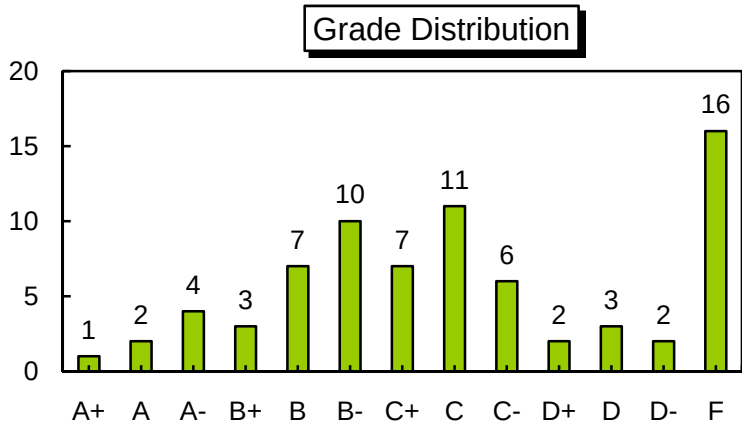
CHEM 393
Spectroscopy and Structure of Organic Compounds

According to Concordia's Centre for Teaching and Learning Services:

- F un
- I nteresting
- R ules
- S yllabus
- T est (pre-)
- C ommunity
- L esson plan
- A xpectations
- S upport
- S mile

Typical class grade distributions in the past

Winter 07 (74)

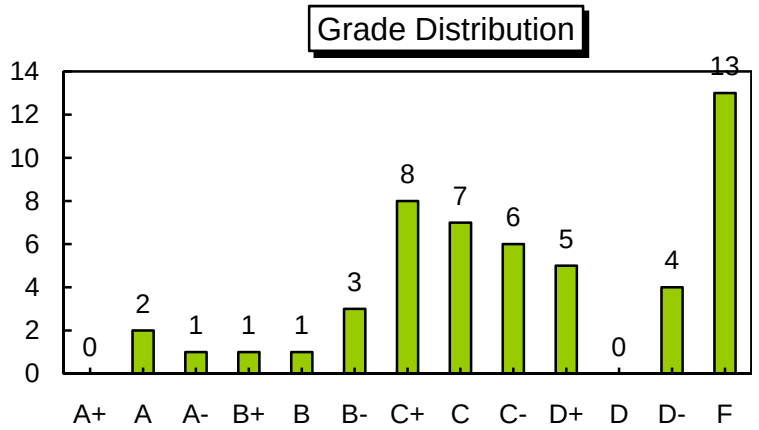


regular practice and reading

no attention to detail

great labs

Winter 06 (51)

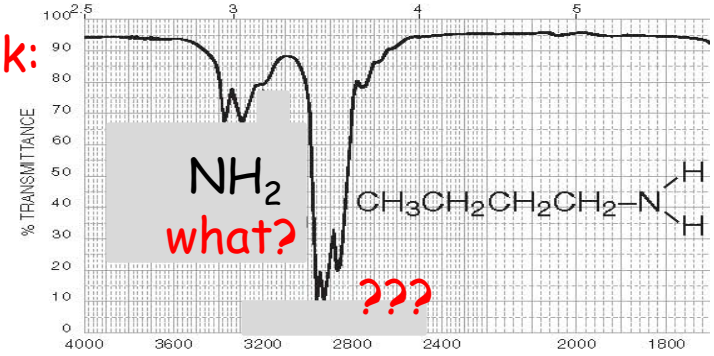


No attention to detail means what?

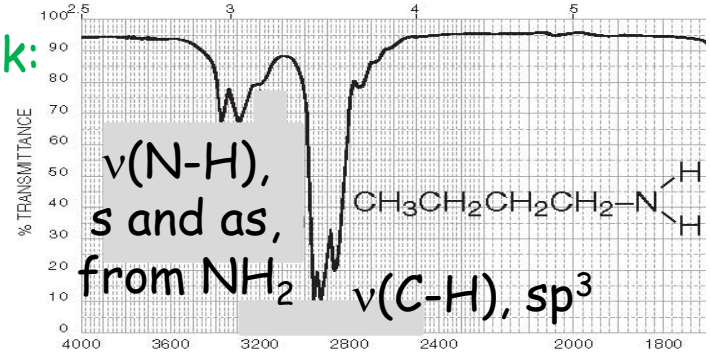
Often caused by not adding to or modifying what you learned in CHEM 222!

- labeling bands either not at all or insufficiently

not ok:



ok:



marks: 0 out of 1

- failing to notice when new information is presented:
  - many students are comfortable with a repeat of coupling information…

    CH_3-CH_2-F: CH_2 couples into a quartet
  - …and cannot follow or work with "more complex coupling":

    H_2C=CHF: CH couples not into a triplet, but into a doublet of doublets

Spectroscopy and Structure of Organic Compounds

Objectives

To provide you with an introduction into the spectroscopic methods used in (organic) chemistry: instrumentation, materials, theoretical background.

