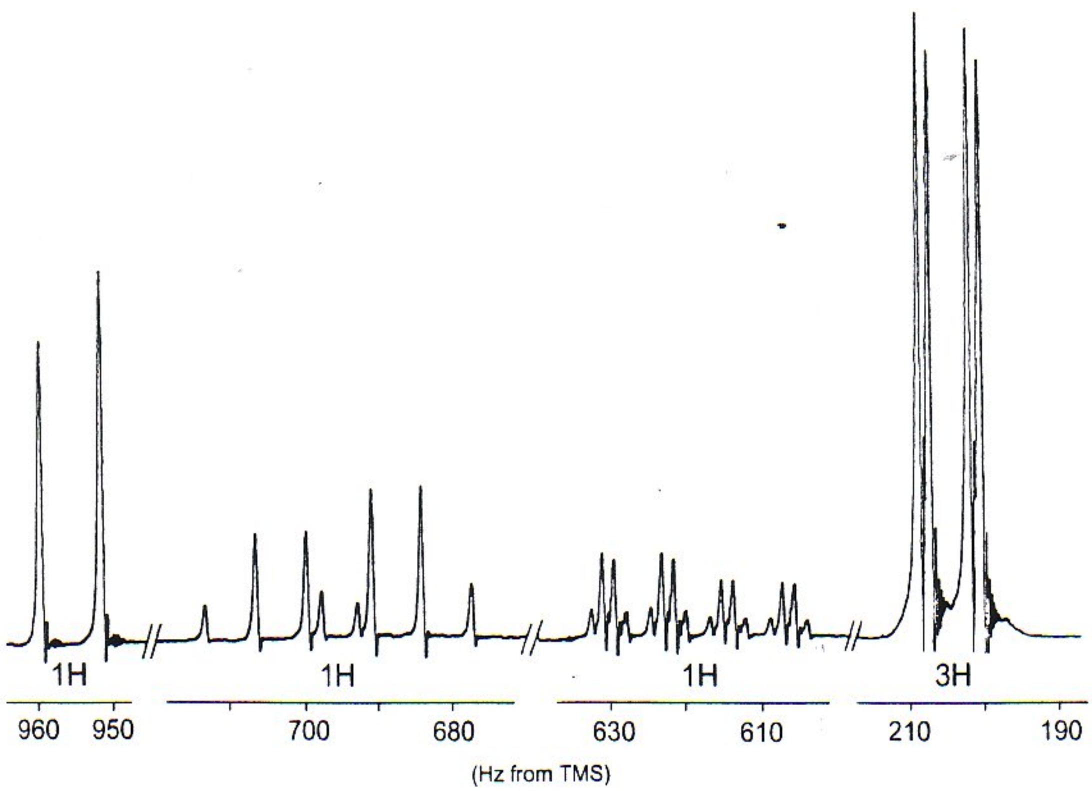
Problem 269

The 100 MHz ^{1}H NMR spectrum (5% in $CDCl_3$) of an α,β-unsaturated aldehyde C_4H_6O is given below.

(a) ~~Draw a splitting diagram and~~ Analyse this spectrum by first-order methods, *i.e.* extract all relevant coupling constants (J in Hz) and chemical shifts (δ in ppm) by direct measurement.

(b) Justify the use of a first-order analysis ~~(see Section 5.6)~~. sp^3-C: $\frac{\Delta\nu}{J} > 10$; sp^2-C: $\frac{\Delta\nu}{J} > 3$

(c) Use the coupling constants to obtain the structure of the compound, including the stereochemistry about the double bond ~~(see Section 5.7)~~.



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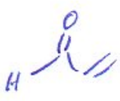
 + CH_3 somewhere : ABMX$_3$

$^3J_{AB}$ 16 Hz

$^3J_{AX}$ 7 Hz

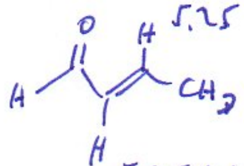
$^3J_{BM}$ 8 Hz

$^4J_{AX}$ 1.5 Hz

$\frac{\Delta\nu}{J} = \frac{(955-695)\ Hz}{8\ Hz} = 32.5 > 10$, ok, first order

even ok for the smaller Δν:

$= \frac{(695-618)\ Hz}{16\ Hz} = 4.8 > 3$, ok, first order



5.25 + 0.44 + 1.13 = 6.82 ppm (exp. 6.95 ppm) ok

5.25 + 1.10 − 0.26 = 6.09 ppm (exp. 6.18 ppm) ok