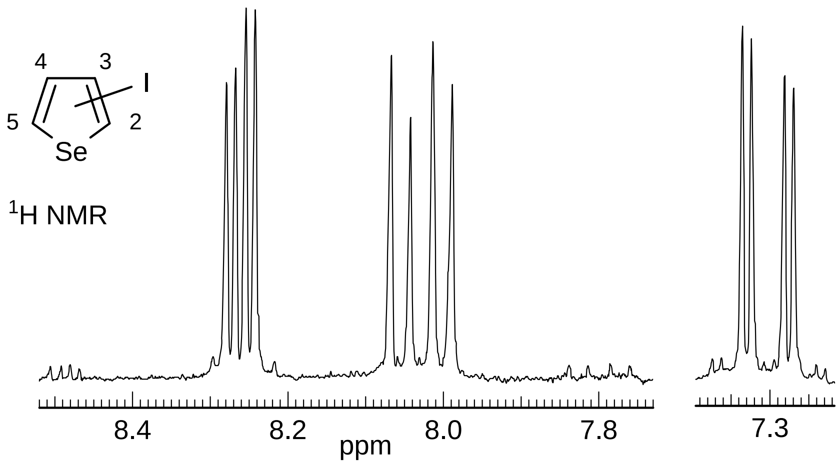
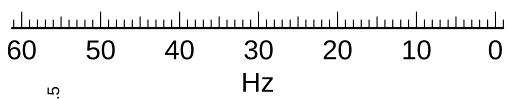
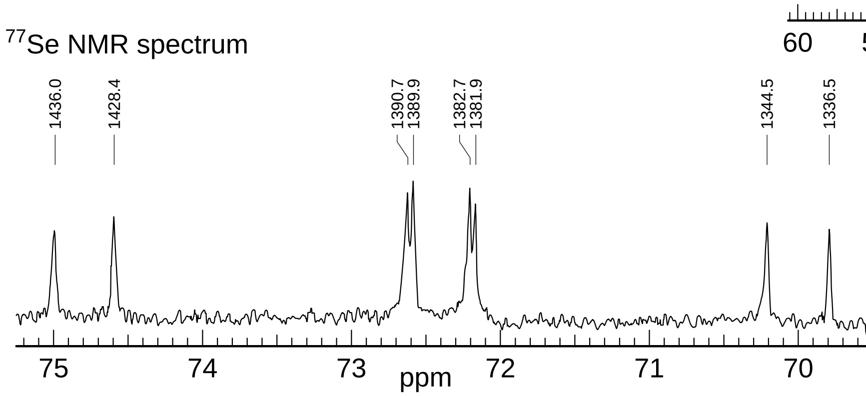
Problem R-12L (C_4H_3ISe). The 100 MHz ^1H and 19.15 MHz ^{77}Se NMR spectra of a mono-iodo selenophene are shown below. Both spectra are at the same Hz scale. Source: Sergeyev *Chem. Scripta* **1975**, *8*, 8.







(a) Interpret the ^1H NMR spectrum, including the various small peaks (e.g., those at 7.8 and 8.5 δ). Report δ and all coupling constants in the standard format.

(b) Interpret the ^{77}Se NMR spectrum. Report all coupling constants. Draw a "coupling tree" on the spectrum.

(c) Draw the structure of **R-12L** below, briefly give your reasoning.