To provide you with the necessary tools for the interpretation of spectra of organic compounds: getting all possible information out of a band.

To enable you to identify organic compounds from their spectra through rigorous analyses.

Spectroscopy and Structure of Organic Compounds

Outline

1 Molecular formula and molar mass

2 Ultraviolet spectroscopy

3 Infrared spectroscopy

4 Nuclear magnetic resonance spectroscopy

5 Mass spectrometry

6 Combined structure problems

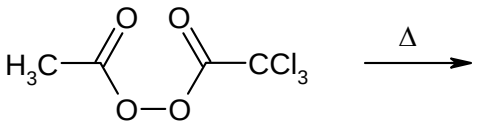
Before we start, you should know (not a comprehensive list!)

- common functional groups.
- the position of the main group elements in the periodic table.
- the approximate atomic masses of H, C, N, O, S, F, Cl and Br.
- the difference between an empirical and a molecular formula.
- what a torsion angle is.
- how to use line drawings of molecules and not forget about H-atoms.
- the difference between shorthand formulae of cyclohexane and benzene.
- that the singular is "spectrum" and the plural is "spectra".
- how to use your calculator.

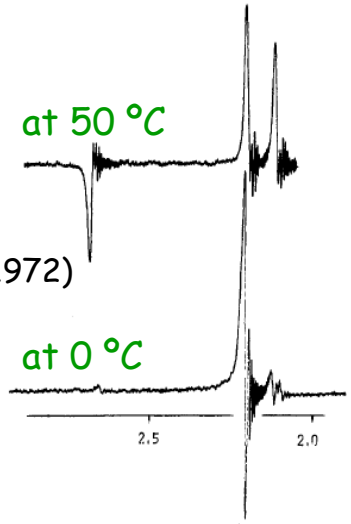
Who needs to know about spectroscopy?

1. The chemist

for fast kinetics, to identify reactive intermediates…

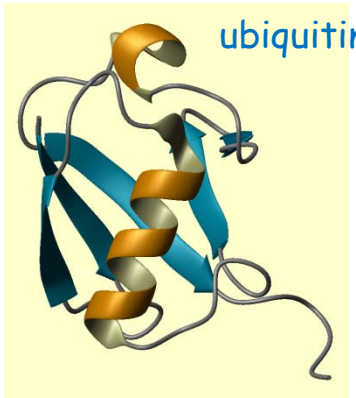


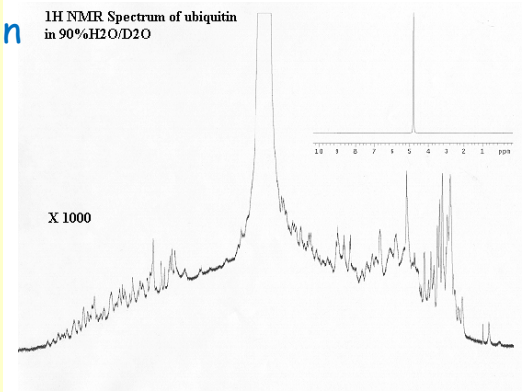
Ward
Acc. Chem. Res. 5, 18 (1972)

