SODAR/Computation of the Unsaturation Number from Molecular Formulae

The SODAR number (Sum or Double Bonds and Rings) is a quick means of determining the "degree of unsaturation" of a molecular composition. By unsaturation we mean the number of rings and/or double bonds that a Lewis structure contains. The can be determined directly from the molecular composition.

Sum of Double Bonds and Rings (SODAR): The number of double bonds and/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. Each of these situations corresponds to a SODAR of 2.

SODAR Recipe for **Hydrocarbons**: Take molecular composition (C_xH_y) and calculate

SODAR = (x + 1) - (y/2).

The SODAR number assumes a valence of 4 for carbon and 1 for hydrogen. Example: C_6H_6 --> (6 + 1) - (6/2) = 7 - 3 = 4.
Thus the SODAR number of C_6H_6 is 4. Any molecular structure with the normal valences for carbon and hydrogen and the composition C_6H_6 must possess a SODAR number of 4 (no more; no less).

Extension of Rule for **oxygen, halogens and nitrogen**:

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

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

Example: C_2H_6O SODAR = 0. $C_2H_6O_2$ SODAR = 0.

B. Halogen (valence of one) is the same as hydrogen, since each halogen can be considered to replace a hydrogen atom.

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

Example: CH_3Cl SODAR = 0. CH_2Cl_2 SODAR = 0. CCl_4 SODAR = 0

C. Nitrogen (valence of three) requires the addition of 1/2 to the SODAR for hydrocarbons for each nitrogen.

$C_xH_yN_z$ --> SODAR = (x + 1) - y /2 + z/2

Example: C_2H_7N SODAR = 0. C_2H_5N SODAR = 1. C_2H_3N SODAR = 2.