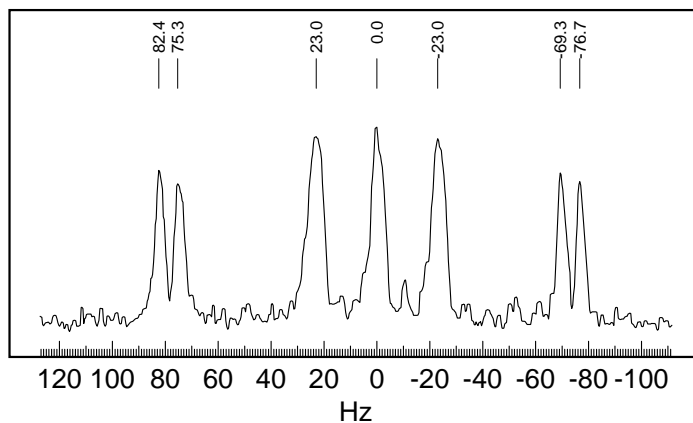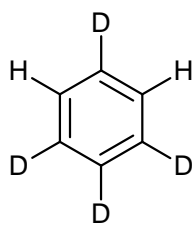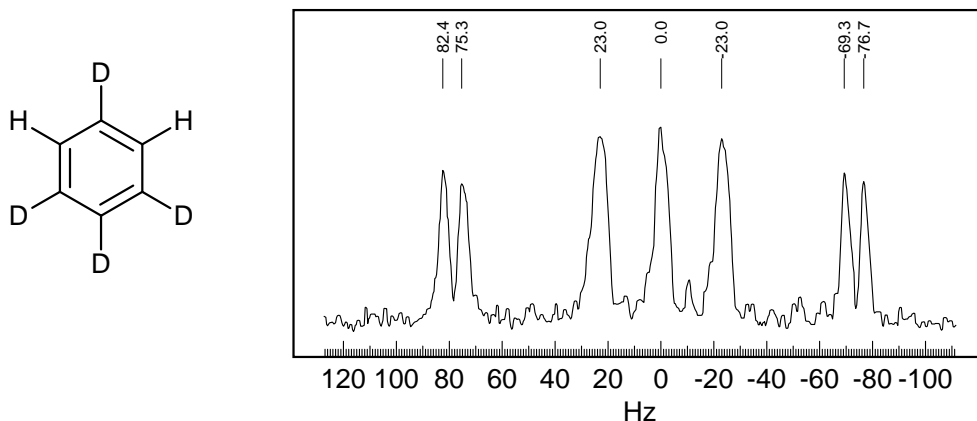Problem R-311 ($C_6H_2D_4$). Assign the peaks in the ^{13}C NMR spectrum below. The spectrum is not ^1H decoupled. Estimate the coupling constants (F. J. Weigert, J. D. Roberts *J. Am. Chem. Soc.* **1967**, *89*, 2967).
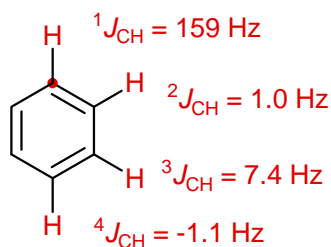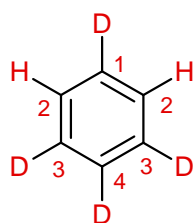
ANSWER

There are four kinds of carbons in this molecule

$^1J_{CH}$ = 159 Hz

$^2J_{CH}$ = 1.0 Hz
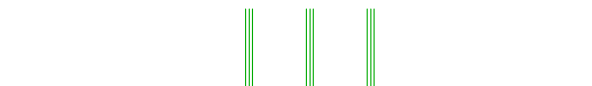
$^3J_{CH}$ = 7.4 Hz

$^4J_{CH}$ = -1.1 Hz

C-1: The only significant coupling is $^1J_{CD}$ = 23 Hz. The $^2J_{CH}$ will be 1 Hz, too small to resolve

C-2: These carbons will be a double intensity dd, with $^1J_{CH}$ = 159 Hz and $^3J_{CH}$ = 7 Hz. There will also be a $^3J_{CD}$ of about 1Hz, too small to resolve

C-3: These will be a double intensity 1:1:1 triplet of 1:1:1 triplets, $^1J_{CD}$ = 23 Hz and $^3J_{CD}$ = 1 Hz

C-4: Carbon 4 will be a 1:1:1 triplet of 1:2:1 triplets, $^1J_{CD}$ = 23 Hz and $^3J_{CH}$ = 7 Hz the outer lines of the triplets are too small to be visible

These outer triplet peaks will be approximately 1/16 of the intensity of the central peaks, hence not detectable at this signal to noise. The central lines are superimposed on C-1 and C-3.