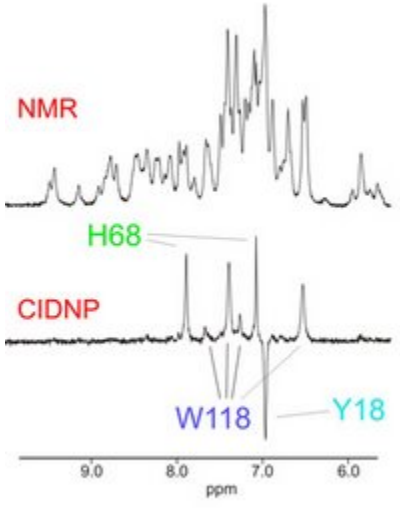


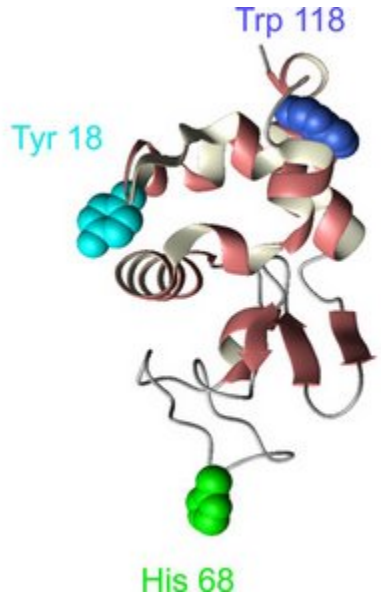
2. The biochemist

protein structure prediction







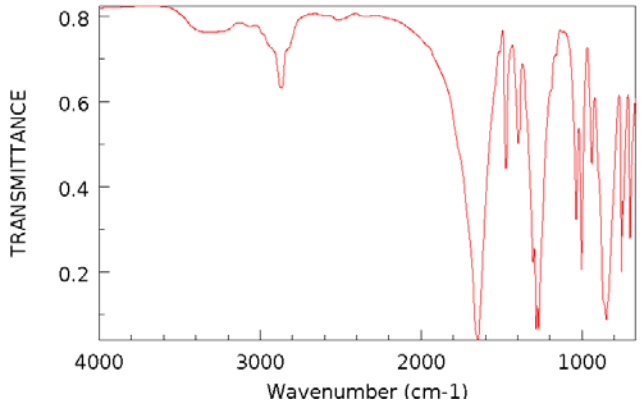


http://bouman.chem.georgetown.edu/nmr/protein.htm

http://http://bioinsilico.blogspot.com/2008/11/protein-structure-prediction_19.html

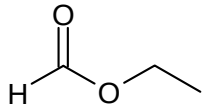
3. The forensic chemist (crime scene investigator)

pentrite, $C(CH_2ONO_2)_4$

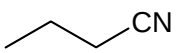


4. The astrochemist

identification of interstellar matter: new molecules in space



found in "a gaseous cloud in the heart of the Milky Way" (Sagittarius B2)



with mm-wavelength spectroscopy by Robin T. Garrod and coworkers, Cornell

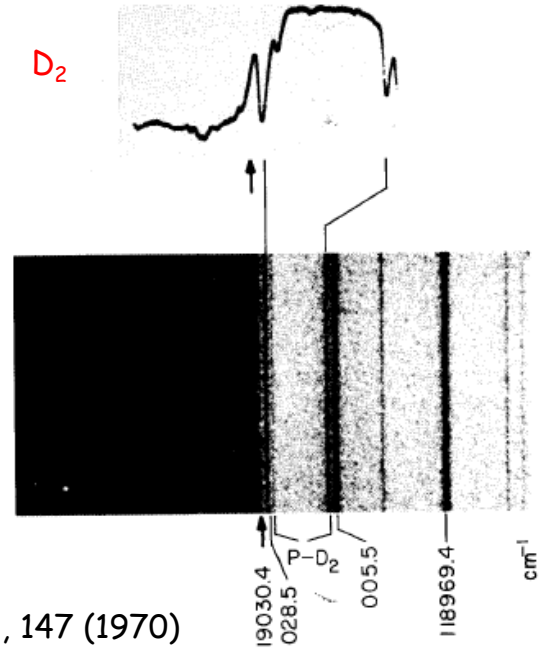
C&E News, April 27, 2009

http://webbook.nist.gov/chemistry

Nobel prizes

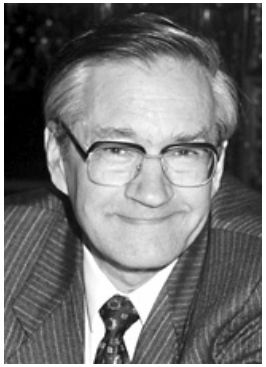
The ultimate prize for recognizing what is "important".

1971
Gerhard Herzberg
for his contributions to the knowledge of
electronic structure and geometry
of molecules, particularly free radicals



Herzberg

J. Mol. Spec. 33, 147 (1970)

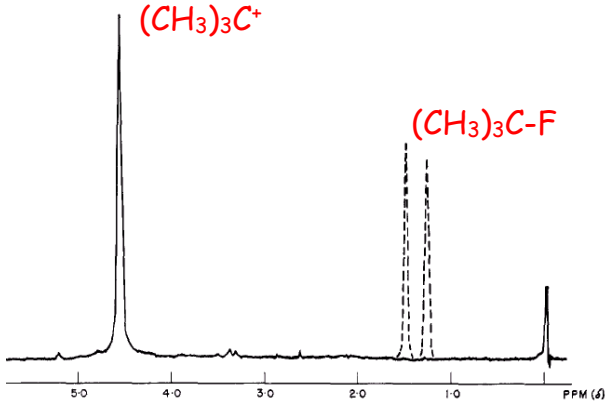


1991
Richard Ernst
for his contributions to the development of the methodology of high-resolution
nuclear magnetic resonance (NMR) spectroscopy

http://nobelprize.org/chemistry/laureates/

Nobel prizes

1994
George Olah
for his contribution to carbocation chemistry



Olah, Baker et al.

J. Am. Chem. Soc. 86, 1360 (1964)

1999
Ahmed Zewail
for his studies of the transition states of chemical reactions
using femtosecond spectroscopy

http://nobelprize.org/chemistry/laureates/