CHEM 361B - Lecture 17 Activity

Hybridised Orbitals

1. Bent's Rules

   Here is a qualitative set of rules, developed by Henry Bent, that you can use to qualitatively estimate bond angles:

   - Central Atoms that obey the octet rule can be classified into three structure types:
     - Central Atoms with four single bonds or electron pairs are to a first approximation described with a tetrahedral (sp^3) geometry
     - Central Atoms with a double bond a any combination of two single bonds or electron pairs are to a first approximation described with a trigonal planar (sp^2) geometry
     - Central Atoms with two double bonds or a triple bond and a single bond or electron pair are to a first approximation described with a linear (sp) geometry
   - The s and p character of each non-equivalent ligand is determined by the electronegativity of the ligand. Electron pairs are considered to have very low electronegativity. Atomic s character concentrates in hybrid orbitals directed towards low electronegative ligands while atomic p character concentrates in hybrid orbitals directed towards high electronegative ligands. The higher the p character in a hybridized orbital, the lower the bond angle.

   Using this information predict

   (a) If the H–O–H bond angle in H_2O is greater than, equal to or less than 109.5°.

   (b) If the X–C–X bond angle in F_2CO is larger or smaller than in H_2CO

   (c) If the H–C–H bond angle in FCH_3 is greater than, equal to or less than 109.5°.

2. We will predict that the angle between sp^2 hybridised orbitals is 120°.

   (a) We can generalise the three sp^2 hybridised orbitals as

   $$\begin{aligned}\xi_1 =& a_1 2s + b_1 2p_x + c_1 2p_y + d_1 2p_z \\ \xi_2 =& a_2 2s + b_2 2p_x + c_2 2p_y + d_2 2p_z \\ \xi_3 =& a_3 2s + b_3 2p_x + c_3 2p_y + d_3 2p_z\end{aligned}$$

   If we were to align all three of these orbitals in the x-z plane, and ξ_1 along the z-axis, argue that $b_1 = c_1 = c_2 = c_3 = 0$.

   (b) Argue that following relationships true

   i.

   $$a_1 = a_2 = a_3$$

ii.

$$a_1^2 + a_2^2 + a_3^2 = 1$$

(c) Using the above relationships, show that $a_1 = a_2 = a_3 = \frac{1}{\sqrt{3}}$

(d) Normalise ξ_1 to show that $d_1 = \sqrt{\frac{2}{3}}$. We have now completely defined ξ_1

(e) Using the fact that ξ_1 and ξ_2 are separate, independent states, show that $d_2 = -\sqrt{\frac{1}{6}}$.

(f) Normalise ξ_2 to show that $b_2 = \sqrt{\frac{1}{2}}$. We have now completely defined ξ_2.

(g) Now that we have two completely defined hybridised orbitals, we can calculate the angle between them

i. For this part of the process calculation, why can we set $\phi = 0$?

ii. To determine the angle between ξ_1 and ξ_2, why is doing the following appropriate

$$\frac{d}{d\theta}\left[\xi_2\right] = 0$$

iii. Show that the angle between between ξ_1 and ξ_2 is 120°.