Intensive Organic Chemistry for Freshmen C3045x

Computation of the Unsaturation Number from Molecular Formulae

Unsaturation / Ring Number: The number of double bonds or rings possessed by a molecule. A triple bond counts as two double bonds, or as one double bond and one ring , or as two rings.

Recipe for Hydrocarbons: Take molecular formula (C_xH_y) and calculate $(x + 1) - (Y / 2)$. The answer is the U / R number. This assumes a valence of 4 for carbon and 1 for hydrogen. Example: C_6H_6 --> $(6 + 1) - (6 / 2) = 7-3 = 4$. Thus the U / R number of C_6H_6 is 4. Any molecular structure with the normal valences for carbon and hydrogen must possess a U / R number of 4 (no more; no less).

Test cases for C_6H_6:

Extension of Rule:

A. Oxygen just gets tacked on (assume valence of two)

$C_xH_yO_z$ --> $(x + 1) - (y / 2)$

1. CH_4O --> $(1 + 1) - (4 / 2) = 2 - 2 = 0$

   CH_3OH saturated

2. C_2H_4O --> $(2 + 1) - (4 / 2) = 1$

   CH_2=CHOH — a C=C double bond

   CH_3CH — a C=O double bond

   CH_2--CH_2 — a ring

3. C_3H_4O --> $(3 + 1) - (4 / 2) = 2$

   H-C C-CH_2OH

   CH_2=CH-CH-O

   CH-CH-CH_3
   O

   CH_2-CH_2
   CHOH

B. Halogen is the same as hydrogen

$C_xH_yX_z$ --> $(x + 1) - (y + z) / 2$

Examples:

1. $CHBr_3$ --> (1 + 1) - (1 + 3) / 2 = O

2. $C_2H_2Cl_2$ --> (2 + 1) - (2 + 2) / 2 = 1

3. $C_3HClBrF$ --> (3 + 1) - (1 + 1 + 1 + 1) / 2 = 4 - 2 = 2

Problems:

1. What is the unsaturation number formula for a compound containing C, H, and N? Containing C, H, and S?
2. Calculate the U / R number for molecules possessing the following molecular formulae and draw three structures corresponding to each example.
   (a) C_7H_9
   (b) C_4H_4
   (c) C_5H_5N
   (d) $C_5H_{10}O$
   (e) $C_8H_{10}O$
   (f) $C_4H_8Br_2O$