$

BOSTON UNIVERSITY

14

Sketch the AO-MO correlation diagram of HO^-

Note: $IE_O > IE_H$

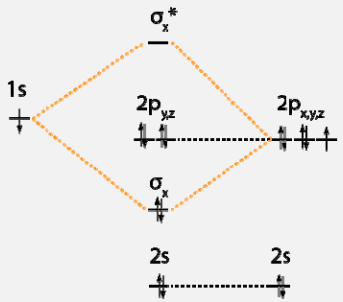


BOSTON UNIVERSITY

15

Sketch the AO-MO correlation diagram of HO^-

Why is the O 2s AO nonbonding?

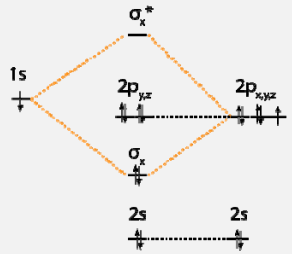


BOSTON UNIVERSITY

16

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

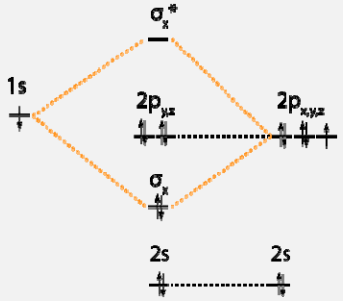
0% 1. it has no net overlap with the H 1s AO
0% 2. It has the wrong symmetry
0% 3. it has a lower ionization energy than the O 2p AOs
0% 4. it has a larger Z_{eff} than the O 2p AOs



BOSTON UNIVERSITY

Sketch the AO-MO correlation diagram of HO^-

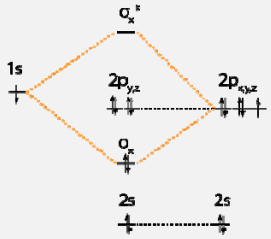
Why are two of the O 2p AOs nonbonding?



BOSTON UNIVERSITY

[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 H 1s AO
25% 4. 2 and 3



BOSTON UNIVERSITY

Response Counter 10

Sketch the AO-MO correlation diagram of HOH

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

BOSTON UNIVERSITY

