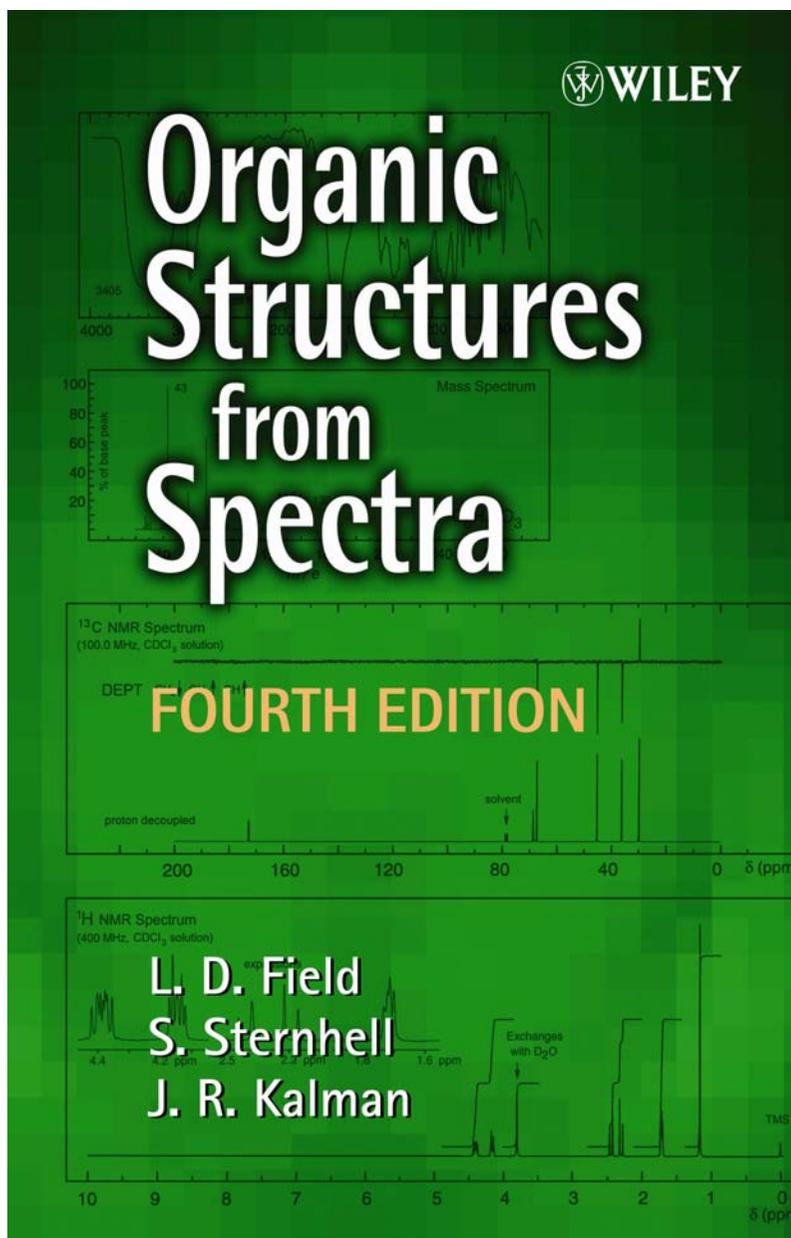


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L D Field, S Sternhell and J R Kalman

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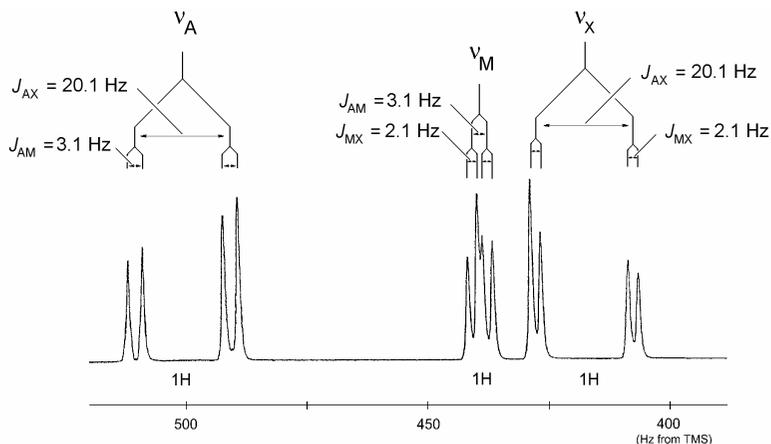
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Problem 315 Spin System AMX



