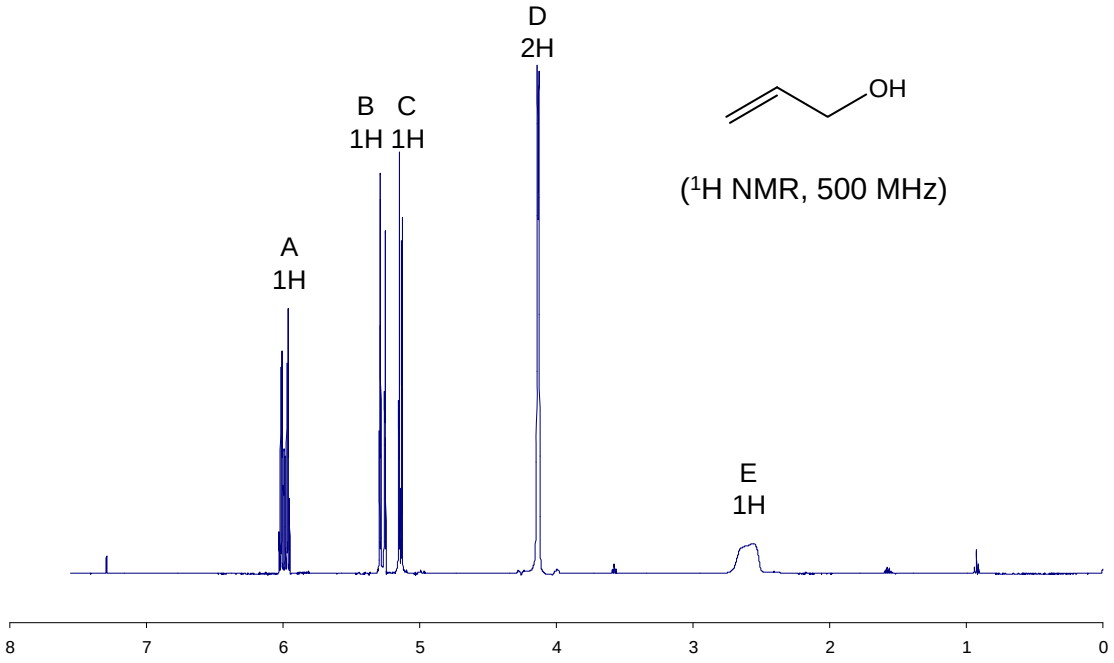
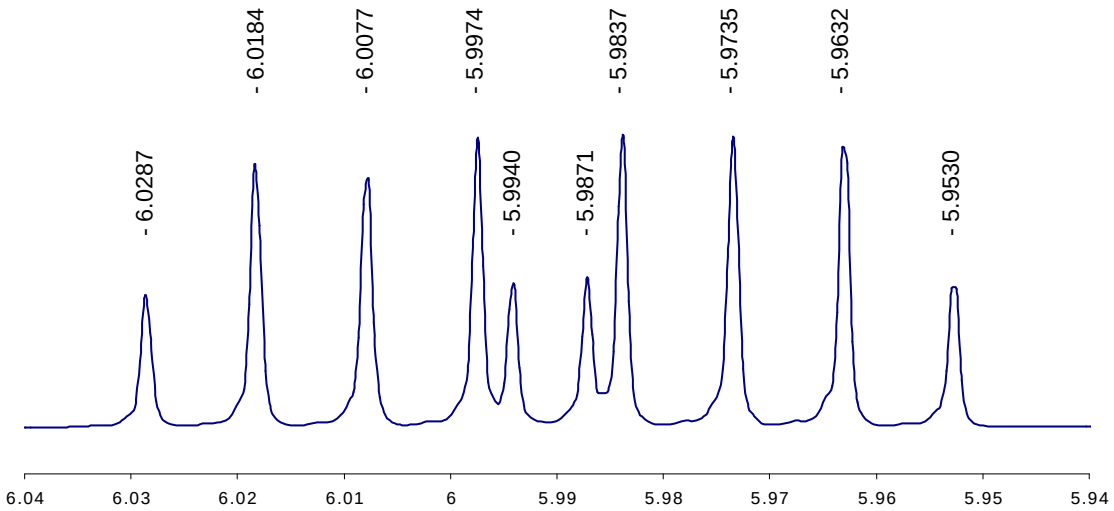
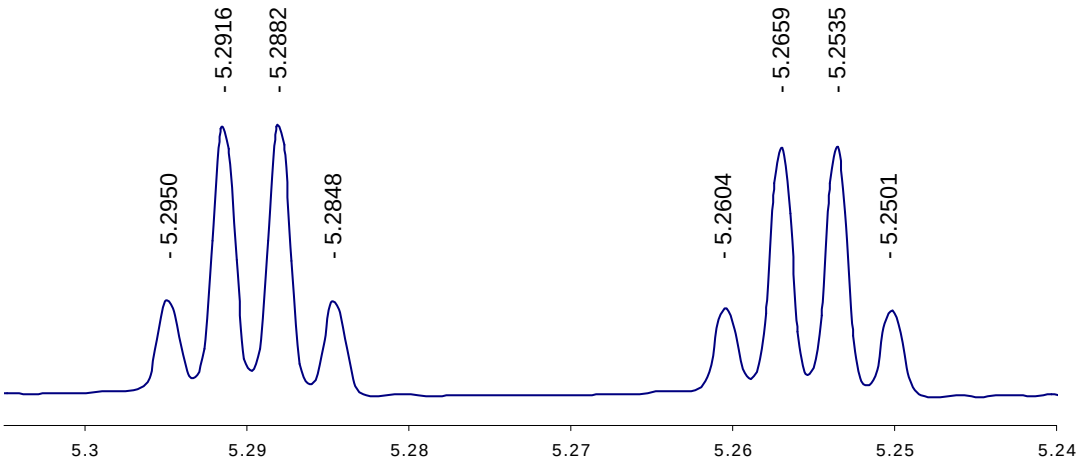
How Do We Deal with Many *J*'s?



