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: \(C_6H_6 \rightarrow (6 + 1) - (6/2) = 7 - 3 = 4\). 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)
\(C_xH_yO_z \rightarrow (x + 1) - (y/2)\)
1. \(CH_4O \rightarrow (1 + 1) - (4/2) = 2 - 2 = 0\)
   \(CH_3OH\) saturated
2. \(C_2H_4O \rightarrow (2 + 1) - (4/2) = 1\)
   \(CH_2=CHOH\) \(\quad CH_3CH\) \(\quad CH_2=CH_2\)
   a C=C double bond \(\quad a\ C=O\) double bond \(\quad a\ ring\)
3. \(C_3H_4O \rightarrow (3 + 1) - (4/2) = 2\)
   \(H-C\ C-CH_2OH\ CH_2=CH-CH-O\ CH-CH-CH_3\ CH_2-CH_2\)
   \(O\ CHOH\)

B. Halogen is the same as hydrogen
\(C_xH_yX_z \rightarrow (x + 1) - (y + z)/2\)
Examples:
1. CHBr\(_3\) --> (1 + 1) - (1 + 3)/2 = 0
2. C\(_2\)H\(_2\)Cl\(_2\) --> (2 + 1) - (2 + 2)/2 = 1
3. C\(_3\)HClBrF --> (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\(_7\)H\(_9\)
   (b) C\(_4\)H\(_4\)
   (c) C\(_5\)H\(_5\)N
   (d) C\(_5\)H\(_{10}\)O
   (e) C\(_8\)H\(_{10}\)O
   (f) C\(_4\)H\(_8\)Br\(_2\)O