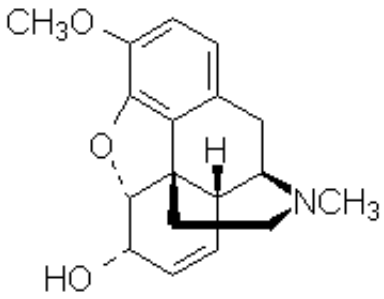
DEPT and APT spectra of codeine

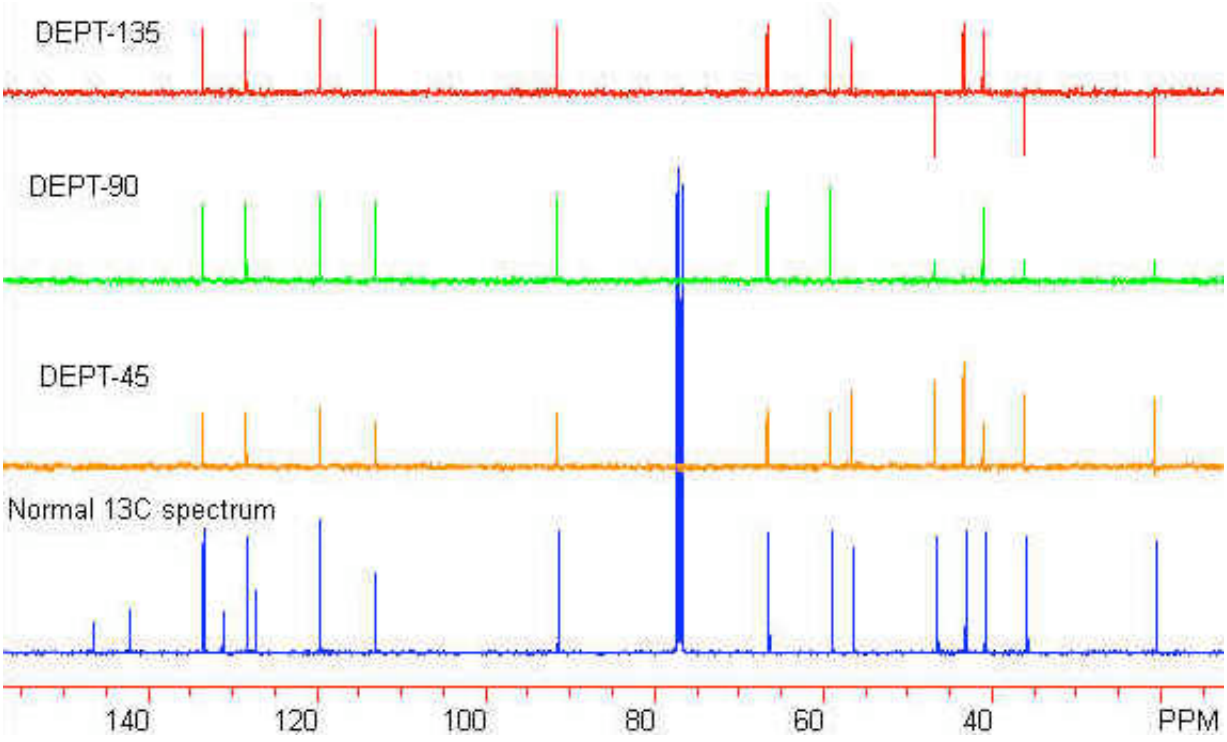
Both experiments are used to identify "multiplicity" (quaternary, CH, CH_2 or CH_3) of peaks in a ^{13}C spectrum. Usually, DEPT is preferred because much less time is required. For DEPT, ^{1}H magnetization is generated first, then transferred to ^{13}C. This "polarization transfer" enhances sensitivity. Also, the experiment repetition rate is dependent on relaxation of ^{1}H, rather than ^{13}C, so a shorter delay is needed. DEPT also can distinguish between CH and CH_3, unlike APT, although quaternary Cs are not observed in DEPT.



