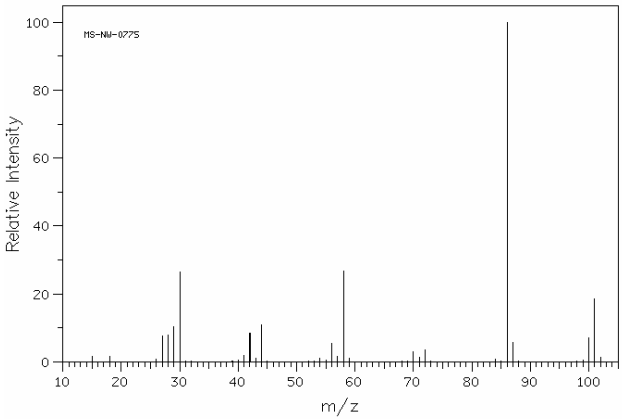
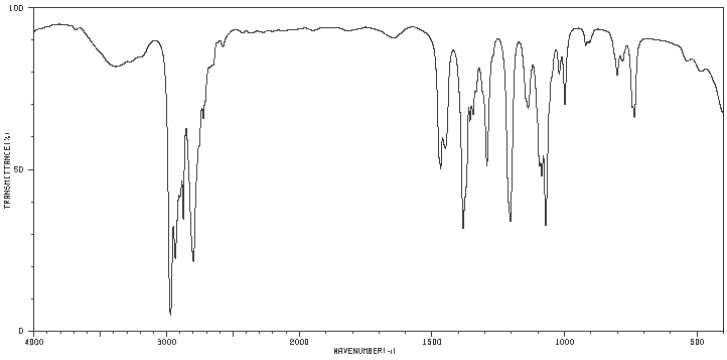
Chem 2061 Fall 2005
Chapter 12 assignment
Due Monday, Oct 24

Answer the following questions on a separate sheet of paper.

A scientist working for a HazMat team arrives at a manufacturing plant where a chemical was spilled. The stench was unbearable, like rotten fish. The scientist took a sample of the chemical and performed GC/MS and IR analysis. The gas chromatogram showed it was a single compound, and the mass spectrum is shown below:




The molecular ion is visible at 101. The infrared spectrum is shown below:

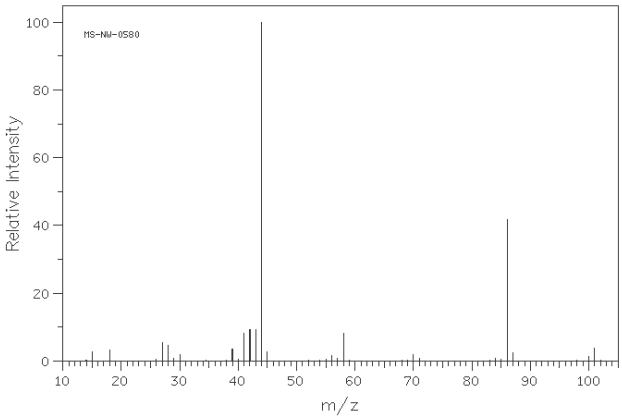



The experimenter assumed that the broad peak above 3000 was too weak to be part of the compound, and was probably just from water.

Assign and rationalize any peaks you can in the above two spectra. Point out any distinctions on the mass spectrum. What common fragments could be lost to give the peaks at 86 and 72?

Draw a few possible structures that could account for the above spectra. How could you confirm your predictions?

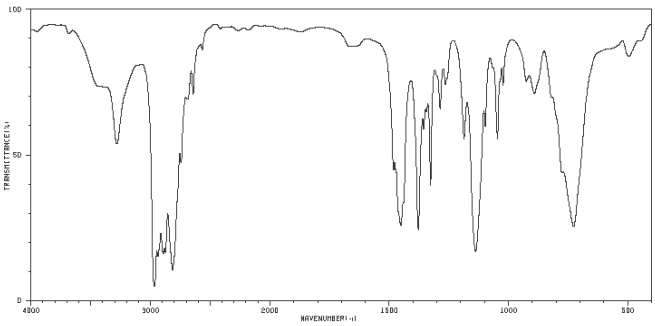
The scientist knew of a smelly compound with a molecular weight of 101 in the supplies at her company, so she analyzed it by GC/MS and IR. Its mass spectrum is shown below:




Like the unknown, it has a molecular ion at 101 and a peak at 86, but she instantly noticed it's missing the peak at 72. Instead there's a peak at 58 that wasn't present in the other compound. What are some fragments that could be lost to give a peak at 58?

Remembering that a molecule only fragments in 1 place to give a peak, refine your above predictions to a molecule that could not have fragment with mass of 72.

The IR is shown below:




The odd peak around 3300 $cm^{-1}$ instantly grabbed her attention. What kind of stretch is it, and why might the compound on the first page not have this peak? (Hint: both the compounds have the same molecular formula)

Using this information, assign a few possible structures to this second compound.