II. Molecular Formula and Degree of Unsaturation

Alkenes are **unsaturated** hydrocarbons because they have fewer than the maximum number of hydrogen atoms per carbon:

General formula for a noncyclic alkane:

General formula for a cyclic alkane:

General formula for an alkene:

General formula for a cyclic alkene:

The general formula for a hydrocarbon is C_nH_{2n+2}, minus two hydrogens for every π-bond and/or ring in the molecule.

☞ *The total number of π-bonds and rings in a molecule gives the degree of unsaturation (or units of unsaturation)*

Given the molecular formula, we can tell the degree of unsaturation:

Example: For a compound with molecular formula C_5H_8, give the degrees of unsaturation and draw a few possible structures for this compound.

This process can be extended to molecules that contain heteroatoms such as O, N, and the halogens.

For O, N and halogens:

- **ignore O**
- **replace each halogen with a H**
- **subtract one H for each nitrogen**

Examples:

C_5H_8O

$C_6H_{11}Cl$
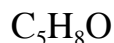
C_8H_9NO

An alternative way to calculate units of unsaturation is to use the following formula:

$$U = \frac{2C + 2 + N - X - H}{2}$$

C = number of carbons
N = number of nitrogens
X = number of halogens (F, Cl, Br, I)
H = number of hydrogens

Redo C_8H_9NO using formula: