

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

Data Worksheet For each of the unknowns, fill in the structure and information below. The possible unknowns are:

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

Structure and name of Possible Unknown	Number of equivalent protons	Number of equivalent carbons

¹H NMR Data: List the chemical shift values for the signals in your proton spectrum. As well, indicate the multiplicity (s, d, t, q...etc), and the value of the integral for each peak. Draw the structure for the proposed compound. Label the hydrogen atoms (using letters) and then assign the hydrogen atoms to the signals in spectrum using the letters. Chemically equivalent atoms should be given the same label.

Structure of Proposed Compound	δ (ppm)	Multiplicity	Integration	Assignment

¹³C NMR Data: List the chemical shift values for the signals in your carbon-13 spectrum. Draw the structure for the proposed compound. Label the carbon atoms (using letters) and then assign the carbon atoms to the signals in spectrum using the letters. Chemically equivalent carbons should be assigned the same letter.

Structure of Proposed Compound	δ (ppm)	Assignment