Problem Set 2. February 2, 2005. **IR Spectroscopy**
CHEM 393
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1. Given below are the IR spectra for 3,4-dimethyl-1-hexene and 2,3-dimethyl-1-pentene.

a) (8 points) Which spectrum belongs to which compound? Label all characteristic bands! see below

b) (1 point) Describe the origin of the bands indicated by an arrow.

A: overtones from bands at 1000 and 900 cm^{-1}

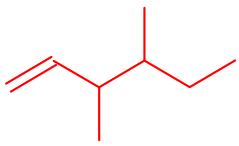
B: overtone from band at 900 cm^{-1}

c) (1 point) Spectrum A shows a band at 1000 cm^{-1} that is missing in spectrum B. Which vibration causes this band in A?

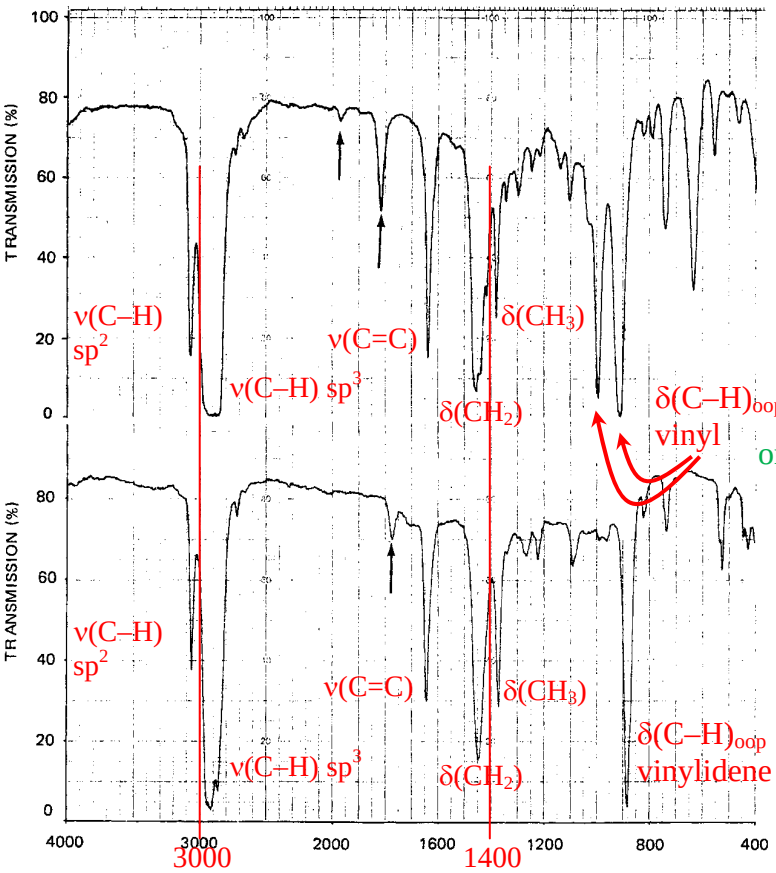
$\delta(C–H)_{oop}$ of the trans H in the vinyl group

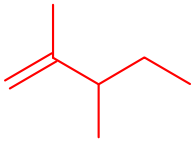
d) (2 points) What is "unacceptable" about spectrum A? Why would you have to rerun it, and how would you improve it?

The band maximum at about 2900 cm^{-1} cannot be observed: there was too much sample. The spectrum would have to be rerun with less sample.



A





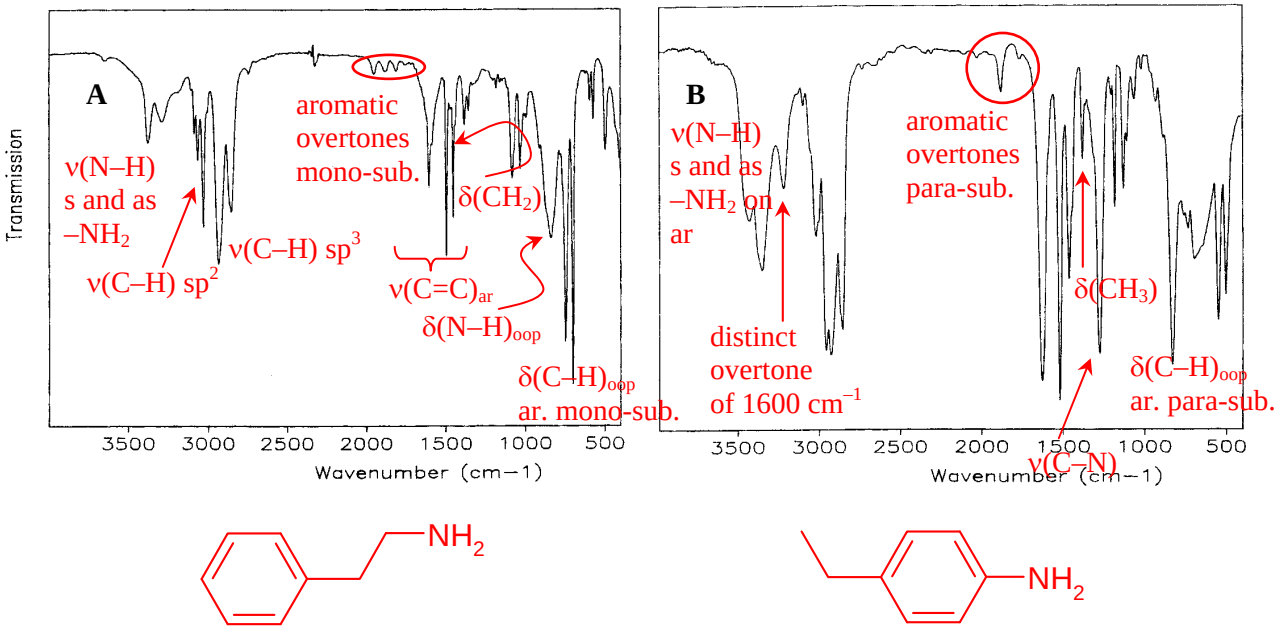
B

It is helpful to draw these particular vertical lines to see whether bands appear on the high or low frequency side!

Notice how the labels are directly at the bands they refer to. If you think I might not understand properly, simply draw an arrow to the band you want labelled!

2. (8 points) Given below are the IR spectra of two isomeric compounds $C_8H_{11}N$, A and B. What are they? Label all characteristic bands.

$$U = 8 + 1 - \tfrac{1}{2}(11 - 1) = 4$$



Only the differences are given in spectrum B; on an exam you should label all characteristic bands!

The ν(C-N) band is not identified in the first spectrum: it occurs between 1350 and 1000 cm^{-1} (towards the low-frequency end of the window for aliphatic amines), so it could be one of two weak bands (not characteristic; you could point them out, anyway). In the second spectrum, there is reason to believe that it would be the strong band at the high-frequency end of the window.

Notice that the answer begins with calculating the unsaturation number: This is alway helpful when dealing with an unknown for which the molecular formula is available!