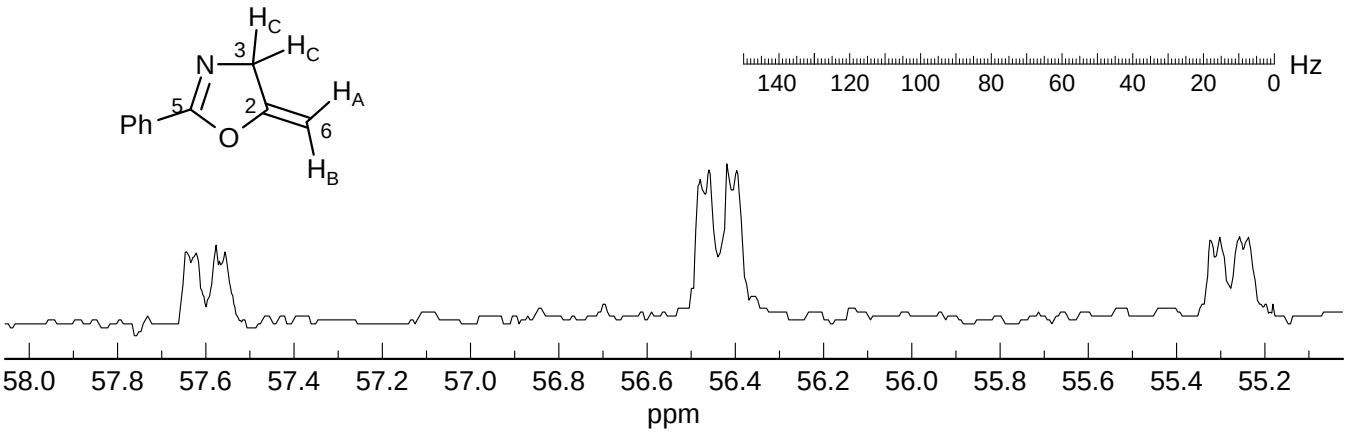
15

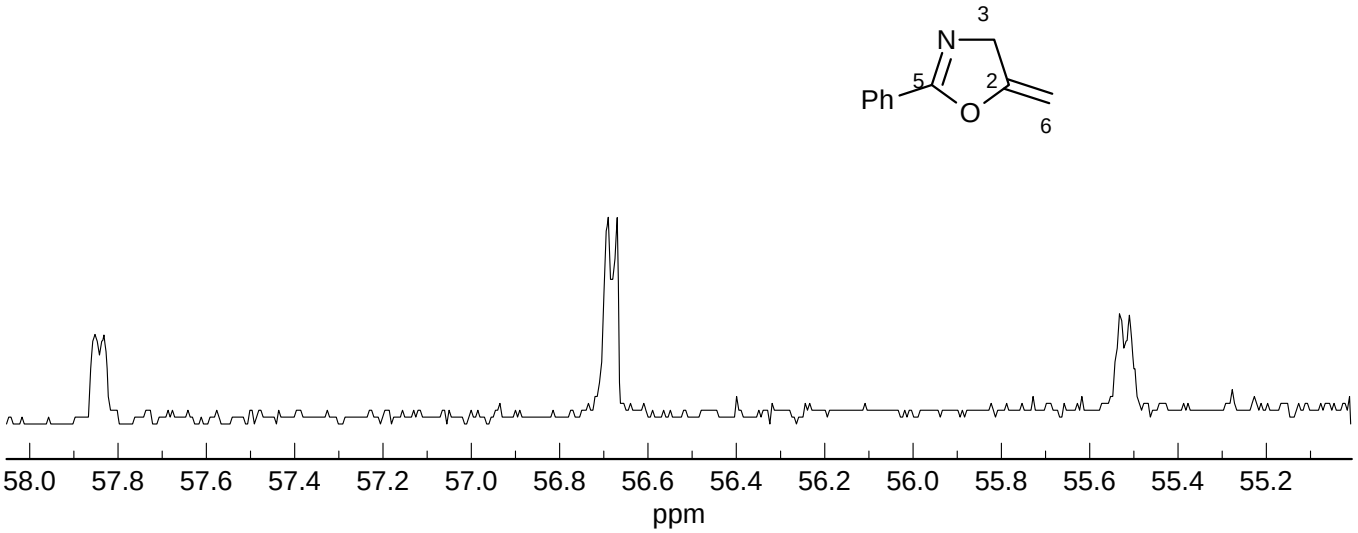
Problem R-12M ($C_{10}H_9NO$). You are asked to interpret the coupled ^{13}C NMR spectrum of an oxazoline Source: Hashmi, A. S. K. *Org. Lett*., **2004**, *6*, 4391.

(a) Which carbon are we looking at? _____



(b) Analyze the spectrum, report all coupling constants in the standard format ($^nJ_{X\text{-}Y}$ = 00.0 Hz).

