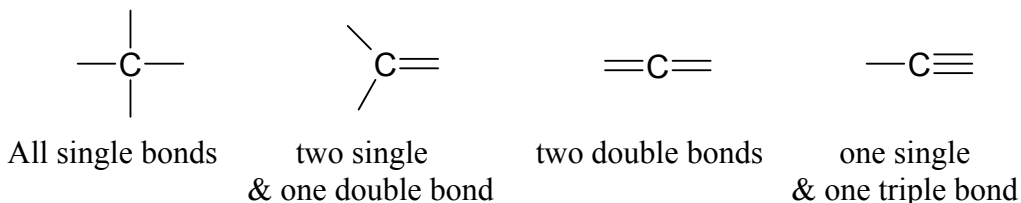


Index of Hydrogen Deficiency (IHD)

(Excerpt from Chem 201 Lab Manual Aug 2005)

There is no simple way of predicting how many isomers a given molecular formula will yield, (it can range from one to many). **Structures are different if they cannot be superimposed upon one another.** Keep in mind that there is rotation about all single bonds not involved in a ring, but not about double bonds. Because all of the formulas that you will be dealing with are based on the C atom, it may be useful to review the ways that C can bond to itself and to other atoms. We will limit ourselves, for now, to the C atom with four bonds. Below are the possible combinations of C having a total of four bonds.



In a hydrocarbon where all the C atoms have only single bonds and no rings are involved, the compound would have the maximum number of H atoms. If any of the bonds are replaced with double or triple bonds, or if rings are involved, there would be a “deficiency” of H atoms. By calculating the *index of hydrogen deficiency* (IHD), we can tell from the molecular formula whether and how many multiple bonds and rings are involved. This will help cut down the possibilities one has to consider in trying to come up with all the isomers of a given formula. Refer to your textbook for a more complete discussion of this. Here is a summary of how the *index of hydrogen deficiency* (IHD) works.

A double bond and ring each counts as one IHD.

A triple bond counts as two IHD.

Hydrocarbons (C_xH_y): $IHD = \frac{2x + 2 - y}{2}$ (where x and y stand for # of C and H respectively.)

Example 1: IHD for C_2H_4 is $\frac{2(2) + 2 - 4}{2} = 1$

This means it can have either one double bond or one ring. It cannot have a triple bond. Since you cannot form a ring with only two C's, it must have a double bond.

Example 2: IHD for C_4H_6 is $\frac{2(4) + 2 - 6}{2} = 2$

This means it can have either one double bond and a ring such as  or two double bonds such as $CH_2=CH-CH=CH_2$ or $CH_2=C=CH-CH_3$

or two rings,  or one triple bond, such as $CH_3C\equiv CCH_3$.

Compounds Containing Elements Other than C and H:

O and S atoms do not affect the IHD.

Halogens (F, Cl, Br, I) are treated like H atoms. (CH_2Cl_2 has the same IHD as CH_4 .)

For each N, add one to the number of C and one to the number H.

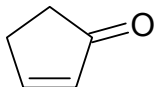
(CH₅N is treated as C₂H₆. CH₄N₂O is treated as C₃H₆ by adding 2 to # of C and 2 to # of H.)

Do not forget that when double bonds and rings are involved, geometric isomers are possible.

Practice problems:

Calculate the IHD for each of the following and see whether it corresponds to the structure shown. (Obviously it should!) Don't peek until you've worked it out yourself, but answers are provided at the bottom.

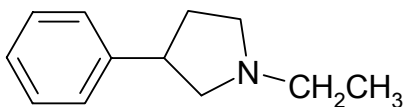
a)



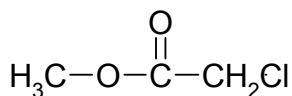
b)



c)



d)



e)



Answers:

- a) IHD = 3
- b) IHD = 2
- c) IHD = 5
- d) IHD = 1
- e) IHD = 3

Note: Brown, Foote & Iverson 4/e talks about this in Chapter 5 (pp.184-185). You may want to go over Examples 5.1, 5.2 and Problem 5.1 and 5.2; and problems from the back of Chapter 5 (#32, 33c, 34d)