Microspectrophotometry

First Derivative Spectra-

Spectra are usually compared by overlaying them to see if they match.

- If they have multiple points of identification e.g. peaks, troughs, shoulders this is easy to do.
- A match can be reported if the peak position and general shape are the same.
- If there is little spectral detail e.g. a broad single peak or if there is a subtle difference when spectra are overlaid, the first derivative spectra may be useful to aid comparison.

- Derivative spectra are usually obtained by Constrained by Constraints of the second signal with respect to the wavelength as the spectrum is scanned.
- The simplest method to produce the first derivative spectrum is by calculating the difference between two points and then smoothing the data before it is differentiated.
- The idea of smoothing was first used by Savitzky and Golay.
- Modern instruments allow first order derivatives to be generated.

• Example – Red Acrylic Fibre.





- A recent study to determine when the technique would be useful involved the following samples:
 - Man-made fibres Red acrylic, Orange polyester, Black polyester, Blue nylon, Blue 'tiger-tail acrylic, blue polyester.
 - Natural fibres Grey lambs wool, yellow cashmere, black cotton, pink wool.
 - Dye Batch fibre samples Brown acrylic (10 batches), Red acrylic (7 batches), Red acrylic (9 batches), Navy blue acrylic (10 batches).

• Problems:

- If different models of instruments are used to generate spectra the results should be viewed with caution.
- Natural fibres exhibit greater variation in absorbance and in the related first derivative spectra.
- 'Tiger-tail' fibres also show great variation.
- Blended samples cause great problems with interpretation.
- Examples will follow .





SET D (3)

MSP800

MSP400





SET D (4)





SET B





SETB





SET F(2)

Benefits:

- When absorbance spectra are broad and featureless their first derivative spectra provide extra points of comparison.
- Subtle differences in the slope of a spectrum can be 'magnified' when first derivative spectra are produced.
- An example follows.











Conclusion:

 First derivative spectra may sometimes be useful but great care should be taken during spectral interpretation to avoid eliminating fibres that originate from the same source.