CHEMDU · COMMUNITY CHEMISTRY · LEVEL 2 ADVANCED

LECTURE L2-12

Spectroscopy

The Rainbow That Identifies Molecules: How a Breathalyzer Knows You've Been Drinking and How an MRI Sees Inside You

Duration: 90 minutes (expanded from 75)

Advanced lecture script — pre-requisite: Level 1

HOOK (3 minutes)

Teacher holds up (or shows photos of):

A bottle of sunscreen (SPF 50 — protects against UV)

A breathalyzer (used by police)

A pregnancy test (color-changing strip)

A glow stick (snap to activate — fluorescence)

An MRI machine (medical imaging — uses NMR)

Teacher says: "How does a breathalyzer know you've been drinking? How does sunscreen protect your skin? How does a pregnancy test show a pink line? How does a glow stick glow? How does an MRI see inside your body without cutting you open?

They all use spectroscopy — the study of how light interacts with matter.

- Today's question: How can scientists identify a chemical — and measure how much is there — just by looking at the light it absorbs, emits, or scatters? *

By the end of this session, you will be able to:

Explain how a spectrophotometer works (light source → sample → detector)

Use the Beer-Lambert Law ($A = \varepsilon bc$) to calculate concentration

Explain how UV light damages skin and how sunscreen blocks it

Understand how a breathalyzer detects alcohol using IR spectroscopy

Explain how glow sticks use fluorescence

Understand how mass spectrometry identifies molecules by their weight

Explain how MRI uses NMR to see inside your body"

SEGMENT 1: What Is Spectroscopy? (5 minutes)

Teacher says: "Before we go deeper, let's define spectroscopy."

Spectroscopy (spek-TROS-koh-pee) is the study of how light (electromagnetic radiation) interacts with matter. Different molecules absorb, emit, or scatter light in unique patterns — like fingerprints.

Teacher: "Think of it this way: Every molecule has a unique 'fingerprint' in light. If you can read that fingerprint, you can identify the molecule — even if you can't see it with your eyes."

The Electromagnetic Spectrum — Quick Refresher

Type of Light	Wavelength Range	Household Connection
Gamma rays	Very short (< 0.01 nm)	Medical imaging (CT scans)
X-rays	0.01 - 10 nm	Dental X-rays, airport scanners
Ultraviolet (UV)	10 - 400 nm	Sunscreen, tanning beds, germicidal lamps
Visible	400 - 700 nm	Colors you see (rainbow)
Infrared (IR)	700 nm - 1 mm	Remote controls, heat lamps, breathalyzers
Microwave	1 mm - 1 m	Microwave ovens, cell phones
Radio waves	> 1 m	Radio, Wi-Fi, Bluetooth, MRI

Teacher: "Different types of spectroscopy use different parts of this spectrum. Today, we'll cover five types you encounter in daily life:

UV-Vis spectroscopy (sunscreen, pregnancy tests)

Infrared (IR) spectroscopy (breathalyzers)

Fluorescence spectroscopy (glow sticks, forensic lights)

Mass spectrometry (drug testing, identifying unknown powders)

NMR spectroscopy (MRI medical imaging)"

SEGMENT 2: How a Spectrophotometer Works (The Instrument) (8 minutes)

Teacher says: "Before we talk about what spectroscopy measures, let's understand the machine that does the measuring — a spectrophotometer."

Spectrophotometer: An instrument that measures how much light a substance absorbs at different wavelengths.

Components of a Spectrophotometer

Draw or show this diagram:

text

Light Source → Monochromator → Sample → Detector → Readout

↓ ↓ ↓ ↓ ↓

Produces Selects Light Measures Displays

light wavelength passes how much result

through light got

through

Component	What It Does	Household Analogy
Light source	Produces light across a range of wavelengths	A light bulb
Monochromator	Selects a single wavelength (color) to shine	A prism or filter
Sample cuvette	Holds the liquid sample	A test tube
Detector	Measures how much light passed through	A light meter
Readout	Displays absorbance or % transmittance	A digital screen

Teacher: "The machine shines light of a specific wavelength through your sample. Some light is absorbed by the molecules. The rest passes through. The detector measures how much light got through.

If the solution is very concentrated (dark blue), very little light gets through. If it's very diluted (pale blue), most light gets through."

