Objective

After completing this section, you should be able to describe the structure of methane in terms of the $sp^3$ hybridization of the central carbon atom.

Key Terms

Make certain that you can define, and use in context, the key terms below.

- bond angle
- hybridization
- $sp^3$ hybrid

Study Notes

The tetrahedral shape is a very important one in organic chemistry, as it is the basic shape of all compounds in which a carbon atom is bonded to four other atoms. Note that the tetrahedral bond angle of $\text{H–C–H}$ is 109.5°.

Bonding in Methane, CH$_4$

Edit section

We are starting with methane because it is the simplest case which illustrates the sort of processes involved. You might remember that the bonding picture of methane looks like this.

There is a serious mismatch between this structure and the modern electronic structure of carbon, $1s^22s^22p_x^12p_y^1$. The modern structure shows that there are only 2 unpaired electrons to share with hydrogens, instead of the 4 which the bonding picture requires.

You can see this more readily using the electrons-in-boxes notation. Only the 2nd level electrons are shown. The 1s$^2$ electrons are too deep inside the atom to be involved in bonding. The only electrons directly available for sharing are the
2p electrons. Why then isn't methane CH$_2$?

**Promotion of an electron**

**Edit section**

When bonds are formed, energy is released and the system becomes more stable. If carbon forms 4 bonds rather than 2, twice as much energy is released and so the resulting molecule becomes even more stable. There is only a small energy gap between the 2s and 2p orbitals, and so it pays the carbon to provide a small amount of energy to promote an electron from the 2s to the empty 2p to give 4 unpaired electrons. The extra energy released when the bonds form more than compensates for the initial input.

![Diagram of electron promotion](image)

The carbon atom is now said to be in an excited state. Now that we've got 4 unpaired electrons ready for bonding, another problem arises. In methane all the carbon-hydrogen bonds are identical, but our electrons are in two different kinds of orbitals. You aren't going to get four identical bonds unless you start from four identical orbitals.

**Hybridization**

**Edit section**

The electrons rearrange themselves again in a process called hybridization. This reorganizes the electrons into four identical hybrid orbitals called sp$^3$ hybrids (because they are made from one s orbital and three p orbitals). You should read "sp$^3$" as "s p three" - not as "s p cubed".

![Diagram of sp$^3$ hybrid orbitals](image)
sp³ hybrid orbitals look a bit like half a p orbital, and they arrange themselves in space so that they are as far apart as possible. You can picture the nucleus as being at the center of a tetrahedron (a triangularly based pyramid) with the orbitals pointing to the corners. For clarity, the nucleus is drawn far larger than it really is.

What happens when the bonds are formed?

Edit section

Remember that hydrogen’s electron is in a 1s orbital - a spherically symmetric region of space surrounding the nucleus where there is some fixed chance (say 95%) of finding the electron. When a covalent bond is formed, the atomic orbitals (the orbitals in the individual atoms) merge to produce a new molecular orbital which contains the electron pair which creates the bond.

Four molecular orbitals are formed, looking rather like the original sp³ hybrids, but with a hydrogen nucleus embedded in each lobe. Each orbital holds the 2 electrons that we’ve previously drawn as a dot and a cross. The principles involved - promotion of electrons if necessary, then hybridization, followed by the formation of molecular orbitals - can be applied to any covalently-bound molecule.

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