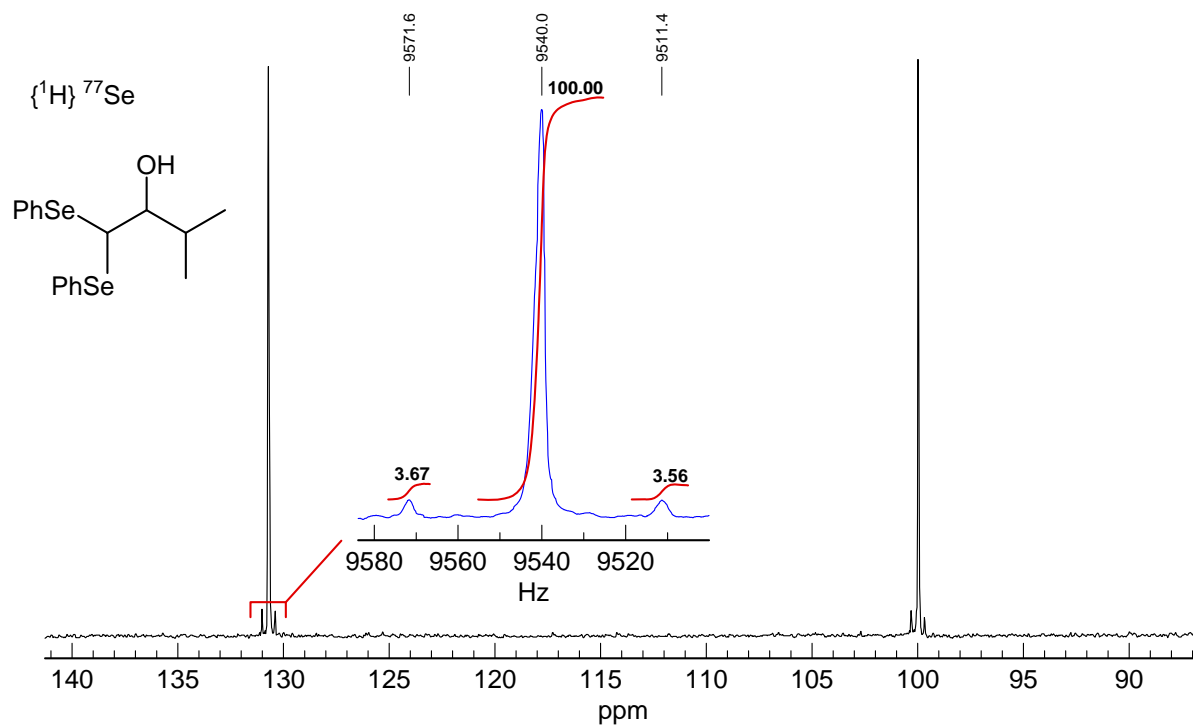
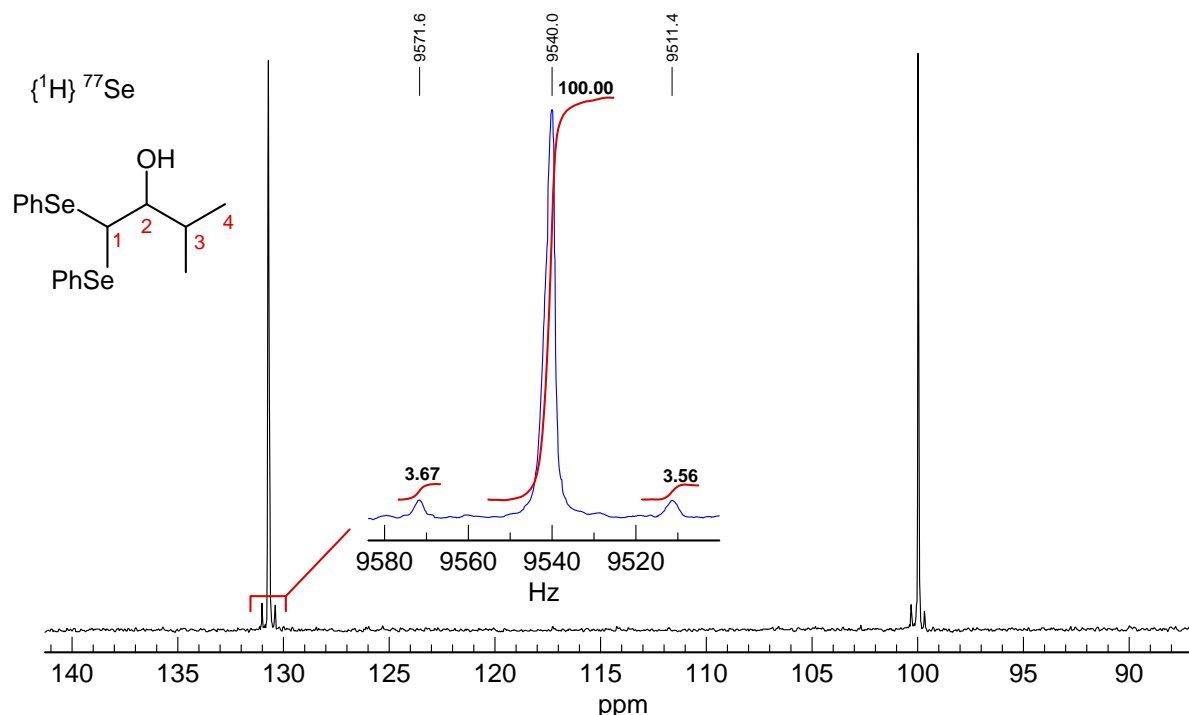


**Problem R-05P** ( $C_{17}H_{20}OSe_2$ ). Reproduced below is the 95.4 MHz proton decoupled  $^{77}Se$  NMR spectrum of 1,1-bisphenylseleno-3-methyl-2-butanol (the chemical shifts are arbitrarily referenced).



- What is the  $^1H$  frequency of the spectrometer?
- Explain why there are two signals.
- Analyze one of the signals (an expansion of the downfield peak is shown).

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(a) What is the  $^1H$  frequency of the spectrometer?

$^{77}Se$   $I = \frac{1}{2}$ , 7.5% abundant, 19.07 MHz ( $^1H = 100$ )

$$^1H \text{ Frequency: } \frac{\gamma_H}{\gamma_{Se}} \times 95.4 = \frac{100}{19.07} \times 95.4 = 500.26 \text{ MHz}$$

(b) Explain why there are two signals.

The asymmetric center at  $C^2$  makes the two PhSe groups diastereotopic ( $\Delta\delta_{Se-Se} = 31$  ppm).

(c) Analyze one of the signals (an expansion of the downfield peak is shown).

The central peak at 9540 Hz is from the fraction of molecules having  $^{77}Se$  in the selenium at 131 ppm, and all the isotopes of the selenium at 100 ppm other than  $^{77}Se$ . The satellites on the 131 ppm peak are from those molecules having  $^{77}Se$  at both seleniums (they add up to 7.23% of the central peak). The two seleniums are coupled to each other:

$$^2J_{Se-Se} = 60.2 \text{ Hz}$$