

Massachusetts Institute of Technology

Organic Chemistry 5.13

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Problem Set #1

This problem set is worth $50/8 = 6.25$ points toward your final grade; each problem is worth **1.25 points**.

NOTE: If mass spectrometry (MS) data are provided, the highest molecular ion given corresponds to the molecular ion (M^+), unless otherwise noted.

1. **Derive** an expression for the **largest possible IHD** for a **neutral** (no overall charge; zwitterions ok), stable compound having n carbon atoms and zero or more H, N, and O atoms (e.g., CH_4O). For the purposes of this problem, "stable" is defined as a structure whose atoms all form the "standard" number of bonds. That is, all of the C atoms have 4 bonds, all the H (if any) have 1, all the N (if any) have, and all the O (if any) have 2.

Express your answer as function of n , and illustrate with **two** specific structures. Calculate and provide the numerical value of the IHD for your examples.

2. What EA, IR, and MS data would you expect for the following 10 common laboratory solvents? Draw the structure of each solvent as part of your answer.
- (a) benzene; (b) toluene; (c) ethanol; (d) tetrahydrofuran; (e) diethyl ether; (f) dichloromethane; (g) chloroform; (h) carbon tetrachloride; (i) acetonitrile; (j) hexane.

3. **Luminol** is the key component in an extraordinarily sensitive chemical test for detecting blood. If you have watched even just one or two episodes of *Forensic Files* or *CSI*, you have probably seen how useful this compound is in the analysis of crime scenes, even where no blood is visible by eye.

Draw the structure of luminol; determine its MF and IHD; calculate the EA data that would you expect for this compound, and list the IR data you would expect to find for this compound.

4. Draw **four (4)** structures that satisfy the following experimental data. Diastereomers (but not enantiomers in this case) **are** considered to be different structures.

EA (found): C, 67.55; H, 12.75; N, 19.69

MS: 71

IR: 2932 cm^{-1}

5. Draw **three (3)** structures that are consistent with the following elemental analysis. Diastereomers (but not enantiomers in this case) **are** considered to be different structures.

EA (found): C, 92.26; H, 7.74