

TETRAVALENT CARBON AND ITS HYBRIDIZATION

A few words

Organic Chemistry is mainly the chemistry of carbon, which is just one element out of the over-hundred elements in the periodic table. But due to its unique position in the periodic table it has become the most important of them all and it's because of carbon and its unique properties that life is as we know it. The three most significant properties of carbon which have overlapping functions are:

1. Its size
2. Tetravalency
3. Property of catenation or forming long chains with itself

Details of these properties can be found in any standard inorganic textbook.

Because of the diversity in organic compounds (they range from acetone in nail polish remover and ethyl alcohol in whisky to complex macromolecules like proteins and nucleic acids which are in comparison monster molecules), it is absolutely imperative to understand in considerable depth how organic molecules react. Understanding the mechanistic profile of different classes of such molecules will not only help us make useful small molecules which can fight cancer, but also help us understand why a certain protein folds in a certain way to develop the cancer in the first place. This may seem a daunting task but surprisingly mechanistic organic chemistry is pretty well developed. A large family of molecules react in the exact same way in similar conditions so several generalizations and rules have been formulated to predict the reactions accurately. So as it rests even a beginner with a basic understanding of structure, reactivity and mechanism can confidently say that he knows the chemical mechanism by which DNA is replicated!

Tetravalent carbon and hybridization

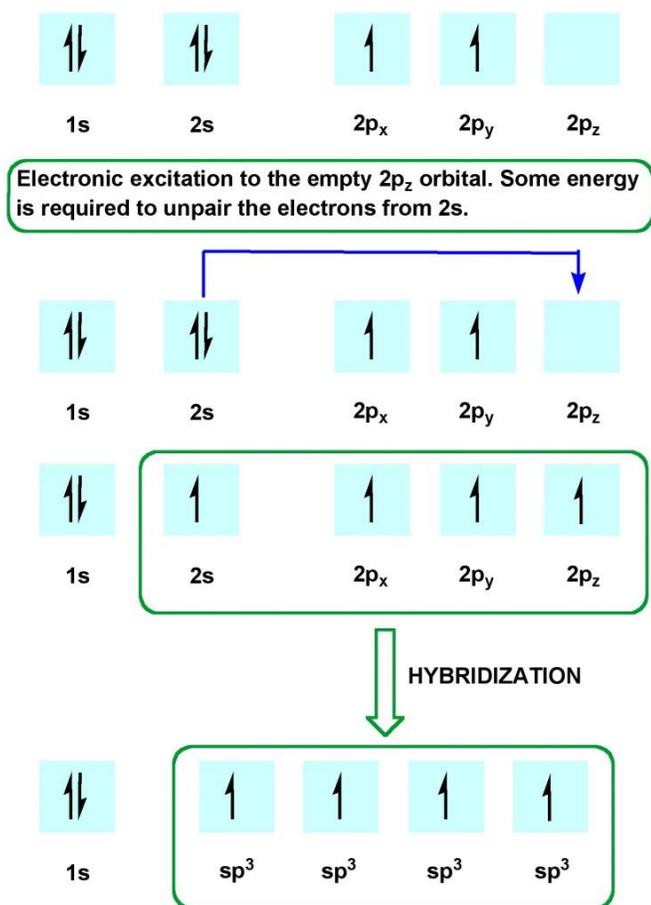


Figure 1. Hybridization of tetraivalent carbon

The ground state electronic configuration of carbon is $1s^2, 2s^2, 2p^2$. So with 4 valence shell electrons it is expected to form 4 bonds. But as we can see the bonds formed by the s orbitals will not be the same as those formed by the p orbitals for the simple reason that their shapes are so different. So for the reaction of C with 4 Hs to form CH_4 , we would have the following bonds: C(s)-H(s), C(s)-H(s), C(p)-H(s), C(p)-H(s). Thus we would have two directional bonds (C(p)-H(s)) and two non-directional bonds (C(s)-H(s)). Also the strengths of the bonds would be different: it would be easier to break the C(p)-H(s) bond than C(s)-H(s) as s orbitals have better electronic overlap. But in reality all the bonds of CH_4 are identical. So we have a problem. To solve this, the concept of hybridization has been used, which is quite popular as it easily explains a lot of bonding but even before we start talking about it it's useful to know that it is an artificial concept which we have created not necessarily something which actually happens in nature. The concept of hybridization has been shown pictorially in figure 1.

