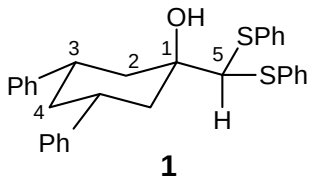
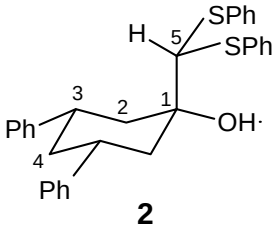
Problem R-06B/C ($C_{31}H_{30}OS_2$). The ^{13}C NMR spectra (Normal and DEPT-135) of two isomers (**1** and **2**) are shown below. Make a reasonable chemical shift argument for which isomer is which. Clearly indicate which carbon signal(s) you are using to make the assignment.

R-06B is isomer____ **R-06C** is isomer____

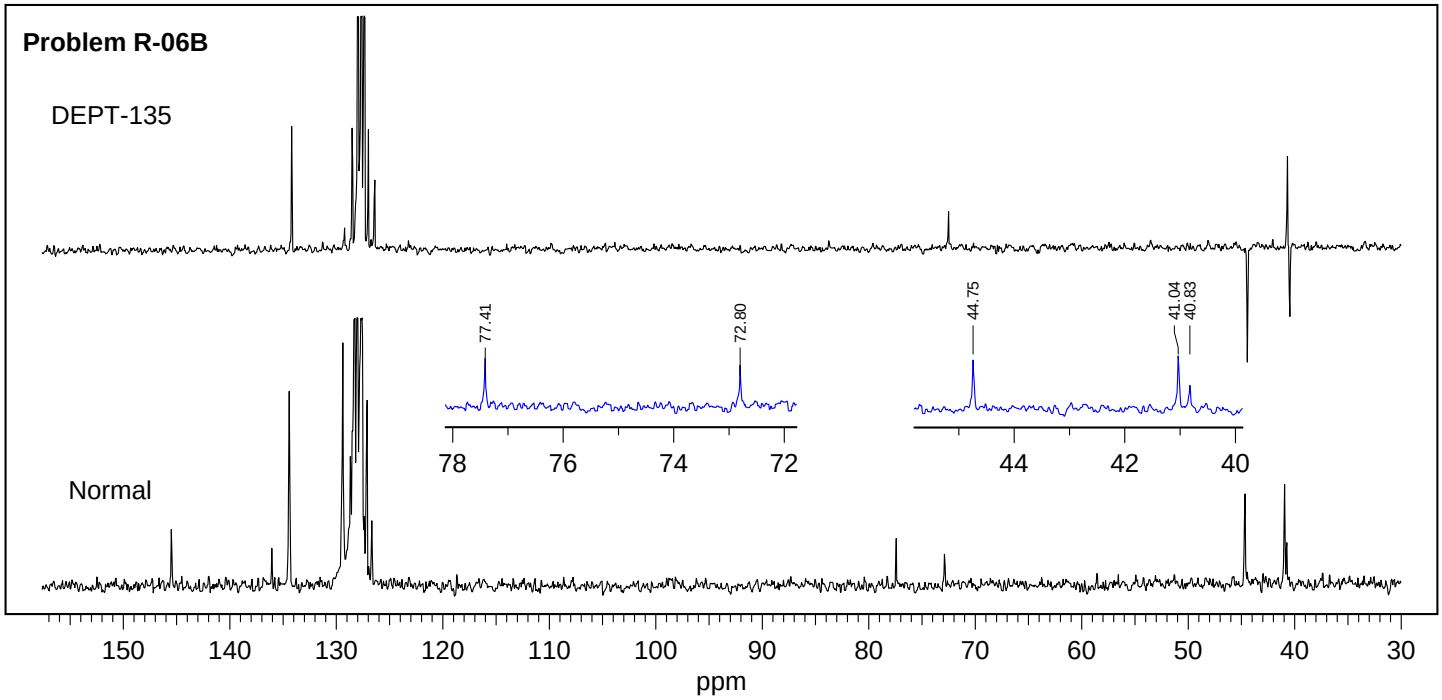


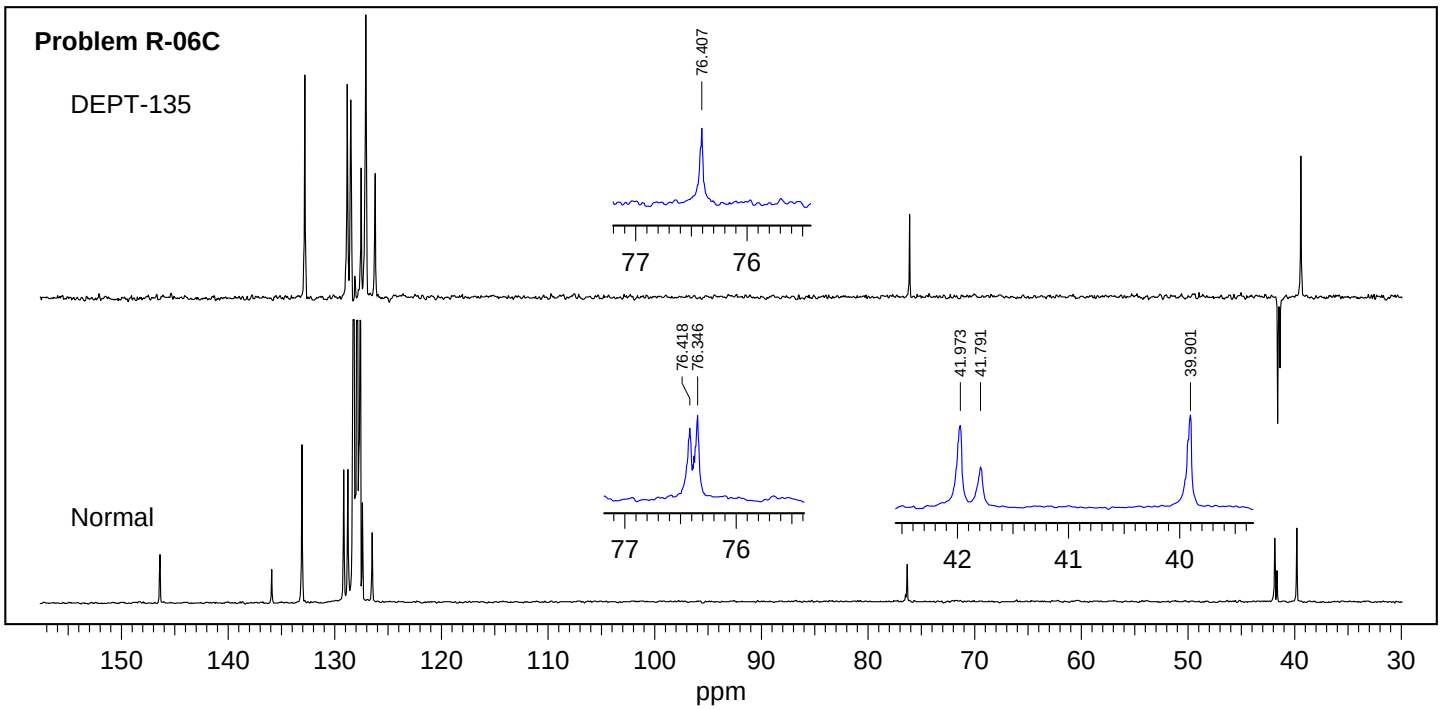
1



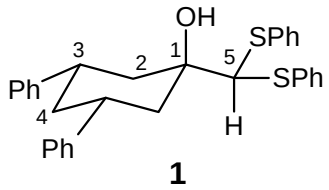
2

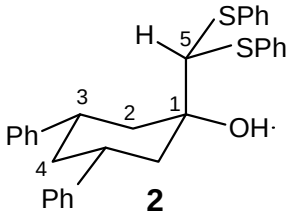
Problem R-06B/C ($C_{31}H_{30}OS_2$).
75.46 MHz ^{13}C NMR spectrum in C_6D_6. Source: Reich/Sikorski g





Problem R-06B/C ($C_{16}H_{18}OS_2$). The ^{13}C NMR spectra (Normal and DEPT-135) of two isomers (**1** and **2**) are shown below. Make a reasonable chemical shift argument for which isomer is which. Clearly indicate which carbon signal(s) you are using to make the assignment.





5 **R-06B** is isomer **2** **R-06C** is isomer **1**

C-5 has two γ-interactions with C-3 in isomer **2**, thus expect C-5 to be upfield. C-5 is at 72.8 in R-06C and at 76.4 in isomer R-06B. Thus R-06B = 2 and R-06C = 1

5 C-3 has a γ-gauche interaction in both isomers, and indeed the shift difference is only 1.1 ppm (41.0, 39.9). Not surprisingly, the γ-OH upfield effect is larger for C-3 in **1** than the γ-C effect for C-3 in **2**

Problem R-06B/C ($C_{31}H_{30}OS_2$).
75.46 MHz ^{13}C NMR spectrum in C_6D_6. Source: Reich/Sikorski g