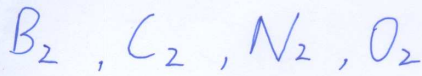


量化的 Quiz 7, 2015, 6, 1

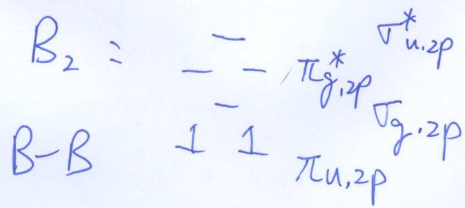
1. Draw molecular orbital diagrams for



60(%)

$B_2: r_e = 1.59 \text{ \AA}, D_e = 190 \text{ kJ/mol} \approx 2.0 \text{ eV}$

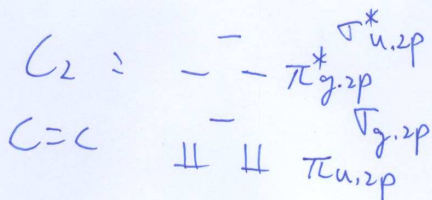
what are their bond order
compare with their r_e, D_e



bond order = $\frac{2-0}{2} = 1$

$r_e = 1.59 \text{ \AA}$

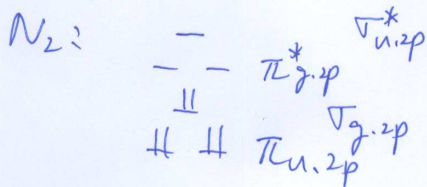
$D_e = 2.0 \text{ (eV)}$



bond order = $\frac{4-0}{2} = 2$

$r_e = 1.24 \text{ \AA}$

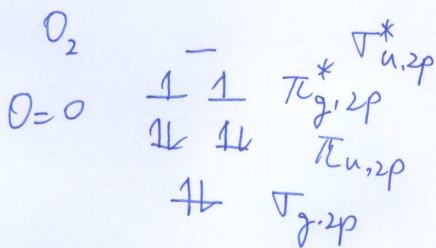
$D_e = 6.3 \text{ (eV)}$



bond order = $\frac{6-0}{2} = 3$

$r_e = 1.10 \text{ \AA}$

$D_e = 9.7 \text{ (eV)}$



bond order = $\frac{6-2}{2} = 2$

$r_e = 1.21 \text{ \AA}$

$D_e = 5.2 \text{ eV}$

bond order: $N_2 > C_2 = O_2 > B_2$

$D_e: N_2 > C_2 > O_2 > B_2$

$r_e: N_2 < O_2 < C_2 < B_2$

因 bond order \uparrow , 鍵的数目 \uparrow

鍵長 \downarrow , 鍵能 \uparrow