In the example three p and one s orbitals mixed or hybridized to give 4 *identical* sp^3 hybrid orbitals. Similar treatment would give rise to sp^2 and sp hybridizations, only differences being in sp^2 only two p orbitals are used, which means one electron in the third p remains unhybridized and there are two such unhybridized p orbitals in case of sp hybridization. It is encouraged that the reader tries to follow the shown approach and perform the hybridization themselves. Also from the VSEPR theory (see any standard inorganic chemistry textbook), it is known that sp^2 and sp hybridized molecules are planar (sp^2 hybridized molecules are trigonal planar and sp hybridized molecules are linear considering three and two groups attached to the central atom respectively), whereas sp^3 centres adopt tetrahedral geometry, which is basically to minimize the energies of the molecules. The angle between each group in case of a tetrahedral geometry is 109.5° , 120° in case of sp^2 and 180° for sp hybridized molecules.

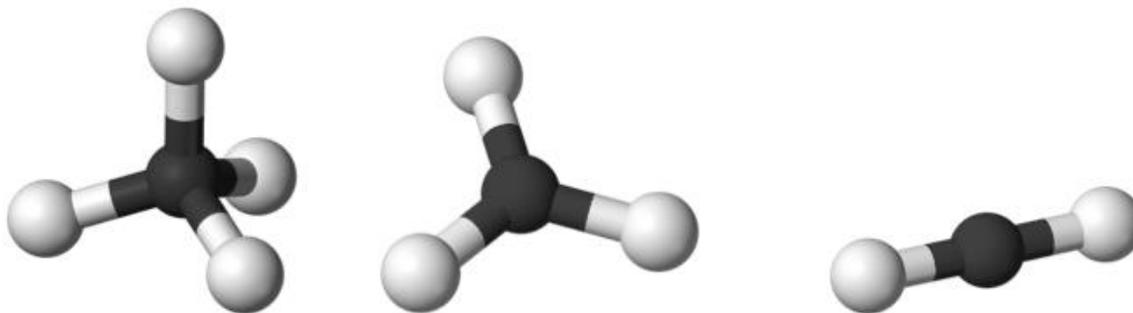


Figure 22. Left: tetrahedral carbon (methane), Center: trigonal planar (ethene), Right: linear (acetylene)

So methane which has an sp^3 carbon is tetrahedral which is indeed what is observed in nature and ethene ($CH_2=CH_2$) and acetylene (C_2H_2) with sp^2 and sp carbons respectively are planar. Now a quick look into the nature of bonding in these molecules before the topic is closed. Since sp^2 and sp Cs have unhybridized p orbitals with an electron in each and the p orbitals are perpendicular to the plane of the molecule (remember p orbitals are always perpendicular to each other as well), in say ethene the two unhybridized p orbitals from each sp^2 C overlap with each other to form a pi bond. So what we know as a double bond in ethene is actually a combination of a sigma (single) bond between two sp^2 orbitals of two Cs and a pi bond between the p orbitals on each C. This is illustrated by the figure 3 below.

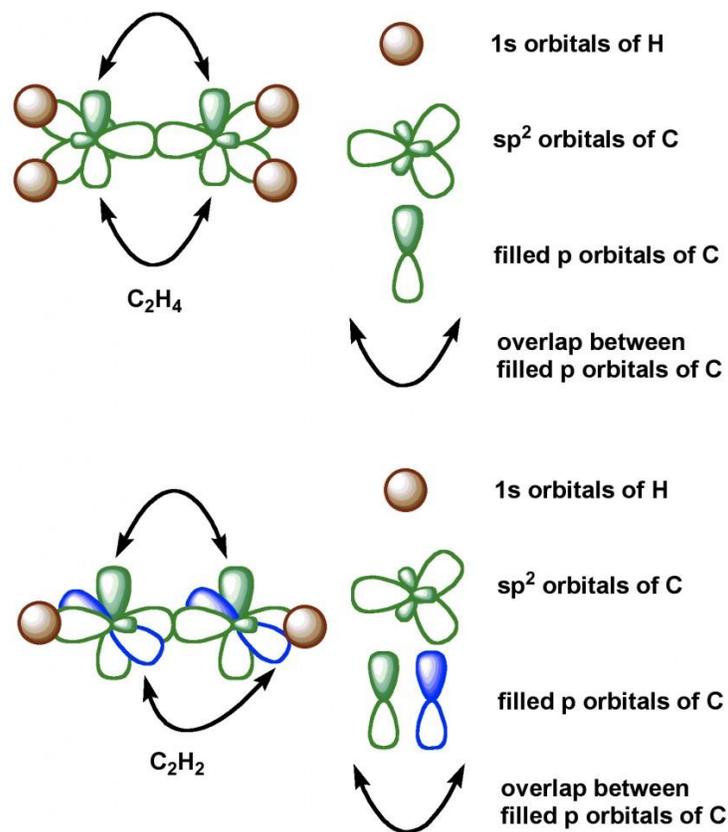


Figure 3. Hybridization of the carbon atoms in ethylene and acetylene

Source : <http://padakshep.org/otp/subjects/chemistry/organic-chemistry/tetravalent-carbon/>