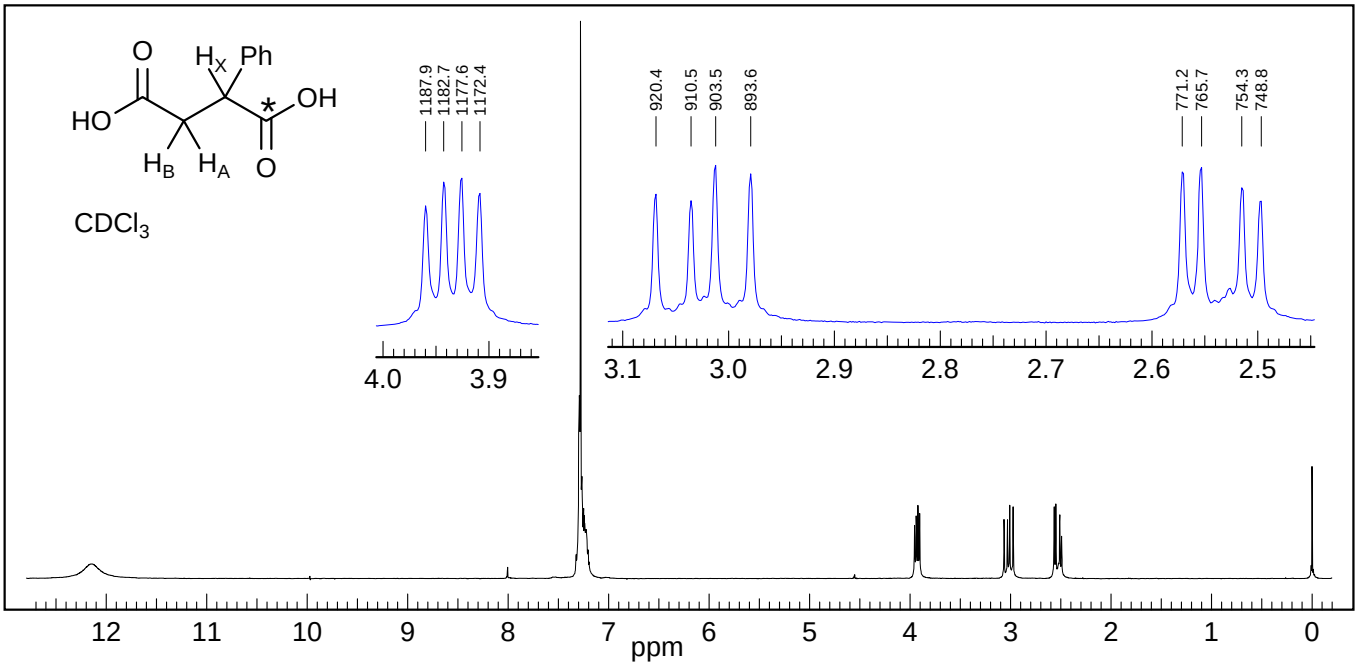
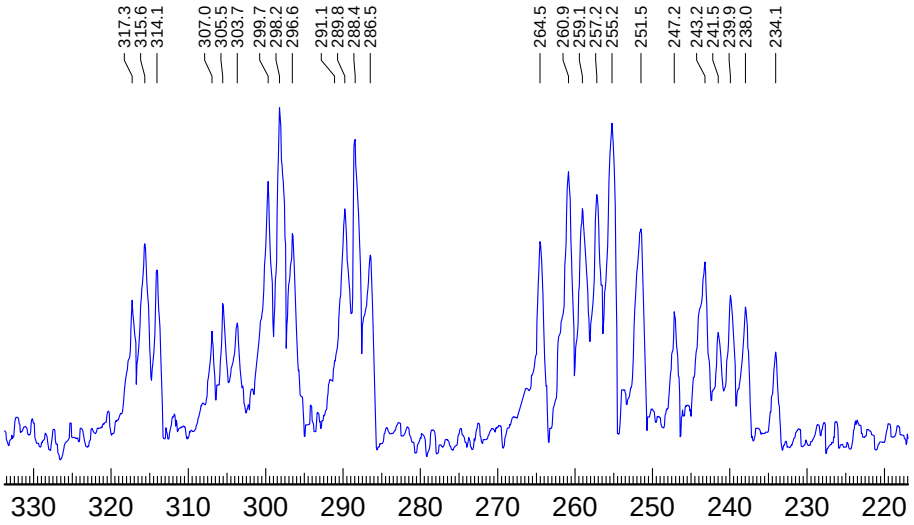
Problem R-65 ($C_{10}H_{10}O_4$). The 300 MHz ^{1}H NMR spectrum of phenylsuccinic acid in $CDCl_3$-DMSO-d_6 is shown below. From the line positions given, calculate the coupling constants J_{ax}, J_{bx} and J_{ab} (Source: Aldrich Spectra Collection).



