Session #10: Homework Solutions

Problem #1

One of the two compounds, NH_3 or BF_3, is found to exhibit a permanent dipole moment. Identify the polar species and account for the different bonding characteristics of the two species. (Make appropriate sketches of the respective bonding configurations.)

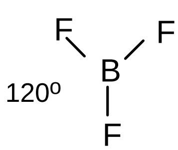
Solution

The answer to this question is found by looking at the valence shell configurations of B and N:

B: $2s^2p^1$

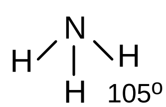
N: $2s^2p^3$

We realize that boron can hybridize into a planar sp^2 bonding configuration and form three σ bonds with fluorine. The compound is expected to be internally polarized, but no permanent dipole will thus result because of the bonding symmetry. Nitrogen has three singly occupied 2p orbitals directed at right angles to each other. Upon σ bond formation in NH_3, we anticipate a pyramidal configuration with nitrogen at the apex. Because of bond polarization (Δx = 0.82), mutual repulsion of the activated hydrogen atoms is anticipated to increase the bond angle (which is found to be 105^o). In fact, the large bond angle observed in NH^3 suggests sp^3 hybridization similar to that invoked in H_2O. In either case, the resulting molecule will exhibit a permanent dipole moment.



(planar)

$\boxed{\text{non–polar}}$



(sp^3 hybridization)

$\boxed{\text{polar}}$

Problem #2

(a) Determine the inter-ionic equilibrium distance between the sodium and chlorine ions in a sodium chloride molecule knowing that the bond energy is 3.84 eV and that the repulsive exponent is 8.

(b) At the equilibrium distance, how much (in percent) is the contribution to the attractive bond energy by electron shell repulsion?

Solution

(a) $E_{equ} = -3.84 \text{ eV} = -3.84 \times 1.6 \times 10^{-19} \text{ J} = -\dfrac{e^2}{4\pi\varepsilon_o r_o}\left(1 - \dfrac{1}{n}\right)$

$$r_o = \frac{(1.6 \times 10^{-19})^2}{4\pi 8.85 \times 10^{-12} \times 6.14 \times 10^{-19}}\left(1 - \frac{1}{8}\right) = 3.3 \times 10^{-10}\text{m}$$

(b) Shell "repulsion" obviously constitutes a "negative" contribution to the bond energy. Looking at the energy equation we find:

the attractive term as: $-E \times (1) = -E$
the repulsion term as: $-E \times (-1/n) = E/n = E/8$

The contribution to the bond energy by the repulsion term = 1/8 x 100 =**12.5%.**

(Since the bond energy is negative, the 12.5% constitute a reduction in bond strength.)

Problem #3

Boron (B) reacts with bromine (Br_2) to form a compound which is not polar (does not have a dipole moment).

(a) Give the compound formed in Lewis notation.

(b) List all bonding orbitals which on orbital overlap lead to the formation of this compound.

(c) Do you expect the compound to exhibit a dipole moment or not? Why?

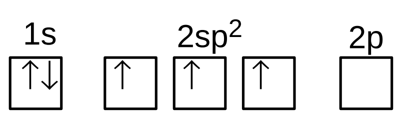
Solution

B: $1s^2 2s^2 2p^1$

Br: [Ar] $4s^2 3d^{10} 4p^5$

(a) If B shares its $2p^1$ electron with Br's $4p^5$ shell, they will both obtain somewhat stable valence shells. However, BBr would be polar.

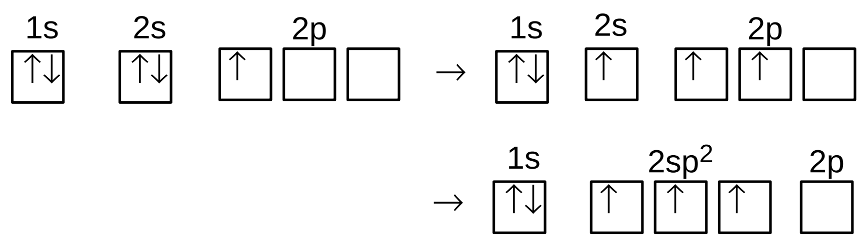
If B hybridizes and its electron shell changes to

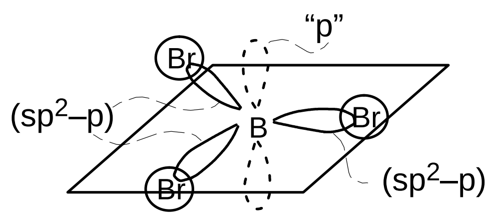


then the B can bond with 3 Br. **BBr_3: 3(sp^2–p overlap) σ bonds**

The symmetry of the hybridized (planar) molecule leads to coincidence of the centers of + and – charges –– the molecule, in spite of three polar covalencies, does not exhibit a dipole moment.

(b)





(c) All three bonds are based on sp^2 orbital overlap, leading to the formation of σ bonds.