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[TP] Atom X have $IE_1 = 17 \text{ eV}$ and atom Y has $IE_1 = 12 \text{ eV}$.
Compared to molecule X:H, ...

20% 1. molecule Y:H has a **greater** dipole moment
20% 2. molecule Y:H has **the same** dipole moment
20% 3. molecule Y:H has a **smaller** dipole moment
20% 4. Neither molecule is polar
20% 5. Cannot know relative polarity without knowing the electronegativities of atoms H, X, and Y.

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Monday, December 12, 2016

- Evaluation
- When atoms are different, which AO's make MO's
- Origin of polarity
- 2p MO's <https://goo.gl/2MEiRA>
- B_2 to Ne_2

Bonding in diatomic molecules <http://goo.gl/1h0S9C>
Questions on Symmetry, Overlap, Energy (SOE) <http://goo.gl/oYEF3b>

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Evaluation

CAS/GRS CH 101 Section: A1

Course Title, Instructor, or Semester/Year: **Not needed**

4. [Do not answer, not applicable]

5. [Do not answer, not applicable]

Reverse side: Comments section: Clear detail will be most helpful

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When atoms are different, which AO's combine?

SOE: Symmetry, Overlap, Energy

- **Symmetry:** Which AO's are able to combine to form MO's?
- **Overlap:** Which AO's combine with the greatest bonding/antibonding effect?
- **Energy:** How does relative AO energy affect composition of MO's?

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Symmetry: Net overlap or not?

- For a pair of AO's to give a (**bonding/antibonding**) pair of MO's, there must be **net overlap** (net in-phase or net out-of-phase).
- If in-phase and out of phase overlap **exactly cancel**, the AO's remain uncombined, as **nonbonding orbitals**.

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Overlap: Greater the better

- The more net overlap, the greater the bonding/antibonding effect.
- Core AO's have least overlap
- Valence AO's have greatest overlap
- Bonding due to MO's made from valence AO's

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Energy: Closer the better

- The **closer** AO's are in energy, the **greater** the bonding/antibonding effect.
- If AO's have **same energy** (identical atoms, homonuclear bond), MO's will be **50% of each AO**.
- If AO's have **different energy** (different atoms, heteronuclear bond), ...
 - **Bonding MO** → contains more of the lower energy AO
 - **Antibonding MO** → contains more of the higher energy AO

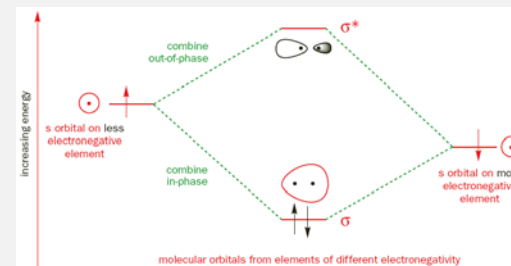
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Energy: Closer the better

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Energy: Closer the better

energy

3s

2p

Na Na⁺ F⁻ F

sodium atom sodium ion fluoride ion fluorine atom

this electron transferred from 3s(Na) to 2p(F)

the atomic orbitals are too far apart to combine with each other to form a new molecular orbital

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Energy: Closer the better

Enegies of AOs both the same

AO on atom B is a little lower in energy than AO on atom A

AO on atom B is a lot lower in energy than AO on atom A

large interaction between AOs

less interaction between AOs

AOs are too far apart in energy to interact

bonding MO much lower in energy than AOs

bonding MO is lowered only by a small amount relative to AO on atom B

antibonding MO is much higher in the energy than the AOs

antibonding MO is raised in energy by only a small amount relative to AO on atom B

both AOs contribute equally to the MOs

electrons in bonding MO are shared equally between the two atoms

the AO on B contributes more to the bonding MO and the AO on A

electrons in bonding MO are shared between atoms BUT are associated more with atom B than A

only one AO contributes to each MO

electrons in the filled orbital are located only on atom B

bond between A and B would classically be described as purely covalent

bond between A and B is covalent but there is also some electrostatic (ionic) attraction between atoms

bond between A and B would classically be described as purely ionic

resistant to break bond into two ions, A⁺ and B⁻, although it is also possible to give two radicals

component already exists as ions A⁺ and B⁻

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[TP] Assume AO_1 and AO_2 have correct relative symmetry, greatest overlap, and are closest in energy. AO_1 has $IE = 5$ eV and AO_2 has $IE = 6$ eV. Which of the following is true?

17% 1. Bonding MO has more AO_1 than AO_2

17% 2. Bonding MO has more AO_2 than AO_1

17% 3. Antibonding MO is almost entirely AO_1

17% 4. Antibonding MO is almost entirely AO_2

17% 5. 1 and 4

17% 6. I do not know how to tell.

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

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Practice

Questions on Symmetry, Overlap, Energy

<http://goo.gl/oYEF3b>



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MO's in B_2 , C_2 , etc.

Build MOs from 2p AO's

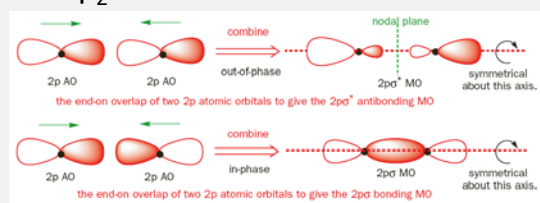


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$2p_z\sigma$ and $2p_z\sigma^*$

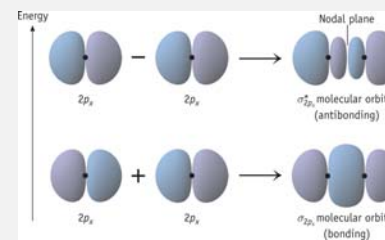


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$2p_z\sigma$ and $2p_z\sigma^*$



Mahaffy et al., Figure 10.23, p. 403



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$2p_z\sigma$ (lower) and $2p_z\sigma^*$ (upper)

$2p_z$ molecular orbitals:
<http://quantum.bu.edu/CDF/101/2pMolecularOrbitals.cdf>

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$2p_x\pi$ and $2p_x\pi^*$

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$2p_x\pi$ and $2p_x\pi^*$

Mahafy et al., Figure 10.24, p. 403

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B_2 to Ne_2

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Homonuclear diatomics, up to N₂

Mahaffy et al., 1e, Figure 10.25

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Homonuclear diatomics, after N₂

the 1s and 1s* MOs are much lower in energy than the other MOs

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Homonuclear diatomics

	Li ₂	B ₂	C ₂	N ₂	O ₂	F ₂	
σ_{2p}^*							σ_{2p}^*
π_{2p}^*, π_{2p}^*							π_{2p}^*, π_{2p}^*
σ_{2p}							
π_{2p}, π_{2p}							π_{2p}, π_{2p}
σ_{2s}^*							σ_{2s}^*
σ_{2s}							σ_{2s}

Laird, University Chemistry, Figure 3.4

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