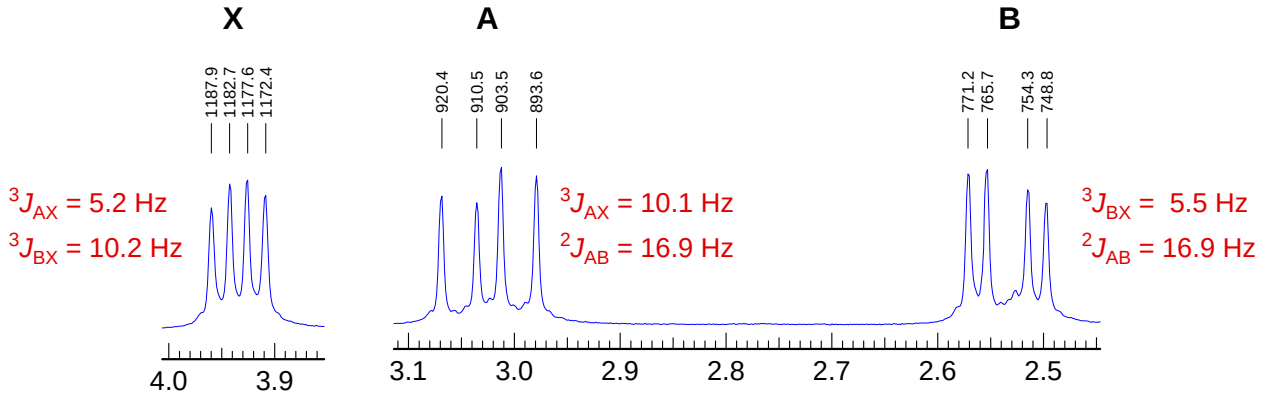
Phenylsuccinic acid partially labeled with ^{13}C at the carboxyl group marked gave the 100 MHz ^{1}H NMR spectrum below (δ 2.2-3.3, acetone-d_6). What is the fraction of ^{13}C incorporation? Estimate the carbon-proton couplings $^3J_{C\text{-}HA}$ and $^3J_{C\text{-}HB}$ from this spectrum. Source: M. E. Rennekamp, C. A. Kingsbury *J. Org. Chem.* **1973**, *38*, 3959 (DOI: 10.1021/jo00962a036).



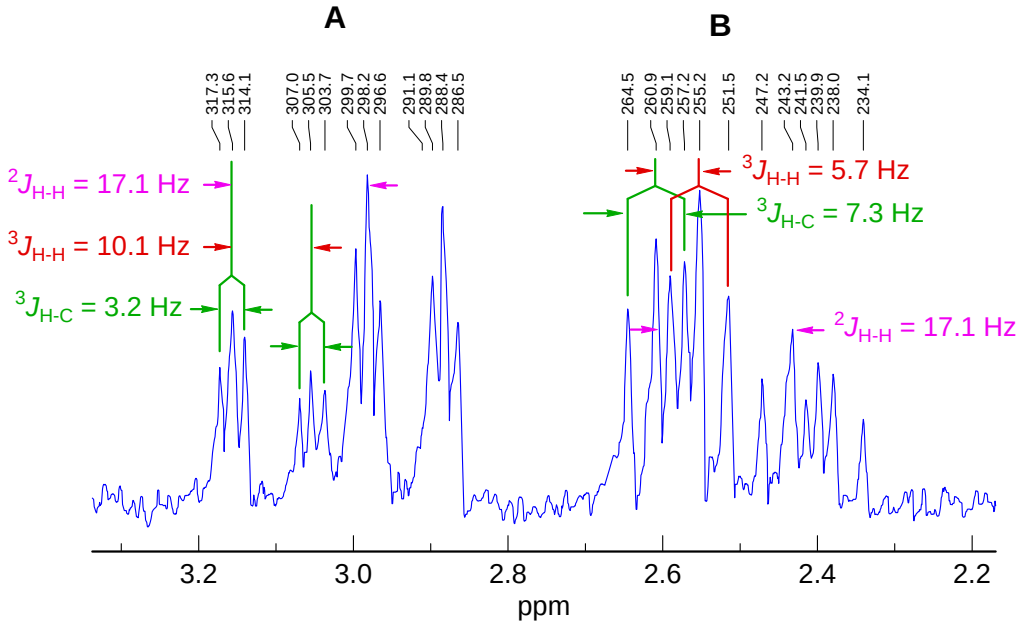
Draw Newman projections for the three possible staggered conformations of phenylsuccinic acid and determine which is the major one in acetone-d_6 solution.

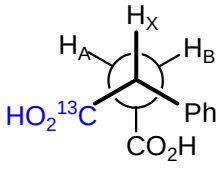
Problem R-65 ($C_{10}H_{10}O_4$). The 300 MHz ^{1}H NMR spectrum of phenylsuccinic acid in $CDCl_3$-DMSO-d_6 is shown below. From the line positions given, calculate the coupling constants J_{ax}, J_{bx} and J_{ab} (Source: Aldrich Spectra Collection).

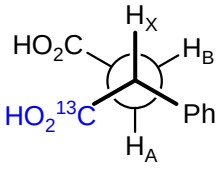
This can be treated as an AMX pattern - first order treatment will give accurate J values ($\nu_{AB} >> 5J_{AB}$)

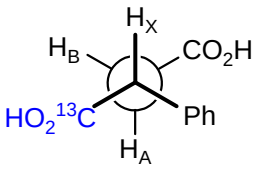


The sample is ca 60% enriched in ^{13}C, from the area of the ^{13}C satellites vs the central peak.









Found:		**Expect:**		**Expect:**		**Expect:**	
J_{AX}	10.1	J_{AX}	small	J_{AX}	large	J_{AX}	large
J_{BX}	5.7	J_{BX}	small	J_{BX}	small	J_{BX}	small
J_{AC}	3.1	J_{AC}	small	J_{AC}	small	J_{AC}	small
J_{BC}	7.3	J_{BC}	large	J_{BC}	large	J_{BC}	small

not true

not true

This is what we see
so this is the major conformation