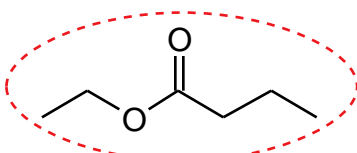


- Checklist for grading rubric; see sample report grading comments: 1) Clearly stated unknown #, physical properties (state, color, odor)
 2) ALWAYS double space your report for easy grading. This allows comments to be added between the lines.
 3) Report IR stretching & bending values to no more than four significant figures; report four significant figures maximum.
 4) Clearly describe your logic (hierarchy process)—beginning with the presence or absence of the carbonyl in identifying your unknown.
 5) Explain in detail how you eliminated other possibilities for your unknown on the list of possibilities given in class.
 6) Precisely & accurately aligned your IR spectrum with an actual spectrum. A help tutorial is provided (click here)

Conclusion

Unknown number O-69 was an ester and was correctly identified as ethyl butyrate.



showed they were capable of using ISIS draw to draw and import an image of a chemical structure

Students are welcome to use similar wording and format with correct flow of logic (hierarchy process) in your analysis as described in the IR tutorials summarizing generic values page 63.

The sample was prepared neat on a (name of instrument) reflectance FTIR and a IR spectral

Thermo-Nicolette iS10 reflectance FTIR

reading was obtained. The presence of a strong sharp stretch for the carbonyl C=O at 1717 cm⁻¹ and C—O at 1170 cm⁻¹ and absorbencies were determined. The absence of

O-H/N-H, and aromatic undertone absorbencies associated with alcohols, amines and aromatics the eliminated these as possibilities and functional groups were no longer considered. The absence of double and triple bonding absorbencies (excluding the

listed the most important absorbencies in the body of the report.

NOTE, these are their measured values

obvious carbonyl) left only the ethers, esters, ketones and aldehydes as possibilities. The determining factor in the identification of unknown O-69 as an ester was the presence of a strong sharp stretch for the C-O at 1170 cm⁻¹ in the C—O region between 1100-1300 cm⁻¹. This characteristic coupled the carbonyl stretch left only the ester and eliminated

ether and aldehyde functional groups as possible matches. The fingerprint region of the original sample was carefully examined and matched alongside to the actual spectrum for ethyl butyrate referenced on the NIST web site¹ which confirmed unknown O-69 as ethyl butyrate.

discussed how their spectrum matched to that of actual

DISCUSS HOW other possibilities were eliminated, describe accurately and precisely your PROCESS & LOGIC!!!!!!!!!!

Ref:

1. <http://webbook.nist.gov/chemistry/form-ser.html>

provided appropriate references

but HOW were possibilities eliminated? don't lose points for not doing.

From our list possibilities given in class, give details and specifics how did you eliminate other possible candidates for your unknown ????

Student points — MISSING in this report — The student lost points for not describing how—names and structures—other possible esters given the list of possibilities were eliminated as possibilities for their unknown.

Where appropriate,
give important bending modes

Give observed measured values

Correlation Table

Specific Functional Group	Observed Frequency Vibration (cm^{-1})	Intensity	Shape
carbonyl C=O	1717	strong	peak
alkene CH_2	1468	moderate	sharp
alkane CH_3	1371	strong	peak
saturated C-C	1300	medium	sharp
ester C-O	1171	strong	sharp

Clearly state how the sample was prepared.

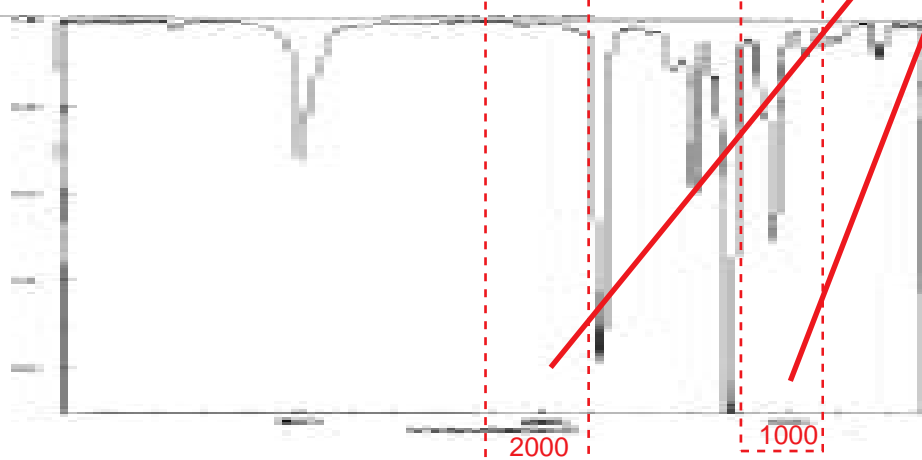
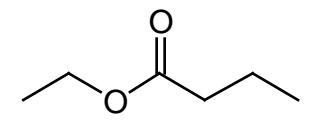
Experimental FT-IR Spectrum - Ethyl Butyrate, Sample Ran Neat

Although in the report the student gave a poor image of their spectrum, they included and aligned it correctly; there was no point



Avoid any point loss align correctly according to our word processing tutorial (click here)