Chemical Shifts

$$\delta_A = 501 \text{ Hz} / 100 \text{ MHz} = 5.01 \text{ ppm}$$

$$\delta_M = 439 \text{ Hz} / 100 \text{ MHz} = 4.39 \text{ ppm}$$

$$\delta_X = 408 \text{ Hz} / 100 \text{ MHz} = 4.08 \text{ ppm}$$

Coupling constants

$$J_{AM} = 3.1 \text{ Hz}$$

$$J_{AX} = 20.1 \text{ Hz}$$

$$J_{MX} = 1.1 \text{ Hz}$$

1st Order Analysis

$$\Delta\nu_{AM} = \nu_A - \nu_M = 501 - 439 = 62 \text{ Hz}$$

$$\Delta\nu_{AE} = \nu_A - \nu_X = 501 - 408 = 93 \text{ Hz}$$

$$\Delta\nu_{ME} = \nu_M - \nu_X = 439 - 408 = 31 \text{ Hz}$$

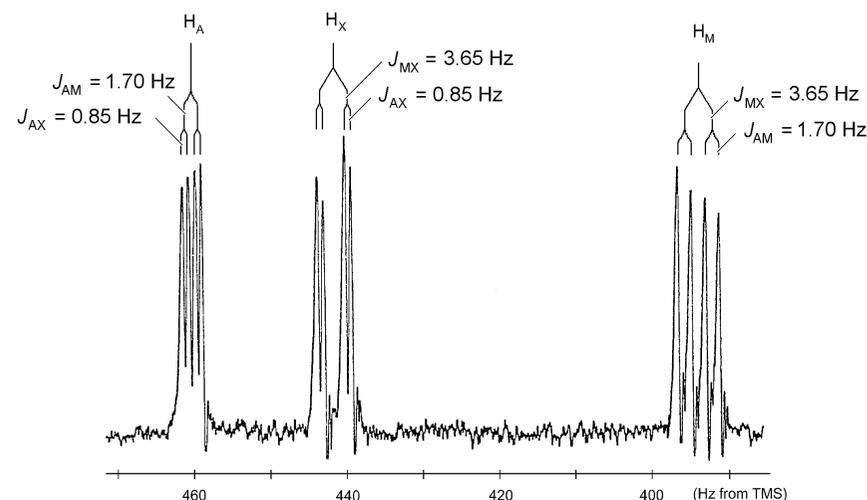
$$\Delta\nu_{AM} / J_{AM} = 62 / 3.1 = 20.0$$

$$\Delta\nu_{AE} / J_{AX} = 93 / 20.1 = 4.6$$

$$\Delta\nu_{ME} / J_{MX} = 31 / 2.1 = 14.7$$

All ratios are greater than 3 so a 1st order analysis is justified.

Problem 316 Spin System AMX



Chemical Shifts

$$\delta_A = 460 \text{ Hz} / 60 \text{ MHz} = 7.67 \text{ ppm}$$

$$\delta_X = 442 \text{ Hz} / 60 \text{ MHz} = 7.37 \text{ ppm}$$

$$\delta_M = 394 \text{ Hz} / 60 \text{ MHz} = 6.57 \text{ ppm}$$

Coupling constants

$$J_{AM} = 1.70 \text{ Hz}$$

$$J_{AX} = 0.85 \text{ Hz}$$

$$J_{MX} = 3.65 \text{ Hz}$$

1st Order Analysis

$$\Delta\nu_{AM} = \nu_A - \nu_M = 460 - 394 = 66 \text{ Hz}$$

$$\Delta\nu_{AE} = \nu_A - \nu_X = 460 - 442 = 18 \text{ Hz}$$

$$\Delta\nu_{ME} = \nu_M - \nu_X = 442 - 394 = 48 \text{ Hz}$$

$$\Delta\nu_{AM} / J_{AM} = 66 / 1.7 = 38.8$$

$$\Delta\nu_{AE} / J_{AX} = 18 / 0.85 = 21.2$$

$$\Delta\nu_{ME} / J_{MX} = 48 / 3.65 = 13.2$$

All ratios are greater than 3 so a 1st order analysis is justified.