Infra-Red

Previously, IR has been used as a fingerprint technique to determine the presence (or absence) of specific functional groups through comparisons of the bands present to IR frequency tables. This is just one use of IR spectra.
Other analysis involves the comparison of multiple spectra to show differences and similarities between patterns of different structures or compounds and attributing these to the different structures.

In the solid state atoms are able to interact with one another in various ways through intermolecular interactions, such as hydrogen bonds and hence give differing environments for different atoms of the same type. The environment of atoms will affect the wavelength of the corresponding band and bands can be shifted as a result whilst showing the same fundamental functional group.

It is important to understand the reasons for the shifts and what is a 'real' shift, opposed to differences which could be due to the machine and data collection process. Overall shape, peak shape and position are all important and should be considered when analysing the various IR spectra.

Data

You have been provided with the IR data for the starting material and two polymorphs generated and can be accessed via LabTrove (and downloaded to your computers).

Analysis

The .csv files provided can be opened with excel. Use these files to compare and contrast the different materials and note key differences in the spectra such as peak shifts, similarities and general observations.
More than one data set can be added to a chart allowing spectra to be overlaid for comparisons. Include suggestions to rationalise your observations and relevant peak wavenumbers where applicable to help support the statements.