

NMR Workshop I Assignment

Step 1. Learn what is meant by “chemically unique” and practice using the replacement test.

The “replacement test” for chemical uniqueness:

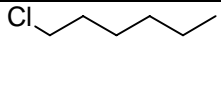
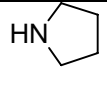
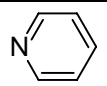
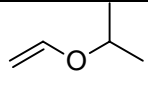
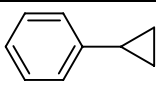
A chemist knows that protons in different chemical environments (“chemically unique protons”) are expected to have different chemical shifts, but he is confused whether H_A and H_B in a given molecule experience different environments. To resolve this, he uses the replacement test:

1. redraw molecule replacing H_A with another element Z (call this “molecule A”)
2. redraw molecule again replacing H_B with another element Z (call this “molecule B”)
3. compare molecule A with molecule B and decide which of the following conditions applies to the molecules:

Molecules A & B are:

- **identical** (or are **conformational isomers**) $\rightarrow H_A$ & H_B experience identical environments on average
- **constitutional isomers** $\rightarrow H_A$ & H_B probably experience different environments
- **diastereomers** $\rightarrow H_A$ & H_B probably experience different environments
- **enantiomers** $\rightarrow H_A$ & H_B are “enantiotopic” and experience identical environments in an achiral medium (the usual situation), but might experience different environments in a chiral medium

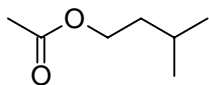
Decide how many chemically unique protons are found in each molecule shown below:

				
			How many alkene _____	How many arene ____
			How many alkane _____	How many cyclopropane _____

Step 3. Learn to process & print NMR data using SpinWorks. Do this for your spectrum of isopentyl acetate by performing these steps:

1. Open [SpinWorks manual](#) (use link on [201 home page](#)). Read manual and perform all steps in the tutorial through **Print (Full) Spectrum** using your isopentyl acetate data.
2. Using the full spectrum, try to complete as much of the chart (below) as you can. (Hint: you won't be able to complete the entire chart, but you should be able to figure out: how many types of H are in your compound and their approximate chemical shifts.)
3. At this point, you will want to print expansions of your spectrum that include peak positions (in Hz) and integrals. You might be able to fit all of this data onto a single page by carefully adjusting the horizontal and vertical scales. However, you might find it more convenient to use two pages, one for the smaller peaks appearing between 1.5-4.3 ppm, and a second for the taller peaks appearing between 0.5-2.5 ppm. Once you have these data, complete the rest of the chart below by inserting integral and coupling pattern data.

Step 4. Interpret your spectrum:



Confounding peaks (if any):

chemical shift (ppm)	#H	coupling pattern (s, d, t, q, ..., m)	J (Hz)	assignment

Step 5 (optional). Learn to write your spectra data for the Experimental section of a lab report. See (online lab manual: appendix: writing a report: Experimental section)

http://academic.reed.edu/chemistry/alan/201_202/lab_manual/appendices/writing_a_report.html#experimental

Write your NMR data on a single line here (this is the same way you will write it in the Experimental section of your lab report):