

FTIR Component Designation Guidelines Updated March 2025

Designate the relative concentration of each substance as major, minor, trace, or unknown. The relative ratio for each substance is based on the relative heights of the peaks compared to one another.

If you would like another technician to review the spectrum please contact the MADDs crew with the sample ID or spectrum directly attached to the email.

- ❖ Major*
 - The substance appears to contribute substantially to the overall composition of the sample.
 - The major substance is the substance that has the clearest, tallest peaks within the spectrum.
 - Substances in major amounts in a sample likely make up more than ~50% of the overall sample composition.
- ❖ Minor*
 - The substance appears to contribute notably to the overall composition of the sample, but not as substantially as a major component.
 - The minor substance has clearly identifiable peaks but are not the tallest peaks within the spectrum.
 - Substances in minor amounts in a sample likely make up 10-50% composition of the sample.
- ❖ Trace*
 - The trace substance is barely visible on the original sample spectrum.
 - There are indications of the substance but it is hard to determine. Typically, a trace substance with very small peaks are visible just above the noise of the baseline.
 - Substances in trace amounts in a sample likely make up 5-10% composition of the sample and is near the limit of detection (LOD)**.
- ❖ Unknown
 - The technician is **NOT** confident in the presence of the substance in the sample.
 - Unknown refers to the technician being uncertain if the compound is in the sample at all. There are indications of the substance in the spectrum but the technician has doubts if the substance is actually present.
 - The uncertainty in the identification can be due to the substance being near the LOD**, noise inhibition, swamping of identification from other substances, etc.

*The technician is **confident** in the presence of the substance based on the FTIR spectrum.

**Limit of Detection (LOD) for the Bruker ALPHA II is ~3% to 5%. Substances under ~3% composition in a sample are unlikely to be identifiable on FTIR.

If you have any questions please contact the MADDs team: (madds@brandeis.edu)