> Quick check (show of hands / chat): "If a solution is very concentrated, does it absorb more or less light?" (More — less light gets through)

SEGMENT 3: The Beer-Lambert Law — Absorbance and Concentration (12 minutes)

> Teacher says: "The Beer-Lambert Law (often just called Beer's Law) is the most important equation in spectroscopy. It tells you that absorbance is proportional to concentration."

$A = \varepsilon \times b \times c$

Where:

A = absorbance (how much light is absorbed — no units)

ε (epsilon) = molar absorptivity (how strongly the molecule absorbs — a constant)

b = path length (how far light travels through the sample — usually 1 cm)

c = concentration (in M, mol/L)

Teacher: *"For a given molecule and a fixed cuvette (b = 1 cm), Beer's Law simplifies to:"*

$A = \varepsilon \times c$ (since b = 1 cm, constant)

What This Means — The Big Picture

Factor	**Effect on Absorbance (A)**
Higher concentration (c ↑)	A increases (more light absorbed)
Longer path length (b ↑)	A increases (light travels through more solution)
Higher ε (molecule absorbs strongly)	A increases (molecule is very 'greedy' for light)

Teacher: "Beer's Law is linear: Double the concentration → double the absorbance. That's why we can use it to find unknown concentrations."

Worked Example 1: Finding Concentration from Absorbance

Problem: A solution of blue dye has ε = 50,000 $M^{-1}cm^{-1}$ (very high — strong absorber). In a 1 cm cuvette, it has A = 1.00. What is the concentration?

Step	**Calculation**
$A = \varepsilon \times b \times c$	
$1.00 = 50{,}000 \times 1 \text{ cm} \times c$	
$c = 1.00 \div 50{,}000$	$= 2.00 \times 10^{-5}$ M

Answer: 2.00×10^{-5} M (very dilute — but still absorbs strongly because ε is large).

Worked Example 2: Finding Unknown Concentration (Standard Curve)

Problem: You have a sample of concentration 0.0001 M (1×10^{-4} M) with A = 0.50. You have an unknown sample with A = 0.75. What is its concentration?

Step	**Calculation**
Since $A \propto c$ (Beer's Law is linear)	
$A_1 / c_1 = A_2 / c_2$	
$0.50 / (1 \times 10^{-4}) = 0.75 / c_2$	
$5{,}000 = 0.75 / c_2$	
$c_2 = 0.75 \div 5{,}000$	$= 1.5 \times 10^{-4}$ M

Answer: 1.5×10^{-4} M (1.5 times more concentrated than the standard).

Worked Example 3: Real-world — Measuring Pollutant in Water

Problem: A water sample contains a pollutant with ε = 10,000 $M^{-1}cm^{-1}$. In a 1 cm cuvette, A = 0.80. What is the concentration in M?

Step	Calculation
A = ε × b × c → c = A ÷ (ε × b)	
c = 0.80 ÷ (10,000 × 1)	= 8.0×10^{-5} M

Answer: 8.0×10^{-5} M (about 0.00008 moles per liter — a tiny amount that can still be measured).

Partner talk (1 minute): "Tell your partner: If you double the concentration of a solution, what happens to absorbance according to Beer's Law?" (It doubles — $A \propto c$)

SEGMENT 4: UV-Vis Spectroscopy — Sunscreen and Beyond (10 minutes)

Teacher says: "UV-Vis spectroscopy uses ultraviolet (UV) and visible light to identify and quantify molecules. It's how sunscreen companies test their products — and how pregnancy tests show results."

UV-Vis spectroscopy: Measures how much UV or visible light a substance absorbs. Different molecules absorb at different wavelengths (colors).

How UV Light Damages Skin

Teacher: "The sun emits UV light in three ranges:

UV Type	Wavelength	Effect on Skin
UVA	315-400 nm	Ages skin, causes wrinkles (penetrates deep)
UVB	280-315 nm	Burns skin, causes sunburn and skin cancer
UVC	100-280 nm	Most dangerous — but blocked by ozone layer

"When UV light hits your skin, it can damage DNA in your skin cells. Over time, this damage can lead to skin cancer."

How Sunscreen Works

Teacher: "Sunscreen contains UV filters — molecules that absorb UV light before it reaches your skin."

