ADVANCED CHEMISTRY

QUANTUM MECHANICS - SPRING - WEEK 4

Chapter 11

(9)

$$\psi_{sp^2(i)} = \frac{1}{\sqrt{3}} 2s + \sqrt{\frac{2}{3}} 2p_z$$

$$\psi^*_{sp^2(i)} = \frac{1}{\sqrt{3}} 2s^* + \sqrt{\frac{2}{3}} 2p_z^*$$

$$\int \psi^*_{sp^2(i)} \psi_{sp^2(i)} d\tau = \int \left(\frac{1}{\sqrt{3}} 2s^* + \sqrt{\frac{2}{3}} 2p_z^*\right)\left(\frac{1}{\sqrt{3}} 2s + \sqrt{\frac{2}{3}} 2p_z\right) d\tau$$

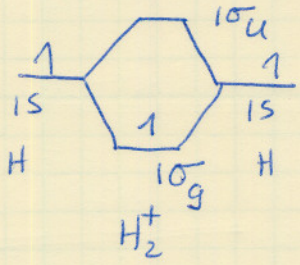
$$= \frac{1}{3}\int \overbrace{2s^* 2s\, d\tau}^{=1} + \frac{\sqrt{2}}{3}\int \overbrace{2s^* 2p_z\, d\tau}^{=0} + \frac{\sqrt{2}}{3}\int \overbrace{2p_z^* 2s\, d\tau}^{=0}$$

$$+ \frac{2}{3}\int \underbrace{2p_z^* 2p_z}_{=1} d\tau$$

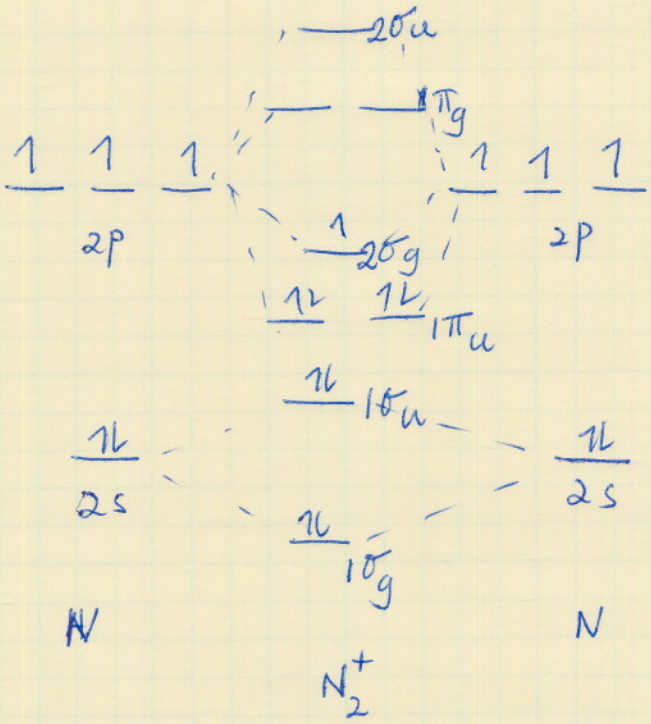
$$= \frac{1}{3}(1) + \frac{\sqrt{2}}{3}(0) + \frac{\sqrt{2}}{3}(0) + \frac{2}{3}(1) = 1$$

$\therefore \psi_{sp^2(i)}$ is normalized

(11)

