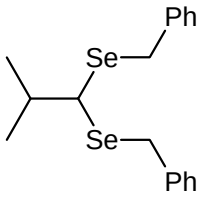
Problem R-11R ($C_{18}H_{22}Se_2$)

200 MHz ^{1}H NMR spectrum in $CDCl_3$.

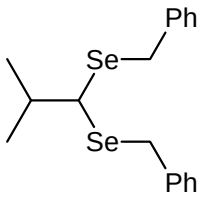
Source: Bob Dykstra/Reich 12/25 (digitized hard copy) g



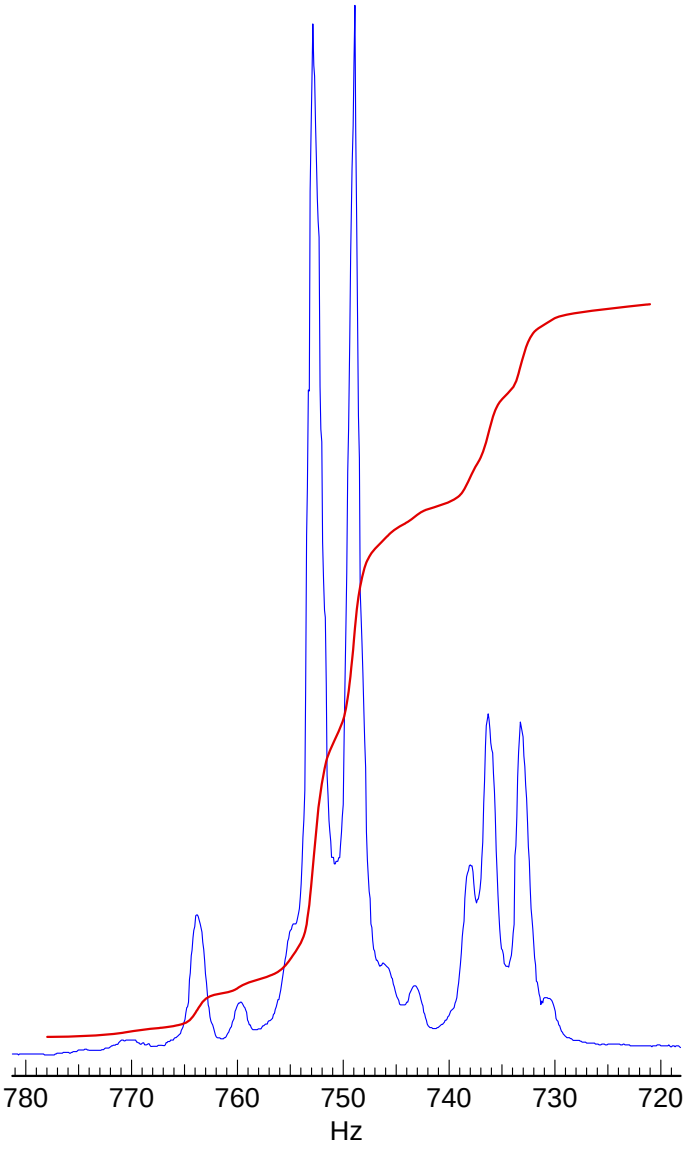
PLT ex-3-2011-12-gq.plt

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 δ 2.1 and report couplings.



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



20

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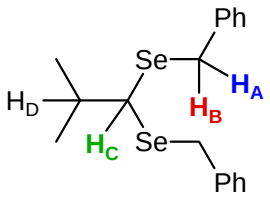


4

Septet of doublets, $^3J_{H\text{-}H}$ = 6.5, 3 Hz (H_D)

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

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

6 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} = 754-753 = 11Hz; 749-738 = 11 Hz

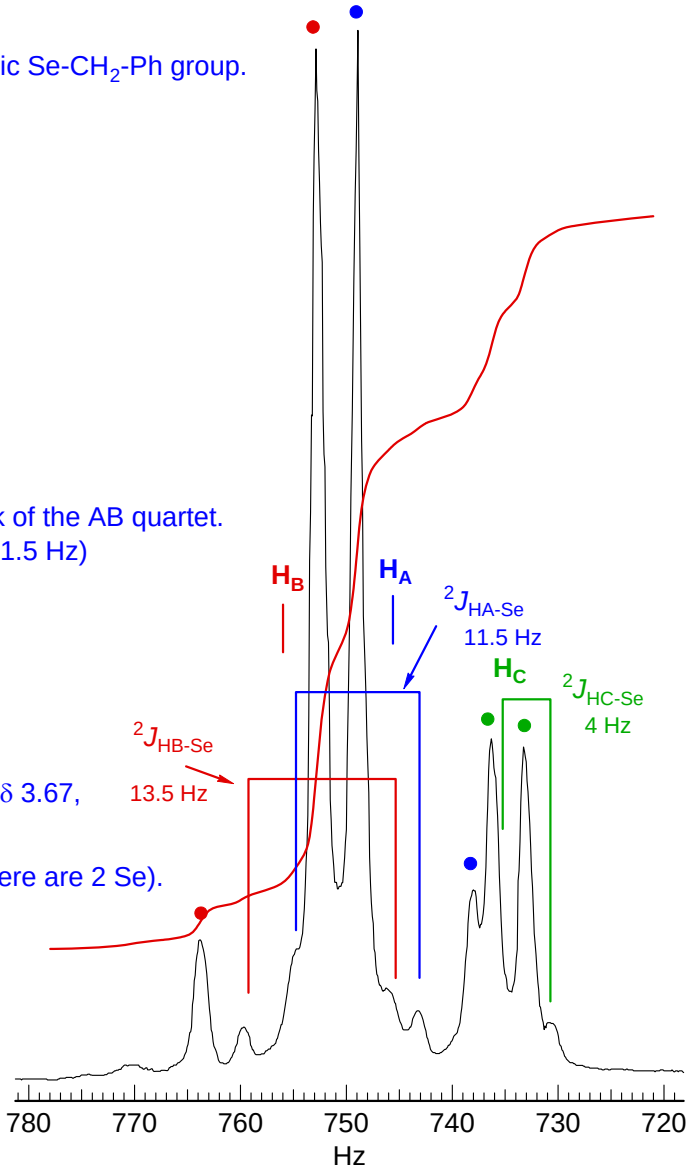
Solve the AB quartet:

ν_{AB} = 10.2 Hz, ν_{center} = 751 Hz

ν_A = 751-5.1 = 746 Hz, δ 3.73

ν_B = 751+5.1 = 756 Hz, δ 3.78

5 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)



3 There is also a doublet for H_C at 735 Hz (marked with •) δ 3.67, ^3J = 3 Hz (to H_D)

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