Two types of sunscreen:

Type	How It Works	Examples
Chemical	Absorbs UV and converts to heat	Avobenzone (UVA), octocrylene (UVB)

Type	How It Works	Examples
Physical (mineral)	Reflects/scatters UV like clothing	Titanium dioxide, zinc oxide

Teacher: "The SPF number (Sun Protection Factor) tells you how much UVB protection the sunscreen provides. SPF 30 blocks about 97% of UVB rays; SPF 50 blocks about 98%."

Household Example: Pregnancy Test

Teacher: "A pregnancy test uses UV-Vis spectroscopy. The test strip contains antibodies that bind to a hormone in urine (hCG). Those antibodies are attached to gold nanoparticles or colored dyes.

When hCG is present, the colored particles move up the strip and concentrate in a line. That line appears because the colored particles absorb specific wavelengths of light — your eyes see the color (e.g., pink or blue)."

> Partner talk (1 minute): "Tell your partner: What's the difference between UVA and UVB?" (UVA = aging/wrinkles, UVB = burning/sunburn)

SEGMENT 5: Infrared (IR) Spectroscopy — The Breathalyzer (12 minutes)

> Teacher says: "Infrared (IR) spectroscopy uses infrared light to identify molecules based on how their bonds vibrate."

IR spectroscopy: Measures which infrared wavelengths a molecule absorbs. Different bonds (O-H, C-H, C=O) vibrate at different frequencies, absorbing specific IR light.

Teacher: "Think of bonds as tiny springs connecting atoms. Each spring vibrates at a specific frequency. When IR light matches that frequency, the bond absorbs the light."

Common Bond Vibrations and Their IR Signals

Bond Type	Wavelength (µm)	What It Tells You	Household Example
O-H (alcohol)	~3.3 µm	Alcohol (ethanol, isopropanol)	Rubbing alcohol, vodka
C-H (hydrocarbon)	~3.4 µm	Organic compounds (fats, oils, plastics)	Olive oil, plastic containers
C=O (carbonyl)	~5.8 µm	Ketones, aldehydes, acids	Acetone (nail polish remover), vinegar
C-O	~9-10 µm	Alcohols, esters	Ethanol, ethyl acetate

How a Breathalyzer Works

Teacher: "Police breathalyzers use IR spectroscopy to detect ethanol (drinking alcohol) in your breath."

Step-by-step:

Step	What Happens
1	You blow into the breathalyzer. Your breath contains ethanol vapor if you've been drinking.
2	An infrared light source shines through the breath sample.
3	Ethanol molecules absorb IR light at specific wavelengths (especially 3.4 μm — C-H bond).
4	A detector measures how much light gets through. Less light = more ethanol.
5	The device calculates blood alcohol concentration (BAC).

Teacher: "Professional breathalyzers use IR because it's very specific — only ethanol absorbs at those exact wavelengths. Other gases (like acetone from diabetics) don't interfere."

Reading an IR Spectrum

Teacher: "An IR spectrum is a graph. The x-axis is wavelength (or wavenumber). The y-axis is percent transmittance (how much light got through). Dips (peaks downward) mean absorption."

Example: Vinegar (Acetic Acid)

Peak at ~3.3 μm → O-H

Peak at ~3.4 μm → C-H

Peak at ~5.8 μm → C=O

Example: Rubbing Alcohol (Isopropanol)

Peak at ~3.3 μm → O-H

Peak at ~3.4 μm → C-H

No peak at ~5.8 μm (no C=O)

Teacher: "Just by looking at which peaks are present, you can tell the difference between vinegar and rubbing alcohol — even if both are clear liquids."

Partner talk (1 minute): "Tell your partner: What bond does a breathalyzer detect in ethanol?" (C-H bond at ~3.4 μm, also C-O at ~9.5 μm)

SEGMENT 6: Fluorescence Spectroscopy — Glow Sticks and Forensics (10 minutes)

Teacher says: "Fluorescence is when a molecule absorbs light at one wavelength and emits light at a longer wavelength (different color)."

Fluorescence: Absorption of high-energy light (UV or blue) followed by immediate emission of lower-energy light (visible, usually green, yellow, or red).

How Fluorescence Works

Teacher draws or shows:

text

Energy

↑

| High-energy light Lower-energy light

| absorbed (UV/blue) emitted (green/red)

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| Electron jumps up → Electron falls down

| | |

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| ↓

| Fluorescence

|_________________________→

Teacher: "The absorbed light has higher energy (shorter wavelength). The emitted light has lower energy (longer wavelength). Some energy is lost as heat — that's why emitted light is always a different color (usually redder/greener than the absorbed light)."

