Problem R-11R \((C_{18}H_{22}Se_2)\)
200 MHz \(^1\text{H}\) NMR spectrum in CDCl\(_3\).
Source: Bob Dykstra/Reich (digitized hard copy)
Problem R-11R \( (C_{18}H_{22}Se_2) \) You are given the structure, and asked to interpret the spectrum (complete spectrum on next page).

(a) Analyze the multiplet at \( \delta 2.1 \) and report couplings.

(b) Analyze the multiplet at \( \delta 3.7 \). Identify all peaks. Obtain exact shifts and report all shifts and couplings in the form: \( \delta 0.00, J_{XY} = 00 \text{ Hz} \). An enlarged copy of the multiplet is shown below. The Hz values are from TMS at 0 Hz.
(a) Analyze the multiplet at $\delta$ 2.1 and report couplings.

Septet of doublets, $^3J_{HH} = 6.5$, 3 Hz (H_D)

No Se satellites due to $^3J_{HD-Se}$ can be seen for this multiplet (satellites of the larger inner peaks are buried under the outer ones)

(b) Analyze the multiplet at $\delta$ 3.7. Identify all peaks. Obtain exact shifts and report all shifts and couplings in the form: $\delta$ 0.00, $^nJ_{XY} =$ 00 Hz. An enlarged copy of the multiplet is shown below. The Hz values are from TMS at 0 Hz.

Main feature is the AB quartet ($H_A$, $H_B$) of the diastereotopic Se-CH$_2$-Ph group.

$764, 753, 749, 738$ Hz (marked with • and ●)

$J_{AB} = 764-753 = 11$ Hz; $749-738 = 11$ Hz

Solve the AB quartet:

$$\nu_{AB} = 10.2 \text{ Hz, } \nu_{center} = 751 \text{ Hz}$$

$$\nu_A = 751-5.1 = 746 \text{ Hz, } \delta 3.73$$

$$\nu_B = 751+5.1 = 756 \text{ Hz, } \delta 3.78$$

There are selenium satellites on both sides of each peak of the AB quartet. The $^2J_{HSe}$ if slightly larger for $H_B$ (13.5 Hz) than for $H_A$ (11.5 Hz)

There is also a doublet for $H_C$ at 735 Hz (marked with ●) $\delta 3.67$, $^3J = 3$ Hz (to H_D)

One satellite only is visible (double intensity because there are 2 Se). It is about 2 Hz from central peak, so $^2J_{HC-Se} = 4$ Hz.