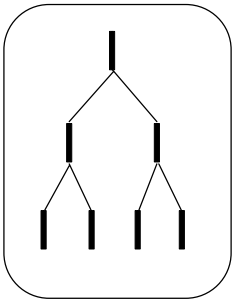
Chem 201, Fall 2006 Name _____

Lab day & box #_____

NMR Workshop III – Coupling Patterns



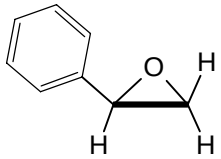
Produce a branching diagram (like the one shown at left) for <u>each</u> of the indicated hydrogens in the two molecules shown below (5 diagrams in all).

Your goals are 1) to make drawings that contain realistic peak heights and separations that will look like the expected coupling patterns for these hydrogens, 2) to use these drawings to assign peaks in the NMR spectra to these H (spectra on web and on separate pages).

Suggestions:

1. Use a ruler or graph paper to measure distances (1 mm = 1 Hz)
2. Begin by marking a single "stick" for the <u>uncoupled</u> hydrogen
3. Underneath the single stick, draw a set of sticks that show the effect of the neighbor(s) that couples <u>most strongly</u> to this hydrogen (largest J).
    a. Mark the distances between sticks accurately (or use graph paper).
    b. Align the sticks properly with the stick(s) on the next higher level
4. Repeat #2 as needed on successive lines, each time using the next weakest coupling until your last level introduces the weakest coupling of all.
5. Name your pattern, "dd", "td", "dt", etc.
6. Assign the peaks in the spectrum
7. If possible, double-check assignments using chemical shifts and integrals

Compound I – Styrene oxide



Typical oxirane couplings: $J_{geminal}$ = 6 Hz, J_{cis} = 4.5 Hz, J_{trans} = 3.1 Hz

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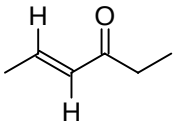
Compound II – *E*-4-hexene-3-one



Typical couplings: J(long-range allylic *H*-C-C=C-*H*) = 1 Hz. $J_{vicinal}$ see lab manual (use values in parentheses)