Nuclear Magnetic Resonance (NMR). Identification of an Unknown Substance.

Reading Techniques 26 and 27 in Pavia (5th edition)**,** Chapter 15 in Klein (3rd edition)

Homework Klein, In-text: 15.1, 15.2, 15.4, 15.6, 15.7, 15.8, 15.10, 15.11, 15.14, 15.15, 15.17, 15.24, 15.25, 15.26, 15.29, 15.30; End-of-chapter: 15.32, 15.33, 15.35, 15.41, 15.43, 15.59;
Integrated Problems: 15.63, 15.64; ACS-style Problems: 15.75-15.77 (don't turn in)

Description

You work for Crime Scene Investigator (CSI) – Laney. You and your partner have recently discovered an unknown substance at a crime scene (used, undoubtedly, for some adverse or otherwise devious act). The identity of the unknown is suspected to be among the following list of possible compounds:

> aspirin, toluene, *m*-xylene, *p*-xylene, 2-butanol, ethyl benzoate, methyl salicylate, diisopropylethylamine, ethyl methacrylate, or *p*-anisidine

As one of the most comprehensive methods of structure analysis found in the CSI-Laney laboratory, NMR spectroscopy is the appropriate method to reveal the identity of the substance (aside from a simple melting point or boiling point - you would use the GC/MS but it is down for maintenance).

Prelab

Using the provided **Data Worksheet**, show the structure for each of the compounds listed above. For each compound indicate the total number of *chemically equivalent* protons (^{1}H) and carbons (^{13}C).

Procedure

Your instructor will demonstrate how to run the NMR instrument during laboratory – use the simple guide provided, which is also found at the class website. Choose one of the unknown samples (note the sample "code"). (The samples have already been prepared for the NMR experiment). Obtain the ^{13}C NMR spectrum, use the guide to phase the spectrum and integrate the peaks, then print. The ^{1}H NMR spectrum will be provided.

To Complete the Experiment

Using the NMR spectra, determine the identity of the unknown compound. Use the **Data Worksheet** to show the structure of your unknown (with labels as indicated) and report the chemical shifts for each type of proton and carbon present. For the proton spectrum report the multiplicity and integration using the appropriate notation. The completed **Data Worksheet** is all that is due for this laboratory report.