

Manual Plotting of DEPT Spectra

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Occasionally, situations arise that require that DEPT spectra be plotted manually. Recall that the DEPT set of spectra typically consists of three subspectra (methyl, methylene, methane), with either a spectrum of the H-bound ^{13}C resonances or a ^{13}C spectrum of quaternary carbon resonances. These data are aligned vertically over one another. One such example is the case in which the subspectra are not properly scaled, causing resonances from one subspectrum to obscure spectral features in the subspectrum directly above. Another example is the case in which quaternary carbons are selected for observation, but the full H-bound set of carbon resonances is needed instead.

The procedure for manually plotting DEPT spectra is described below – note that the command or string to be typed is designated using bold font:

1. Type **process** to convert the DEPT data into processed/aligned subspectra.
2. Type **ds(4)** to view the plot with methyl carbon subspectrum ($-\text{CH}_3$).
3. Type **vo?** to evaluate the vertical offset (vo) value (typically around 40).
4. Type **vp?** to evaluate the current vertical position (vp) value (around 125).
5. Type **vp=125** (or whatever value was generated in the previous step).
6. Type **pl** to send the methyl carbon subspectrum to the plot queue.
7. Type **ds(3)** to view the plot with the methylene carbon subspectrum ($-\text{CH}_2$).
8. Type **vp=vp-vo** and then **pl** to send the methyl carbon subspectrum to the plot queue.
9. Type **ds(2)** to view the plot with the methylene carbon subspectrum ($-\text{CH}_2$).
10. Type **vp=vp-vo** and then **pl** to send the methylene carbon subspectrum to the plot queue.
11. Type **wft** to generate a spectrum of all H-bound carbon resonances.
12. Type **vp=vp-vo** and then **pl pscale page** to send the DEPT plots to the printer. This procedure should generate a plot output with the three carbon subspectra aligned vertically (methyl, then methylene, then methane), and with the all H-bound carbon spectrum at the bottom.
13. Alternatively, type **vp=vp-vo** and then **pl pscale page('MyDEPT.ps')** to send the DEPT plots to an output file named MyDEPT.ps. This output file can be converted to various graphics formats (jpeg, tif, pdf, etc., using Adobe Illustrator or any of the many alternatives).