The sample is 18 mg of codeine in .65 ml $CDCl_3$

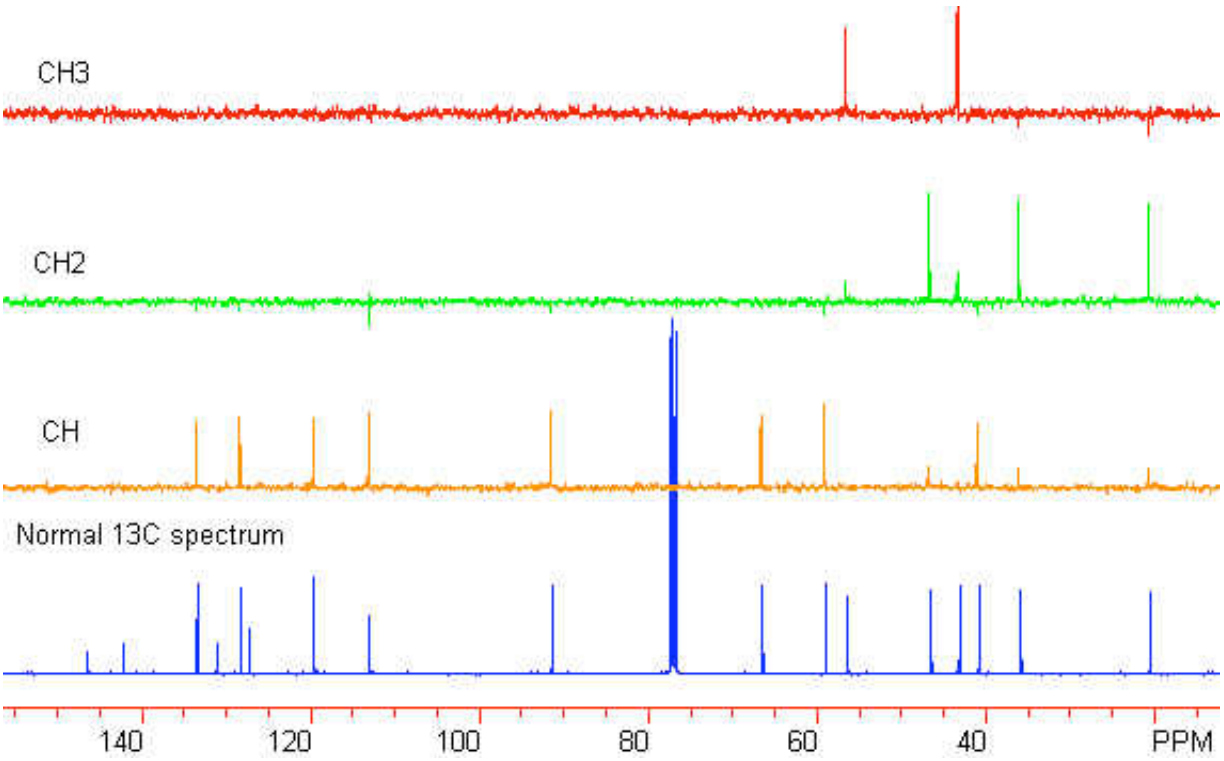
DEPT spectra shown in the figure below are, from top to bottom:

DEPT-135	CH and CH_3 peaks up, CH_2 peaks inverted
DEPT-90	CH peaks only
DEPT-45	all protonated carbons
normal ^{13}C spectrum	



The 3 DEPT spectra were acquired in less than 10 min each. From the DEPT-135, CH_2 peaks are identified as the 3 inverted peaks. DEPT-90 contains only CHs. Any positive peaks in DEPT-135 which don't appear in DEPT-90 are CH_3s.

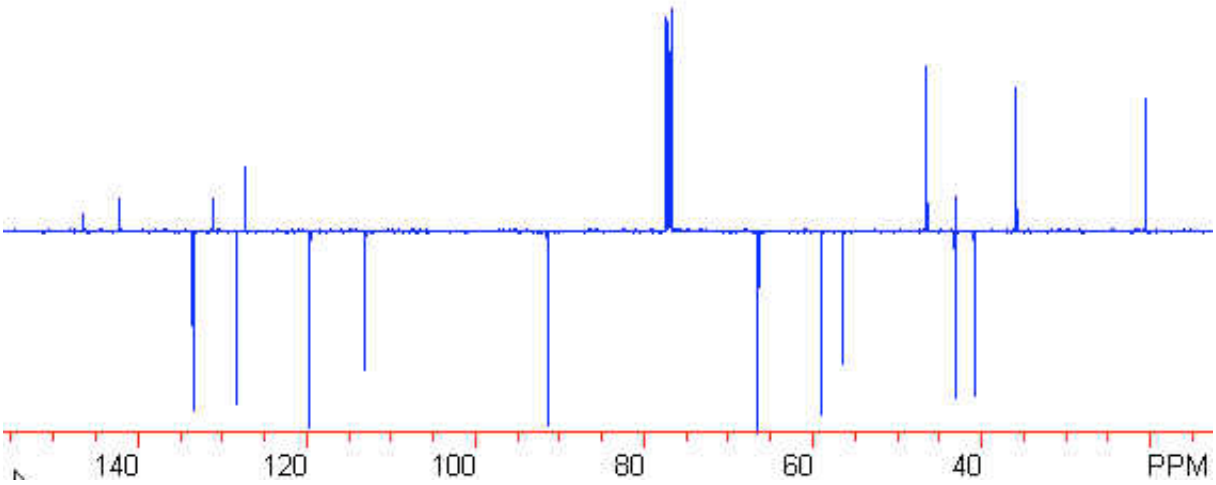
The 3 DEPT spectra can be combined by addition and subtraction with appropriate coefficients to yield "edited DEPT" spectra, in which each spectrum contains only peaks of one multiplicity (CH, CH_2 or CH_3), as shown below.



The subtraction is not perfect, most likely due to slightly imperfect pulse widths, but multiplicity of all peaks can be readily determined.

In practice, creation of the edited display is not necessary, as multiplicity of all peaks can be easily assigned from just a DEPT-135 and, if needed, a DEPT-90 to distinguish CH and CH_3.

An APT spectrum provides nearly equivalent information. Quaternary and CH_2 peaks are positive, CH and CH_3 peaks are inverted. For codeine, the APT clearly resolves the 2 peaks at 43 ppm, a quaternary and a CH. The APT experiment is simpler to set up, as it does not require calibration of a proton 90 degree pulse. Also, many older generation spectrometers are not capable of accurate phase shifts of the decoupler channel, needed for DEPT. The disadvantages of APT are its lower sensitivity, the need to wait between scans for ^{13}C relaxation, and no means of distinguishing CH from CH_3 peaks.



This spectrum was acquired in 2.5 hrs.

Last updated: 06/24/2005

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