Infrared Analysis of Product

In this exercise we will use infrared (IR) spectroscopy to confirm the presence of acetylsalicylic acid (Aspirin) in the sample as well as to assay the sample for impurities.

The most probable impurities in the synthesized sample according to the SUSB-028 procedure are salicylic acid and water. The amount of water is minimized by thoroughly drying the sample before obtaining the IR spectrum. The Structures and spectra of salicylic acid and aspirin are shown on the next page. Note that both molecules have many structural features in common, and thus show similar peaks in the spectra. For example, each has a strong peak near 1689 cm⁻¹ due to stretching of the C=O bond of the acid group [-\(\text{C=O}\)-O-H]. Each also shows peaks near 1605 cm⁻¹ due to a skeletal vibration of the benzene ring.

Other features of the spectra are quite different. Most obviously, acetylsalicylic acid shows two strong peaks in the carbonyl (C=O) stretching region (1650 – 1800 cm⁻¹), since it has two carbonyl groups. The higher frequency peak at about 1750 cm⁻¹ can be assigned to the acetyl [-\(\text{O-(C=O)-CH}_3\)] group (why?).

In this exercise, you will obtain the infrared spectrum of your synthesized ASA sample. Overall comparison with the spectra of authentic samples given on the following page will be helpful in verifying qualitatively that the product you have synthesized really contains ASA. You will also see if you detect any SA present in the sample as an impurity. Impurities will result in extra peaks such as the OH peak near 3230 cm⁻¹ in salicylic acid.

RESULTS:

1.) What does your infrared spectrum indicate about the purity of your product?

2.) Based on the spectrum of the 50/50 mixture of ASA and SA on the next page, can you detect any SA in your sample? What is your best estimate of the minimum or maximum SA that might be present?
Salicylic Acid (SA)

Acetylsalicylic Acid (ASA) (Aspirin)

50/50 Mixture of SA & ASA