(c) The spectrum below is of the same compound with one H replaced by D. Where is the deuterium? Place it on the structure, and explain briefly.



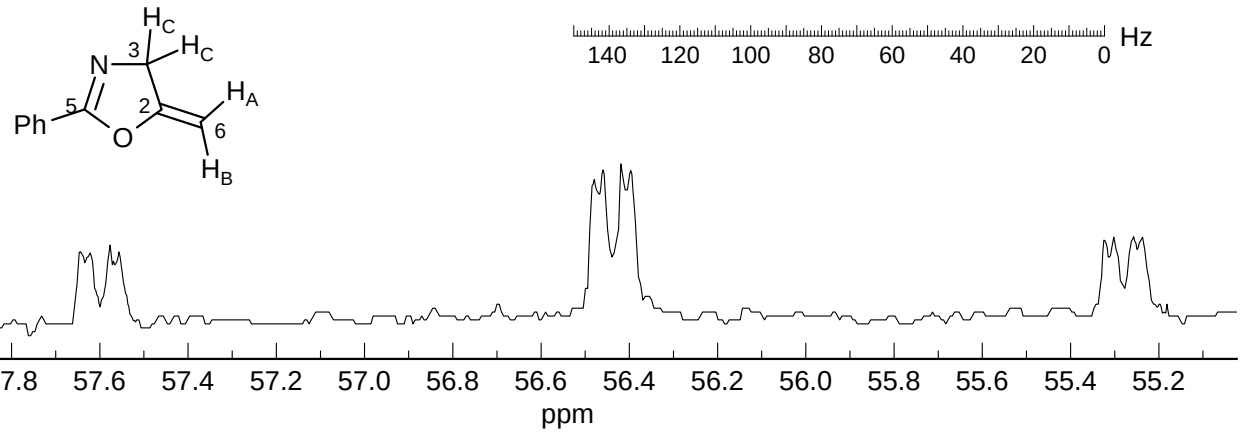
(d) What is the proton NMR frequency of the spectrometer they were using?_____

15

Problem R-12M ($C_{10}H_{09}NO$). You are asked to interpret the coupled ^{13}C NMR spectrum of an oxazoline.

(a) Which carbon are we looking at? C3

2



(b) Analyze the spectrum, report all coupling constants in the standard format ($^{n}J_{X\text{-}Y}$ = 00.0 Hz).

tdd, *J* = 146, 8, 3

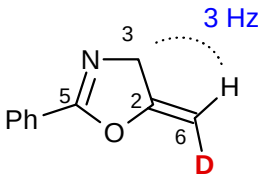
$^{1}J_{C\text{-}H}$ = 146 Hz

5 $^{3}J_{C\text{-}H}$ (trans) = 8 Hz

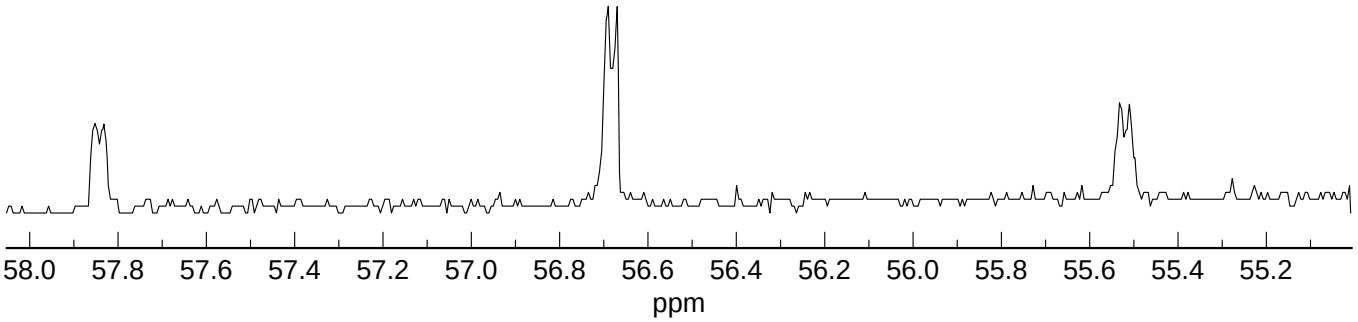
$^{3}J_{C\text{-}H}$ (cis) = 3 Hz

(c) The spectrum below is of the same compound with one H replaced by D. Where is the deuterium? Place it on the structure, and explain briefly.

Only the small cis $^{3}J_{C\text{-}H}$ remains in the deuterated compound, so the trans proton must have been replaced by deuterium. The C-D coupling would be only 1.3 Hz, so is not detectable at this resolution.



5



(d) What is the proton NMR frequency of the spectrometer they were using? 497 MHz

1 ppm = 125 Hz in the ^{13}C NMR spectrum, so the ^{13}C frequency is 125 MHz. Thus the proton frequency is 125x(100/25.14) = 497.2 MHz

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