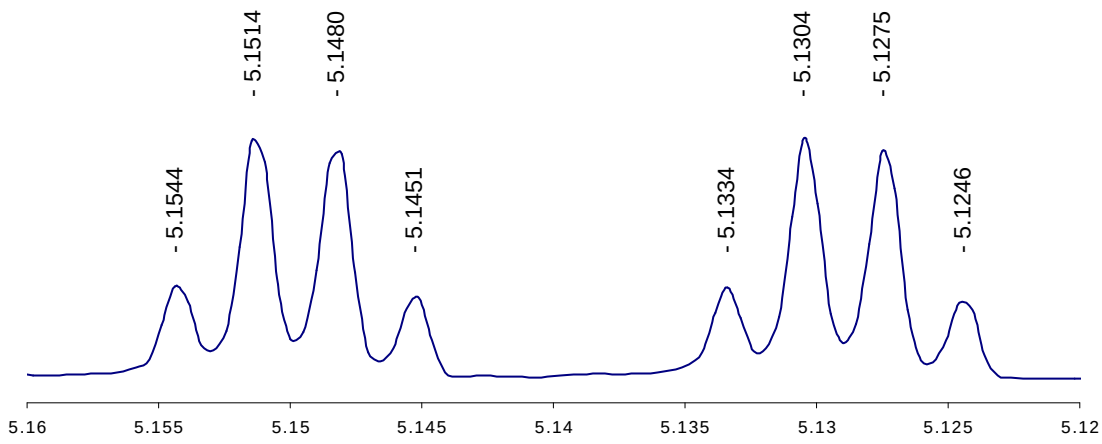
H_A: 1H



H_B: 1H


- 5.2916
- 5.2882
- 5.2659
- 5.2535
- 5.2950
- 5.2848
- 5.2604
- 5.2501
5.3
5.29
5.28
5.27
5.26
5.25
5.24

H_C: 1H


- 5.1514
- 5.1480
- 5.1304
- 5.1275
- 5.1544
- 5.1451
- 5.1334
- 5.1246
5.16
5.155
5.15
5.145
5.14
5.135
5.13
5.125
5.12

Shortcut for Determining *J* Values

1. Determine relative peak sizes
   - First peak is always intensity 1
   - Number all positions in order (a peak with intensity of 2 will have 2 numbers, etc.)
   - Sum of peak sizes must add up to 2^n
   - n = number of J values
2. Distance from 1 → 2 = J_1
3. 1 → 3 = J_2
4. Cross out number representing $J_1 + J_2$
5. 1 → n + 1 = J_n
6. Cross out all additive combinations of J_1, J_2 … J_n that haven't been crossed out yet (should be 2^{n-1} combinations)
7. Repeat 5, 6 …

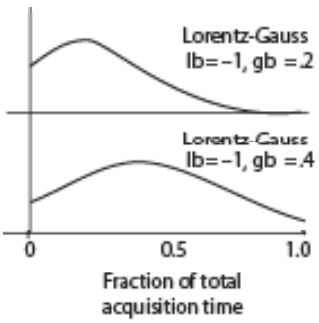
Resolution Enhancement with Window Functions

Problem:

End of FID contains noise that reduces frequency resolution.

