^{13}C NMR – 6 Things to Know

1) Signals are much weaker (μ of ^{13}C is 25% of ^{1}H; ^{13}C only 1% abundant)

2) Signals in ^{13}C NMR are almost always singlets (sharp)
   a) C-C splittings are extremely low intensity because C is 99% ^{12}C
   b) C-H splitting are eliminated by "decoupling"

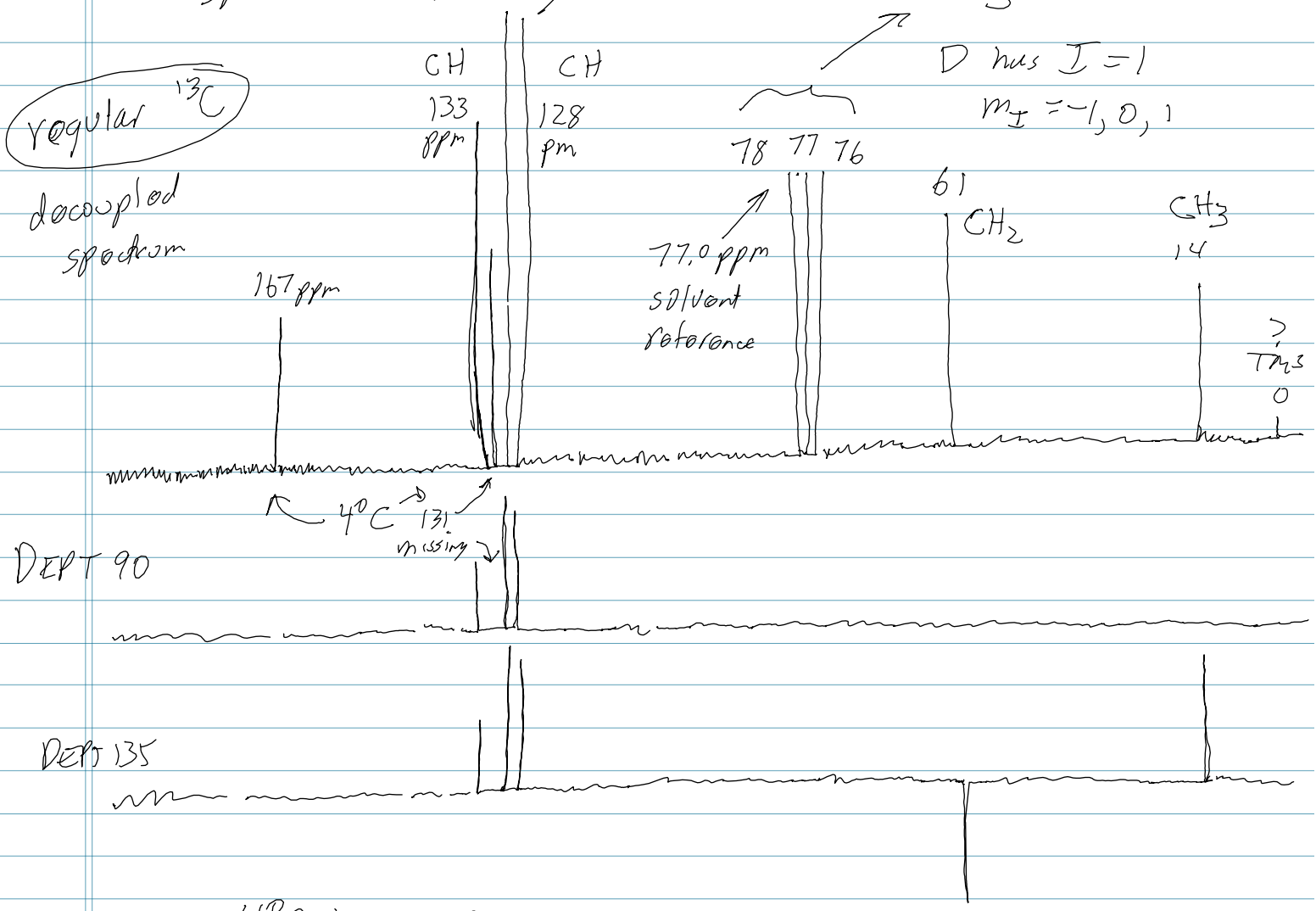
3) Chem shift range is 20× larger than ^{1}H (230 ppm → 0 ppm)
   a) sp^2 C: 230 ppm → 100 ppm (230 → 165 are C=O)
   b) sp^3 or sp C: 100 → 0 ppm (heteroatoms cause downfield shift)

4) Integration unreliable, but...
   a) peak due to 2 equiv C ≈ 2× as large.
   b) C not bound H (quaternary C, 4°) have small signals (≈30 to 50%)

5) DEPT (distortionless enhanced polarization transfer)
   ⇒ show # of attached H
   a) DEPT 90 – see only C with one H attached (CH, ternary, 3°)
   b) DEPT 135 – see CH, CH_3 peaks (3°, 1°) rightside up
      CH_2 (2°) upside down
   c) regular ^{13}C + DEPT 90 + DEPT 135
      ⇒ 4°, 3°, 2°, 1°
      C CH CH_2 CH_3

6) Accidental pk overlap are very rare
   ⇒ # of peaks = # of unique C environments
   (4°, 3°, 2°, 1°) ⇒

^{13}C spectrum of Ethyl Benzoate in $CDCl_3$



4°C : 2	C
3°C : 3	CH
2°C : 1	CH_2
1°C : 1	CH_3