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## Training Procedure for Infrared Spectroscopy

- 1.0 Purpose** – This section will introduce the principles of Infrared (IR) Spectroscopy. The IR spectrophotometer measures the reflectance, transmittance or absorbance of a substance as a function of wavelength of infrared light. The energy absorbed or reflected by a substance can be recorded as an IR spectrum which can be used to identify a substance (e.g., different drugs absorb at different wavelengths of the electromagnetic spectrum). IR can be used as a Category A Technique in the identification of controlled substances. (See the [Drug Chemistry Technical Procedure for Drug Chemistry Analysis](#).) The Forensic Scientist shall become familiar with the basic principles of IR Spectroscopy through the completion of study questions and the analysis of a set of known substances.
- 2.0 Scope** - This procedure applies to trainees in Drug Chemistry at the Raleigh, Triad and Western locations of the State Crime Laboratory.
- 3.0 Procedure**
- 3.1 Objectives**
- 3.1.1** Be knowledgeable of the principles of IR spectroscopy.
  - 3.1.2** Be able to operate the IR spectrophotometer properly and change the desiccant.
  - 3.1.3** Successfully perform all calibration and quality control procedures contained in the procedures listed in the [Drug Chemistry Technical Procedure for Infrared Spectroscopy](#).
  - 3.1.4** Review the [Technical Procedure for Drug Chemistry Analysis](#) as it relates to the use of infrared spectroscopy.
  - 3.1.5** Be able use the IR spectrophotometer to identify controlled substances. (Tutorial software is available for the ATR Attachment.)
  - 3.1.6** Review the instrument software used to electronically subtract spectra on the FTIR. Complete a practical exercise utilizing this skill.
  - 3.1.7** Review the Infrared section of the Drug Chemistry worksheet in FA with the Infrared Coordinator (or his/her designee).
  - 3.1.8** Successfully complete a written exam on FTIR spectroscopy.
- 3.2 Study Questions**
- 3.2.1** What is the range for the Infrared Region of the Electromagnetic Spectrum? What is the range used for the determination of controlled substances?
  - 3.2.2** What is the wavelength range scanned for FTIR spectra at the NC State Crime Laboratory?
  - 3.2.3** Explain what happens when infrared electromagnetic radiation impinges on a molecule.
  - 3.2.4** Draw a simple diagram of an IR spectrophotometer and describe the basic components.

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- 3.2.5 Explain in general a Fourier Transform Infrared (FT-IR) spectrophotometer and the advantages of using one over another technique.
- 3.2.6 Explain how an interferometer works.
- 3.2.7 What is an interferogram?
- 3.2.8 What is the function of the laser in the FT-IR spectrophotometers?
- 3.2.9 Explain how an ATR (Attenuated Total Reflectance) Infrared Spectrophotometer works.
- 3.2.10 Can spectra from an ATR be compared to ordinary absorption spectra for purposes of identification?
- 3.2.11 Where do the following functional groups absorb in the infrared spectrum?
- C-H Aliphatic
  - C-H Aryl
  - O-H
  - C=O
  - Secondary amine (N-H)
  - Sulfate stretch
- 3.2.12 What is a wave number?
- 3.2.13 How do you convert the wave number  $4000\text{ cm}^{-1}$  to a wave length in microns ( $\mu$ )?
- 3.2.14 What is the fingerprint region in IR spectroscopy?
- 3.2.15 What region of the IR shows the difference between salt and base forms of drugs?
- 3.2.16 T or F – FTIR can distinguish between enantiomers.
- 3.2.17 T or F - FTIR can distinguish between diastereomers.

### 3.3 Practical/Laboratory Exercises

- 3.3.1 Using the IR Spectrophotometer, test a set of known standards provided by the Drug Chemistry Training Coordinator and record the results. Be able to recognize specific spectra, the difference between IRs of the base and the salt forms of drugs, and identify the functional groups associated with IR peaks.
- 3.3.1.1 Example of Standards to Test Using IR Spectrophotometer (depending upon availability)
- 4-Methylmethcathinone (Mephedrone)
  - Acetaminophen
  - Amphetamine HCl
  - Aspirin
  - Cathinone
  - Cocaine base

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- Cocaine HCl
  - Codeine with aspirin
  - Codeine sulfate
  - Creatine
  - Diltiazem
  - Dimethylsulfone
  - Ephedrine HCl
  - Heroin base
  - Heroin HCl
  - Inositol
  - Ketamine HCl
  - Lactose
  - Lidocaine HCl
  - Mannitol
  - Methamphetamine HCl
  - MDA HCl
  - MDMA
  - MDPV
  - Oxycodone
  - Phentermine
  - Pseudoephedrine
  - Sodium bicarbonate (baking soda)

**3.3.2** Using the IR Spectrophotometer, practice using the subtraction software on a set of mixtures provided by the Training Coordinator or Infrared Key Operator.

#### **4.0 Required Reading**

- Technical Note, “FT-IR Spectroscopy: Attenuated Total Reflectance (ATR).”  
[www.perkinelmer.com](http://www.perkinelmer.com)  
(See Drug Chemistry Shared Drive/Sharepoint)

#### **5.0 References**

Skoog, Douglas A. *Principles of Instrumental Analysis*. 3<sup>rd</sup> Ed. CBS College Publishing: 1985.

Smith, Brian. *Infrared Spectral Interpretation: A Systematic Approach*. CRC Press LLC: 1999.

<http://www.perkinelmer.com>

#### **6.0 Records**

- Drug Chemistry Training Checklist
- Section Completion Summary

#### **7.0 Attachments – N/A**

Revision History		
Effective Date	Version Number	Reason
09/17/2012	1	Original Document
12/06/2013	2	Added issuing authority to header
10/19/2015	3	<b>Header</b> – Revised issuing authority <b>3.1.4</b> – Added objective to review Technical Procedure for Drug Chemistry Analysis. <b>3.1.6</b> – Added objective to review software and perform practical exercise on subtraction of spectra <b>3.1.7</b> – Clarified requirements for combined written spectroscopy exam. <b>3.2</b> – Edited study questions to illicit more specific information on answers.
08/17/2018	4	Add FA portion to objectives <b>3.2.9, 3.2.14</b> – removed <b>3.3.1.1</b> – edited examples of standards for more relevant ones <b>3.2.2, 3.2.16, 3.2.16</b> – added new questions