Hybridization
Hybridization of Carbon

\[ \begin{align*}
  &\text{s} \\
  &\text{z} \\
  &\text{y} \\
  &\text{x} \\
  &\mathbf{p}_x \\
  &\mathbf{p}_y \\
  &\mathbf{p}_z
\end{align*} \]
Carbon has, outside its nucleus, six electrons and therefore the ground state electronic configuration of carbon is:

\[ 1S^2 \ 2S^2 \ 2P^2 \]

This, however, represent the ground state of the carbon atom in which only two unpaired electrons are available for bond formation with other atoms, i.e. at first sight carbon might appear to be only divalent.
A typical C-H has a bond strength of 100 Kcal/mol

Net-Energy change = (400-97) Kcal/mol = 300 Kcal/mol

In the excited state carbon has four unpaired electrons and can form four bonds with hydrogen.
Methane - sp$^3$ Hybridized

What is the nature of the four C-H bonds in methane?

Since excited carbon uses two kinds of orbitals (2s and 2p) for bonding purpose, we might expect methane to have two kinds of C-H bonds.

\[
1s^2 \quad 2s^1 \quad 2p_x^1 \quad 2p_y^1 \quad 2p_z^1
\]

In fact this is not the case.

A large amount of evidence show that all four C-H bonds in methane are identical in terms of their length and strength.
The valence orbitals of a carbon atom are neither s or p but a hybrid or mixture of orbitals.

Since three p orbitals are mixed with one s-orbital, we call the hybrid orbitals sp³, meaning that each of them has one-fourth s-character and three-fourth p-character.
Each bond in CH$_4$ is formed by overlap of an sp$^3$ hybrid orbital of carbon with a 1s orbital of hydrogen. These four bonds point to the corners of a tetrahedron.

Bond strength = 104 Kcal/mol
The tetrahedral shape of an sp³ hybridized carbon
All four C – H bonds in methane are sigma (δ) bonds, because the electron density is concentrated on the axis joining C and H and are formed by head on overlap of orbitals.
Ethane (C$_2$H$_6$) – sp$^3$ Hybridization

We can picture the ethane molecule by assuming that the two carbon atoms bond to each other by sigma overlap of an sp$^3$ hybrid orbital from each carbon.
Structure of Ethane

- **sp³ carbon**
- **sp³ carbon**
- **sp³–sp³ sigma bond**
Ethane \((\text{C}_2\text{H}_6)\) – \(\text{sp}^3\) Hybridization
Ethylene (C$_2$H$_4$)-sp$^2$ Hybridization
sp² hybridization of a carbon

ground state

excited state

sp² hybridized state

unhybridized p orbital
sp² hybridized carbon

120°
δ Bond are formed by end-on overlap of two sp$^2$ hybrid orbitals. π bond are formed by side-by-side overlap of two 2p orbitals.

The electron density in a π bond is farther from the two nuclei, π bonds are usually weaker and therefore more easily broken than δ bonds.
Planar shape
The carbon-carbon double bond is rigid and bond rotation can not occur. For rotation to occur the $\pi$-bond must be broken. The energy barrier for bond rotation in ethene (ethylene) is 235 kJ/mol while for ethane is only 12 kJ/mol.

The rigidity of the double bond gives rise to the possibility of stereoisomerism (geometric isomerism) which is commonly referred to as cis-trans isomerism in alkenes.

*Cis* isomer cannot become *trans* without a chemical reaction occurring.
$cis = \text{The substituents are on the same side of the double bond.}$

$trans = \text{The substituents are on opposite side of the double bond.}$
Examples

\[
\begin{align*}
\text{Cl} & \quad \text{Cl} \\
\text{C} & \quad \text{C} \\
\text{H} & \quad \text{H}
\end{align*}
\]

\[
\begin{align*}
\text{Cl} & \quad \text{H} \\
\text{C} & \quad \text{C} \\
\text{H} & \quad \text{Cl}
\end{align*}
\]

\textit{cis-1,2-dichloroethene} \quad \textit{trans-1,2-dichloroethene}
Ethyne (C$_2$H$_2$)-sp-Hybridization
sp hybridization of a carbon

**ground state**

- $2s$
- $2p_z$

**excited state**

- $2s$
- $2p_z$

**sp hybridized state**

- $2p_y$
- $2p_z$

unhybridized $p$ orbitals

<table>
<thead>
<tr>
<th>s</th>
<th>+</th>
<th>p</th>
</tr>
</thead>
</table>

Hybridization

2 $sp$
sp hybridized carbon

\( \text{sp} \) hybridized carbon

\( p_y \)

\( p_z \)

\( \text{sp} \)

\( \text{sp} \)

\( \text{sp} \)

\( x \)

\( y \)

\( z \)
Alkynes have a linear geometry with C-C bond angles of 180°.
Comparison of Carbon-Carbon and Carbon-Hydrogen bonds in methane, ethane, ethylene and ethyne.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Bond</th>
<th>Bond strength (Kcal/mol)</th>
<th>Bond length (Å)</th>
<th>S-character (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methane, CH₄</td>
<td>C&lt;sub&gt;SP3&lt;/sub&gt;-H&lt;sub&gt;1s&lt;/sub&gt;</td>
<td>104</td>
<td>1.10</td>
<td>25</td>
</tr>
<tr>
<td>Ethane, CH₃-CH₃</td>
<td>C&lt;sub&gt;SP3&lt;/sub&gt;-C&lt;sub&gt;SP3&lt;/sub&gt;</td>
<td>88, 98</td>
<td>1.54, 1.10</td>
<td>25, 25</td>
</tr>
<tr>
<td>Ethylene, H₂C≡CH₂</td>
<td>C&lt;sub&gt;SP2&lt;/sub&gt;-C&lt;sub&gt;SP2&lt;/sub&gt;</td>
<td>152</td>
<td>1.33, 1.076</td>
<td>33, 50</td>
</tr>
<tr>
<td>Ethyne, HC≡CH</td>
<td>C&lt;sub&gt;SP&lt;/sub&gt;-C&lt;sub&gt;SP&lt;/sub&gt;</td>
<td>200</td>
<td>1.20, 1.06</td>
<td>50</td>
</tr>
<tr>
<td></td>
<td>C&lt;sub&gt;SP&lt;/sub&gt;-H&lt;sub&gt;1s&lt;/sub&gt;</td>
<td>125</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Problem

I. Locate and identify the functional groups in the following molecules:

a)  

\[
\text{H} - \text{N} - \text{CH}_{2}\text{OH}
\]

d)  

\[
\text{CH}_3\text{CH}_{\text{C}}\text{C} = \text{OH}
\]

II. Indicate bond angle at each carbon in the following compounds

a.  

\[
\text{O} \quad \text{C} \quad \text{C} \quad \text{C}
\]

b.  

\[
\text{C} \quad \text{C} \quad \text{C}
\]