Actual FT-IR Spectrum * - Ethyl Butyrate, Neat

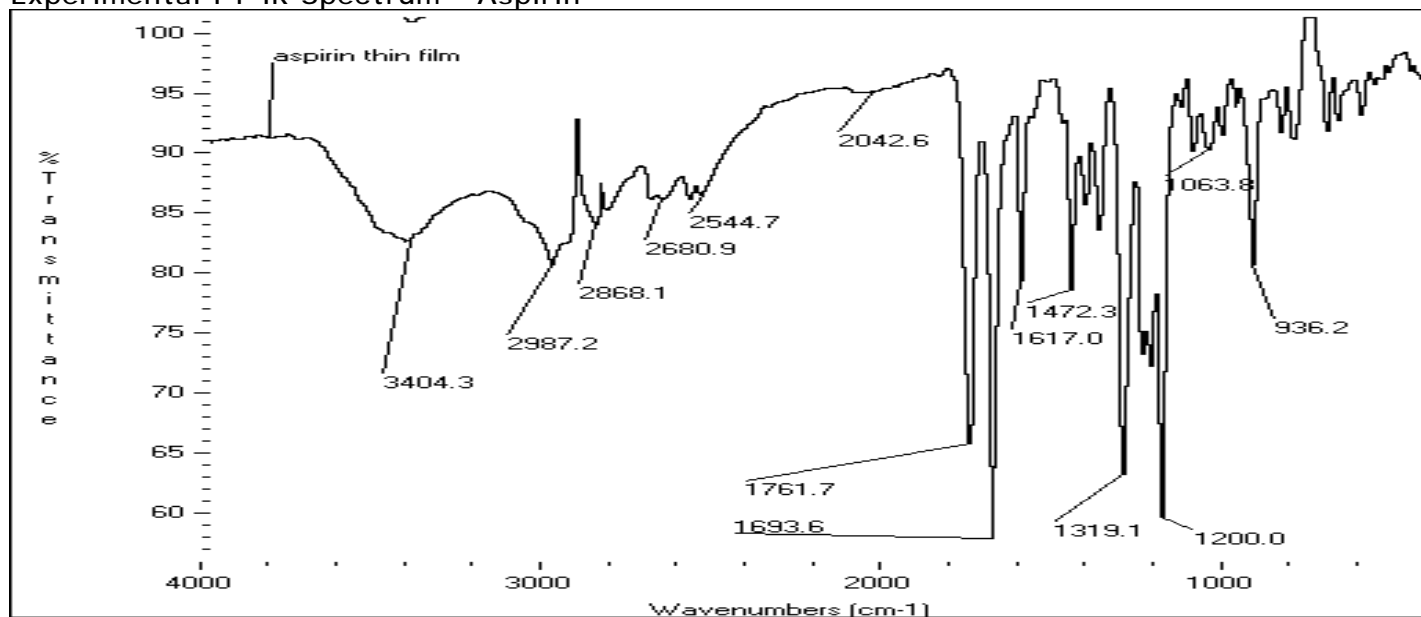
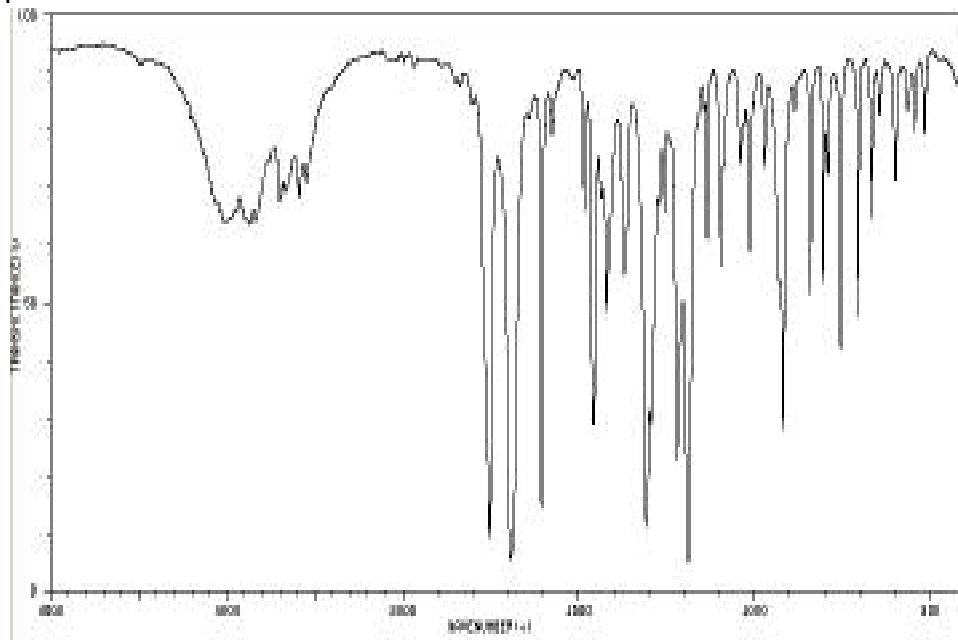
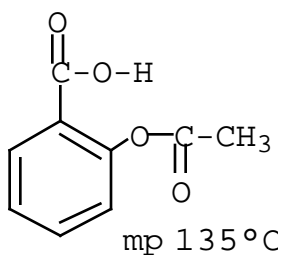


Correctly scaled the actual and measured spectra so the 1000 and 2000 cm^{-1} regions matched for easy comparison

* Source: <http://webbook.nist.gov/chemistry>

Specific Functional Group	Observed Frequency Vibration (cm ⁻¹)	Intensity	Shape
acid O-H	3500-2800	moderate	broad
ester C=O stretch	1762	strong	sharp
acid C=O stretch	1694	strong	sharp
C=C stretch	1617	weak	sharp
C-O stretch	1200	strong	sharp
C-H bend	1472	weak	sharp

Experimental FT-IR Spectrum - Aspirin

Actual FT-IR Spectrum - Aspirin¹1. <<<http://aist.go.jp/RIODB/SDBS/sdbs>>>