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

![Chemical structure of \(\left(C_6H_2D_4\right)\)](image)

**ANSWER**

There are four kinds of carbons in this molecule

![Carbon labels and coupling constants](image)

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

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

C-3: These will be a double intensity 1:1:1 triplet of 1:1:1 triplets, \(1J_{\text{CD}} = 23\) Hz and \(3J_{\text{CD}} = 1\) Hz

C-4: Carbon 4 will be a 1:1:1 triplet of 1:2:1 triplets, \(1J_{\text{CD}} = 23\) Hz and \(3J_{\text{CH}} = 7\) 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.