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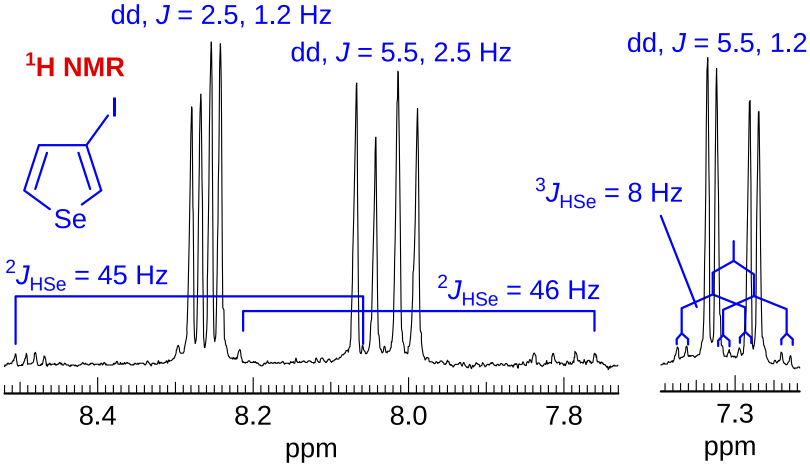
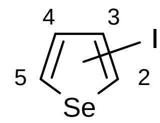
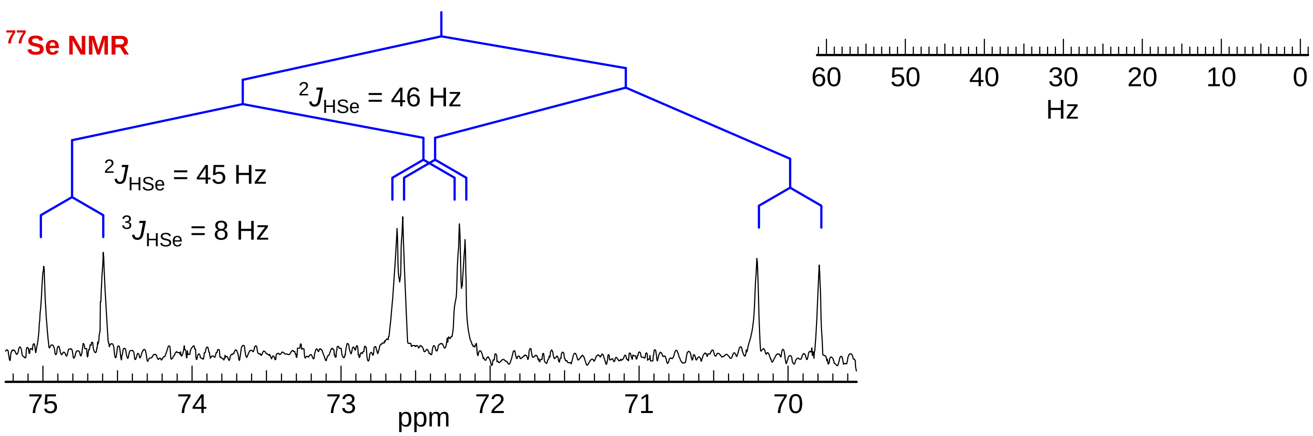
Problem R-12L (C_4H_3ISe). The 100 MHz ^{1}H and 19.15 MHz ^{77}Se NMR spectra of a mono-iodo selenophene are shown below. Both spectra are at the same Hz scale. Source: Sergeyev *Chem. Scripta* **1975**, *8*, 8.





^{77}Se I = 1/2, 7.5% abundant

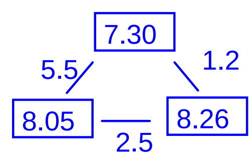


(a) Interpret the ^{1}H NMR spectrum, including the various small peaks (e.g., those at δ 7.8 and 8.5). Report δ and all coupling constants in the standard format.

δ 7.30, dd, J = 5.5, 1.5 Hz. Se satellites: $^3J_{HSe}$ = 8 Hz

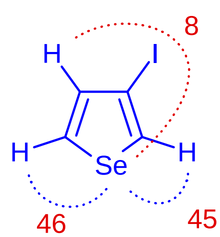
8 δ 8.05, dd, J = 5.5, 2.5 Hz. Se satellites: $^2J_{HSe}$ = 46 Hz

δ 8.26, dd, J = 2.5, 1.2 Hz. Se satellites: $^2J_{HSe}$ = 45 Hz



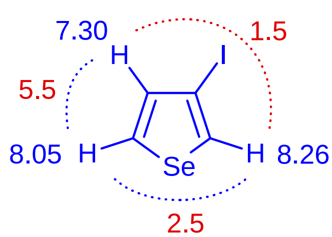
(b) Interpret the ^{77}Se NMR spectrum. Report all coupling constants. Draw a "coupling tree" on the spectrum.

6 δ 72.4, ddd, J =46, 45, 8 Hz



(c) Draw the structure of **R-12L** below, briefly give your reasoning.

6



The two large Se-H couplings require I to be at the 3 position (if know that $^2J >> ^3J$ - see examples under Selenophene in HDATA). This substitution also fits the proton couplings - would have expected J of 5.5 and 3.8 for 2-iodoselenophene.

Chemical shift arguments also favor this structure - the two most downfield protons have the large Se-H coupling