

Lecture 2 218. Distortionless Enhanced Polarization Transfer Spectra

Answer these questions on your spectra if possible. No additional sheets are necessary.

What is the known number _____ and compound.

How many different C's are present? (from the number of peaks in the C spectrum) How many C's are associated with each peak? (from the height of the peaks. How many attached hydrogens are there on that C?

Attach the decoupled C spectrum (the normal C spectrum) and the DEPT Spectrum. Label the peaks A, B, etc corresponding to your answer above.

Draw the structure of the known alcohol and give its name and label the carbons in the structure so that the correspond to the table above.

What is the unknown number _____

How many different C's are present? (from the number of peaks in the C spectrum) How many C's are associated with each peak? (from the height of the peaks. How many attached hydrogens are there on that C?

Attach the decoupled C spectrum (the normal C spectrum) and the DEPT Spectrum. Label the peaks A, B, etc corresponding to your answer above.

Draw the structure of the unknown alcohol and give its name and label the carbons in the structure so that the correspond to the table above.

1. Solve the following structures from their C-13 spectra:

Molecular Formula	chemical shifts (dept results, intensity) u-up n- not there d-down three results from bottom to top on dept spectra. Starred values indicate
a) C ₄ H ₉ Br	12(unu,1) 26(unu,1) 34(und,1)

	53(uuu,1)
b) C ₅ H ₁₁ Cl	9.5(unu,1) 32(unu,2) 39(und,1) 71(nnn,1?)
c) C ₅ H ₁₁ Cl	22(unu,2) 26(uuu,1) 42(und,1) 43(und,1)
d) C ₉ H ₁₂	24(unu,2) 34(uuu,1) 126(uuu,1) 126.5(uuu,2) 128(uuu,2) 149(nnn,1?)
f) C ₄ H ₈ O ₂	184(nnn,1?) 34(uuu,1) 19(unu,2)
g) C ₄ H ₈ O ₂	161(uuu,1) 67(uuu,1) 22(unu,2)

DEPT Spectra

DEPT (distortionless enhanced polarization transfer) spectra are series of three C-13 that are usually arrange from bottom to top as follows:

The bottom spectrum shows all carbons with hydrogens attached to them.

The middle spectrum shows all carbons with 1 H and only one hydrogen attached to them.

The top spectrum shows carbons with odd numbers of hydrogens as up peaks and even numbers of hydrogens with down peaks.

Interpretation of the DEPT spectra then allows you to assign each peak in the spectrum to a C with no hydrogens, one hydrogen, two hydrogens or three hydrogens.

Obtain the DEPT spectra as follows:

1. After you have gotten a good C-13 spectrum on your sample Enter the PNMR program. Type <DEPT> in the command line followed by return. The program will ask you for the Name of file. Just hit return if you wish to use the file My_dept for your data. If you want to call it something else- do so but remember what you called it.

2. The program now acquires three sets of data. So just wait. When it is done, it will put up another question box. This just gives you time to read the processing instructions. Hit return when you've read them.

3. Enter the *NUTS* program. Nut commands are just two letters in main program with NO following enter.
4. Process the data first spectrum. [a1] ("a" one)
5. Phase it. [ap]
- .6. Now put all three of the spectra of the screen. [Cntrl F11]
7. Adjust scale by using scroll bar on right
8. Plot the data [p]