Household Example 1: Glow Sticks

Teacher: "A glow stick contains two chemicals in separate compartments:

Hydrogen peroxide (in a glass vial inside)

Phenyl oxalate ester (in the outer solution)

A fluorescent dye (determines the color)

When you snap the glow stick, the glass breaks. The chemicals mix. The reaction produces energy. That energy excites the fluorescent dye. The dye emits light (fluorescence).

Different dyes give different colors:

Dye	Emitted Color
9,10-Diphenylanthracene	Blue
Rubrene	Yellow
Rhodamine B	Red
Chlorophyll (from plants)	Red

Household Example 2: Forensic UV Lights

Teacher: "Forensic investigators use UV lights to find bodily fluids (blood, semen, saliva) at crime scenes. Many biological fluids are naturally fluorescent — they glow under UV light.

Also, many security features on money, passports, and credit cards use fluorescent inks that are invisible in normal light but glow under UV."

Celebrity example: "Black lights at concerts or bowling alleys make white clothes glow — that's fluorescence!"

Difference Between Fluorescence and Other Light Interactions

Type	What Happens	Example
Absorption	Light is taken in (not re-emitted)	Sunscreen (UV absorbed, no visible light emitted)
Fluorescence	Absorbs → emits immediately (different color)	Glow stick, black light poster
Phosphorescence	Absorbs → emits slowly (glows in the dark)	Glow-in-the-dark stars on ceiling
Scattering	Light bounces off (no absorption)	Blue sky (Rayleigh scattering)

Partner talk (1 minute): "Tell your partner: What's the difference between fluorescence and phosphorescence?" (Fluorescence = emits immediately; phosphorescence = emits slowly, glows after light source removed)

SEGMENT 7: Mass Spectrometry (MS) — Weighing Molecules (8 minutes)

Teacher says: "Mass spectrometry (MS) doesn't use light. Instead, it measures the mass of molecules. It's one of the most powerful techniques for identifying unknown compounds."

Mass spectrometry: Measures the mass-to-charge ratio (m/z) of ions. Gives you the molecular weight (molecular mass) of a compound.

How a Mass Spectrometer Works (Simplified)

Step	What Happens
1	Sample is vaporized (turned into gas)
2	Molecules are ionized (given a charge, usually positive)
3	Ions are accelerated through a magnetic or electric field
4	Lighter ions are deflected more; heavier ions are deflected less
5	Detector measures how many ions hit at each mass

Teacher: "The output is a mass spectrum — a graph with mass on the x-axis and abundance on the y-axis."

What a Mass Spectrum Tells You

Feature	What It Means
Highest mass peak (M^+)	Molecular weight of the compound
Fragmentation pattern	How the molecule breaks apart — like a fingerprint
Isotope patterns	Clues about how many chlorine or bromine atoms are present

Household Example 1: Drug Testing in Sports

Teacher: "Mass spectrometry is the gold standard for drug testing in athletes. It can detect minute amounts of banned substances in urine or blood, and it can tell the difference between natural and synthetic hormones."

Household Example 2: Identifying Unknown Powders

Teacher: "If you find an unknown powder, you can put it in a mass spectrometer. The resulting mass spectrum will match a library of known compounds. This is used in forensics, hazmat, and pharmaceutical quality control."

Household Example 3: Breathalyzers (Some Use MS)

Teacher: "Some advanced breathalyzers use a miniature mass spectrometer to detect alcohol and other drugs instantly — no need for a blood draw. They're portable and fit in a suitcase."

Partner talk (1 minute): "Tell your partner: What does mass spectrometry measure?" (The mass-to-charge ratio, which gives the molecular weight)

SEGMENT 8: NMR Spectroscopy — MRI Medical Imaging (8 minutes)

Teacher says: "NMR spectroscopy (Nuclear Magnetic Resonance) is the most sophisticated type of spectroscopy. It's used in chemistry labs to determine the 3D structure of molecules — and in hospitals for MRI (Magnetic Resonance Imaging)."

NMR spectroscopy: Measures how atomic nuclei (usually hydrogen, ^1H) behave in a magnetic field. Different hydrogens in different chemical environments absorb at slightly different frequencies.