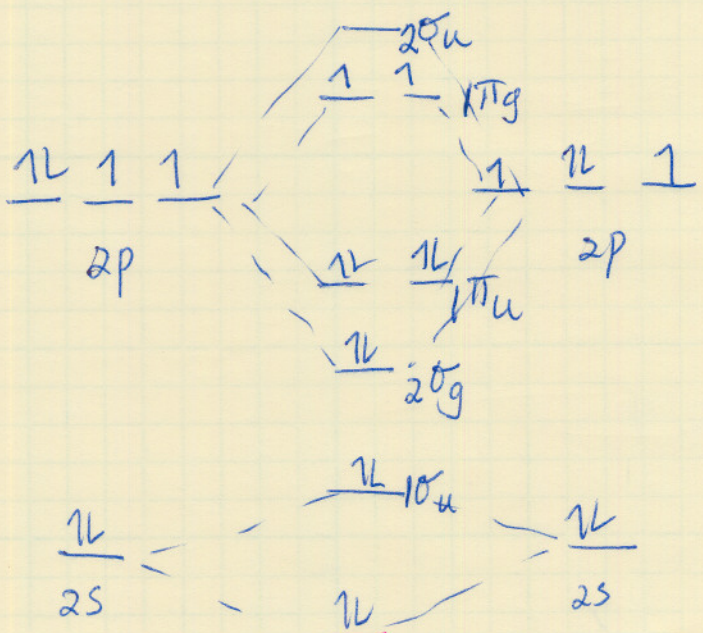


Bond order = $\frac{1}{2}(1-0) = \frac{1}{2}$



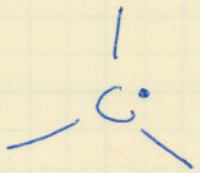
Bond order for N_2^+ = $\frac{1}{2}(7-2)$ = 2.5

Bond order for N_2 = $\frac{1}{2}(8-2)$ = 3

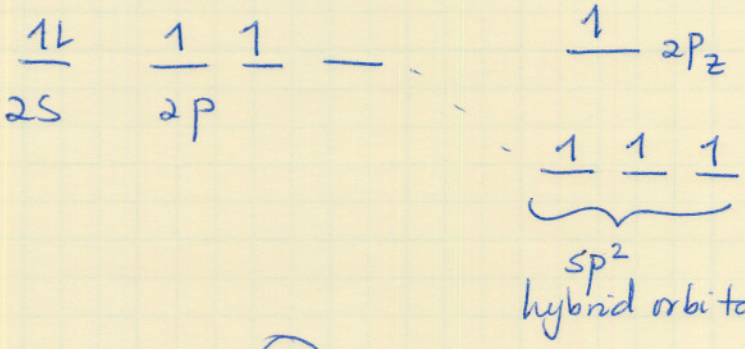


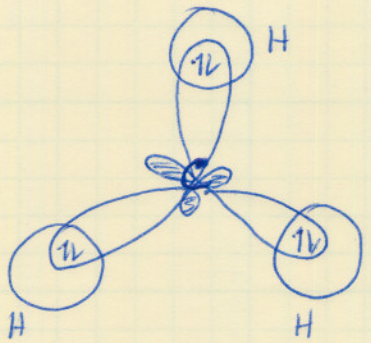
Bond order = $\frac{1}{2}(8-4)$ = 2

(12)



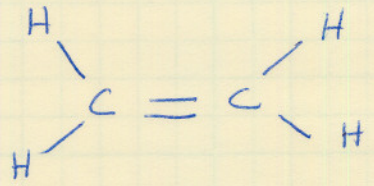
C atom is sp^2 hybridized.
CH_3 is a planar radical.





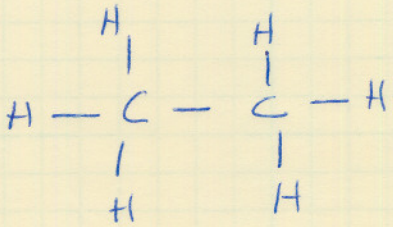
The sp^2 hybrid orbitals contain a single electron that then overlaps with the 1S orbitals (containing a single electron) to form three C–H single bonds. The unhybridized p_z orbital, perpendicular to the plane of the CH_3 radical contains the unpaired electron.