Solution:

Multiply FID by a function that de-emphasizes problem areas.



Consequence:

Integrals no longer proportionate.

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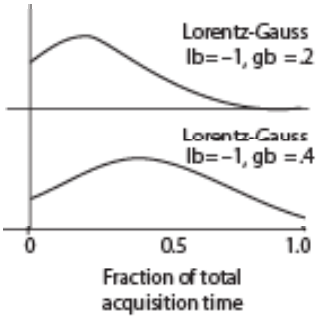

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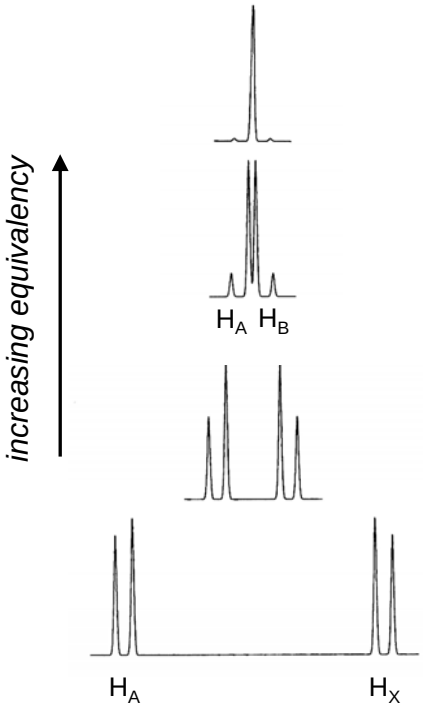
Spectral Distortions at Low $\Delta\nu/J$

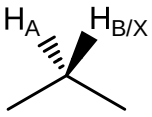


$\Delta\nu/J$ = 0.4

$\Delta\nu/J$ = 1.0

$\Delta\nu/J$ = 4.0

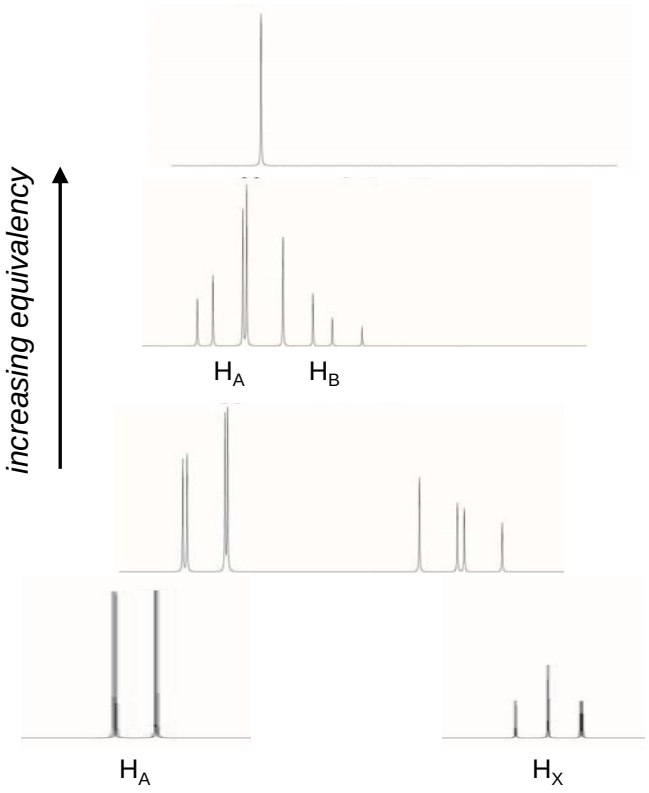
$\Delta\nu/J$ = 15.0

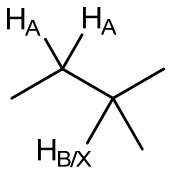


- Say H's are coupled, inequivalent, but not very inequivalent.
- Multiplet intensities are distorted towards each other.
- As long as this is the only issue, *J* can sometimes still be determined by inspection.

Lambert has more discussion.

Spectral Distortions at Low $\Delta\nu/J$





- But sometimes multiplets get too complicated to evaluate *J*'s.

Important takeaway:

Inequivalent protons with identical chemical shift do not split one another.