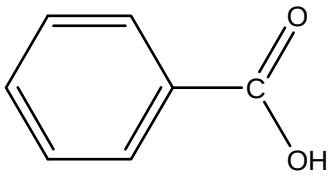
T2 Practice problems (Refer to page C13 in the online manual)

1. Draw the structure of benzoic acid.



Benzoic acid (C_6H_5COOH)

2. Predict the positions of the major IR bands due to the functional groups in benzoic acid.

O-H stretch, acid	***2400-3400 cm^{-1} very broad***
C=O stretch, conjugated acid	***1710-30=1680 cm^{-1} strong***
C-H bend, mono-substituted benzene ring	***690, 700 cm^{-1}***

3. Find an IR spectrum of benzoic acid and assign the major bands.
Hint: there is one in your manual or try a website such as "SDBS".
manual page 28: 2400-3200 (OH); 1675 (C=O); 690 sh, 700 s mono-Ar
SDBS: 2564-3073 (OH), 1689 (C=O), 708, 685 (=CH bend)

4. Why are the cells for infrared spectroscopy not made of glass? Why is it important to keep all IR equipment away from the sink?
Glass (fused silica) does not transmit light below 2500 cm^{-1}.
NaCl and KBr are highly soluble in water (hygroscopic).

5. If you want to observe a band at 520 cm^{-1} for a solid sample, which would be the best choice - a Nujol mull between sodium chloride disks, or a potassium bromide pellet? Explain the reasons for your choice.
NaCl absorbs light below 625 cm^{-1}, thus no information can be obtained using NaCl and Nujol.
AND/OR
KBr absorbs below 385 cm^{-1}, so a KBr disk will allow a band at 520 cm^{-1} to be observed.

6. Is the energy at 4000 cm^{-1} greater or less than that at 2000 cm^{-1}? Explain.
$E = hc/\lambda$ and wavenumber = $1/\lambda$; so energy is directly proportional to cm^{-1}.
Therefore, energy is greater at 4000cm^{-1} than at 2000 cm^{-1}.

For further information watch the Royal Society of Chemistry video on IR instrumentation on the tutorial website, or go to http://www.youtube.com/watch?v=DDTIJgIh86E.