Bond order and bond energy

CH101 Fall 2012
Boston University

BOSTON UNIVERSITY

[TP] Which of the following has the **highest bond order**?

0% 1. Li_2^{2+}
0% 2. Li_2^{+}
0% 3. Li_2^{-}
0% 4. Li_2^{2-}
0% 5. Li_2^{+} and Li_2^{-}
0% 6. Li_2^{2+} and Li_2^{2-}

BOSTON UNIVERSITY

0 of 5

10 Countdown Timer On Slide

2

Bond order and bond energy

The lowest energy (most stable) s AO of atom X has energy −10 eV.

X_2 has a σ (bonding) MO of energy −12 eV and a σ* (antibonding) MO of energy −7 eV.

Draw the correlation diagram.

BOSTON UNIVERSITY

3

Bond order and bond energy

The lowest energy (most stable) s AO of atom X has energy −10 eV.

X_2 has a σ (bonding) MO of energy −12 eV and a σ* (antibonding) MO of energy −7 eV.

X_2^+ has one electron in the σ MO and none in the σ* MO.

Calculate the bond order of X_2^+.

Calculate the bond energy of X_2^+.

E_{far} = 1 x (−10 eV) = −10 eV

E_{close} = 1 x (−12 eV) = −12 eV

Bond strength = $E_{far} - E_{close}$ = +2 eV

BOSTON UNIVERSITY

4

Bond order and bond energy

The lowest energy (most stable) s AO of atom X has energy −10 eV.

X_2 has a σ (bonding) MO of energy −12 eV and a σ* (antibonding) MO of energy −7 eV.

X_2^- has two electrons in the σ MO and one in the σ* MO.

Calculate the bond order of X_2^-.

Calculate the bond energy of X_2^-.

E_{far} = 2 x (−10 eV) + 1 x (−10 eV) = −30 eV

E_{close} = 2 x (−12 eV) + 1 x (−7 eV) = −31 eV

Bond energy = $E_{far} - E_{close}$ = +1 eV

BOSTON UNIVERSITY

5

Bond order and bond strength

The lowest energy (most stable) s AO of atom X has energy −10 eV.

X_2 has a σ (bonding) MO of energy −12 eV and a σ* (antibonding) MO of energy −7 eV.

X_2^- has two electrons in the σ MO and one in the σ* MO.

X_2^+ and X_2^- have the same bond order 1/2

X_2^+ had bond strength 2 eV: $X_2^+ \rightarrow X + X^+$ ΔE = 2 eV

X_2^- has bond strength 1 eV: $X_2^- \rightarrow X + X^-$ ΔE = 1 eV

BOSTON UNIVERSITY

6

[TP] Which of the following has the **largest bond energy**? (the **strongest bond**)?

0% 1. X_2^{2+}
0% 2. X_2^{+}
0% 3. X_2^{-}
0% 4. X_2^{2-}
0% 5. X_2^{+} and X_2^{-}
0% 6. X_2^{2+} and X_2^{2-}

BOSTON UNIVERSITY

0 of 5

10 Countdown Timer On Slide

7

[TP] Use the same approach we used for analysis of diatomic ions of X to determine which of the following has the **largest bond energy** (**strongest bond**)?

0% 1. Li_2^{2+}
0% 2. Li_2^{+}
0% 3. Li_2^{-}
0% 4. Li_2^{2-}
0% 5. Li_2^{+} and Li_2^{-}
0% 6. Li_2^{2+} and Li_2^{2-}

BOSTON UNIVERSITY

0 of 5

10 Countdown Timer On Slide

8

Bond order and bond energy

The lowest energy (most stable) s AO of atom X has energy −10 eV.

X_2 has a σ (bonding) MO of energy −12 eV and a σ* (antibonding) MO of energy −7 eV.

X_2^{2+} has no electrons in the σ MO and none in the σ* MO.

Calculate the bond order of X_2^{2+}.

Calculate ΔE for the reaction $X_2^{2+} \rightarrow X^+ + X^+$.

Explain whether your answer makes physical sense.

BOSTON UNIVERSITY

9

Bond order and bond energy

The lowest energy (most stable) s AO of atom X has energy −10 eV.

X_2 has a σ (bonding) MO of energy −12 eV and a σ* (antibonding) MO of energy −7 eV.

X_2^{2-} has two electrons in the σ MO and two in the σ* MO.

Calculate the bond order of X_2^{2-}.

Calculate ΔE for the reaction $X_2^{2-} \rightarrow X^- + X^-$.

Explain whether your answer makes physical sense.

BOSTON UNIVERSITY

10