

## *Helpful Hints For Mass Spectrometry and Compound Identification*

### **Degrees of Unsaturation**

From a molecular formula, we can calculate how many rings and/or multiple bonds (equals the “degrees of unsaturation”) are contained in a given molecule.

1. Count the total number of carbon atoms. If nitrogen atoms are present, count each nitrogen atom as 1/2 of a carbon atom (sounds weird, but it works).
2. If oxygen or sulfur atoms are present, ignore them.
3. Count the total number of hydrogen and halogen atoms.

Then use:

$$\text{Degrees of Unsaturation} = \frac{(2 \times \text{carbon atoms} + 2) - (\text{hydrogens} + \text{halogens})}{2}$$

### **The “M+1” Rule**

As long as our mass spectrum is of reasonable quality, then we can get an idea of the number of carbon atoms in our compound by:

$$\frac{\text{M} + 1 \text{ peak intensity (as a \%)}}{\text{M}^+ \text{ peak intensity (as a \%)}} \div 1.1 \times 100 = \text{approximate number of carbon atoms}$$

### **The “Nitrogen Rule”**

Because nitrogen has an even atomic mass (14) but an odd valence (3), compounds containing an odd (and non-zero) number of nitrogen atoms will have an odd molecular mass. In other words:

*If the mass of a compound is even, then the compound contains either zero or an even number of nitrogen atoms (0, 2, 4, 6, etc. nitrogens). If the mass of a compound is odd then the compound contains an odd number of nitrogen atoms (1, 3, 5, 7, etc. nitrogens). The "nitrogen rule" holds true for all neutral compounds containing any elements from the first or second period, sulfur (but not phosphorus) and all of the halogens.*