(13) (a)



there are 5 σ bonds (10 electrons) and one π bond (2 $\bar{e}$)

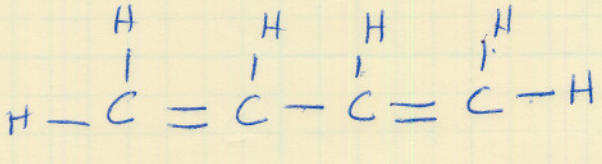
(b)



7 σ bonds (14 $\bar{e}$)

no π bonds

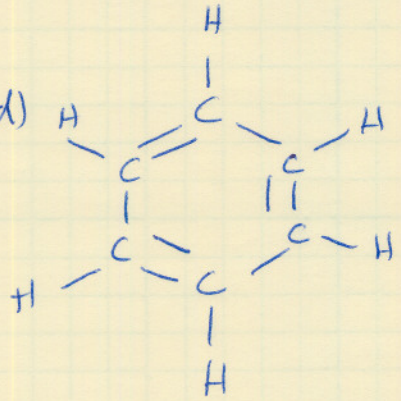
(c)



9 σ bonds (18 $\bar{e}$)

2 π bonds (4 $\bar{e}$)

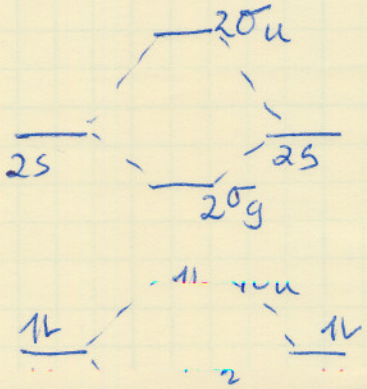
(d)



12 σ bonds (24 $\bar{e}$)

3 π bonds (6 $\bar{e}$)

(25)



$(1\sigma_g)^2 (1\sigma_u)^1 (2\sigma_g)^1$

S = 0, 1 (singlet or triplet states possible)

bond order = $\frac{1}{2}(3-1) = 1$

From the worksheet

H_2^+ $\underline{1}\ \sigma_g$ $S = 1/2$ $\Lambda = 0$ $^2\Sigma_g^+$

H_2 $\underline{1\downarrow}\ \sigma_g$ closed orbital $^1\Sigma_g^+$

He_2^+ $(1\sigma_g)^2 (1\sigma_u)^1$ $\underline{1}\ 1\sigma_u$ $S = 1/2$ $\Lambda = 0$ $^2\Sigma_u^+$

He_2 closed orbital $^1\Sigma_g^+$

Li_2 $2\sigma_u$ — $\underline{1}$ (2s) $\quad$ $\underline{1}$ (2s) $1\sigma_g$ — $\underline{1\downarrow}$ $2\sigma_g$ closed orbital $^1\Sigma_g^+$

Be_2 $(2\sigma_g)^2 (2\sigma_u)^2$ closed orbital $^1\Sigma_g^+$

B_2 $3\sigma_u$ — $1\pi_g$ — $\underline{1}$ (2p) $\quad$ $\underline{1}$ (2p) $3\sigma_g$ — $\underline{1}\ \underline{1}\ 1\pi_u$ π^2 configuration

$S = 0, 1$

$\Lambda = 2, 0$

possible terms $^1\Sigma^+$ $^3\Sigma^-$ $^1\Delta$

$^3\Sigma_g^-$ is ground state

C_2 $(1\pi_u)^4$ closed orbital $^1\Sigma_g^+$

N_2^+ $(3\sigma_g)^1$ $^2\Sigma_g^+$

N_2 $(3\sigma_g)^2$ closed orbital $^1\Sigma_g^+$

O_2^+ $(1\pi_g)^1$ $^2\Pi_g$ (regular)

O_2 $(1\pi_g)^2$ π^2 configuration $^1\Sigma_g^+$ $^3\Sigma_g^-$ $^1\Delta_g$

ground state is $^3\Sigma_g^-$

F_2 $(1\pi_g)^4$ Closed orbital $^1\Sigma_g^+$

Ne_2 $(3\sigma_u)^2$ closed orbital $^1\Sigma_g^+$