How NMR Works (Simplified)

Step	What Happens
1	The sample is placed in a very strong magnetic field
2	Radio waves (RF) are pulsed at the sample
3	Hydrogen nuclei (protons) absorb the RF energy and flip their spin
4	When they relax back, they emit RF energy — slightly different frequencies depending on their chemical environment
5	A computer processes the signal into an NMR spectrum

What NMR Tells You

Feature	What It Means
Number of peaks	How many different types of hydrogen atoms are in the molecule
Chemical shift (ppm)	What kind of environment each hydrogen is in (near oxygen, near carbon, etc.)
Splitting pattern	How many neighboring hydrogens are nearby
Integration (peak area)	How many hydrogens of each type

Household Example: MRI (Magnetic Resonance Imaging)

Teacher: "MRI is NMR applied to the human body. Your body is mostly water (H_2O). The hydrogen atoms in water give a strong NMR signal.

An MRI scanner maps where those hydrogens are. Different tissues (muscle, fat, bone, brain) have different water content, so they appear different in the image.

MRI is used to diagnose:

Brain tumors

Torn ligaments in knees

Spinal cord injuries

Heart problems

Celebrity example: "When an athlete tears their ACL, the MRI shows exactly where the tear is without surgery."

NMR vs. MRI

Technique	Used For	Sample	Household Example
NMR spectroscopy	Determining molecular structure	Small molecules in solution	Identifying unknown chemicals
MRI	Medical imaging	The human body	Diagnosing torn ligaments, brain tumors

Partner talk (1 minute): "Tell your partner: What does MRI stand for, and what does it measure?" (Magnetic Resonance Imaging — measures hydrogen atoms in water in the body)

SEGMENT 9: Putting It All Together — Identifying a Mystery Liquid (8 minutes)

Teacher says: "Let's practice being analytical chemists. You find a clear liquid in an unlabeled bottle in your kitchen. You run three tests. What is it?"

Test Results

Test	Result
Smell	Sharp, pungent odor
UV-Vis	No significant UV absorption above 250 nm
IR spectrum	Strong C=O peak (~5.8 μm), O-H peak (~3.3 μm), C-H peaks (~3.4 μm)
Mass spectrum	M^+ peak at 60 m/z (molecular weight = 60)

Step-by-step reasoning:

Step	Analysis
1	Strong C=O peak indicates a carbonyl compound (ketone, aldehyde, or acid)

Step	Analysis
2	O-H peak suggests either an alcohol or a carboxylic acid
3	Combination of C=O + O-H = carboxylic acid (not just an alcohol)
4	Sharp smell and household location → Vinegar (acetic acid)
5	Molecular weight of acetic acid = 60 g/mol → matches mass spec

Answer: The liquid is vinegar (acetic acid, CH_3COOH).

> *"In a real lab, you'd confirm by comparing to a reference spectrum — the peaks would match exactly."*

SEGMENT 10: New Technology — Smartphones as Spectrometers (6 minutes)

Teacher says: "Traditionally, spectrometers were large, expensive, and only found in labs. Today, they're shrinking. Some can even fit in your pocket."

Miniaturization of Spectrometers

Time Period	Spectrometer Size	Cost	Accessibility
1980s-1990s	Tabletop (20-50 kg)	$50,000+	Only research labs
2000s-2010s	Shoebox (2-5 kg)	$10,000-30,000	Universities, industry
2020s	Smartphone attachment (50-100 g)	$200-1,000	Consumers, schools
Future	Built into phone	< $100	Everyone

What You Can Do with a Pocket Spectrometer

Application	What It Measures	How It Helps
Food safety	Sugar content in fruit	Pick the ripest apple
Olive oil authenticity	Spectral fingerprint	Detect fake olive oil
Medicine verification	Compare to authentic spectrum	Spot counterfeit drugs
Plastic sorting	Identify polymer type	Recycle correctly

Application	What It Measures	How It Helps
Gemstone ID	Raman fingerprint	Tell real diamond from cubic zirconia

Teacher: *"This technology is called NIR spectroscopy (near-infrared). By 2030, your phone might be able to tell you if your olive oil is real, if your vitamins are genuine, and if your avocado is ripe — just by scanning it."*

CLOSING — The 60-Second Challenge (6 minutes)

Teacher says: *"Pair up. Person A: 60 seconds — explain Beer's Law (A = εbc) and what each variable means. Person B: 60 seconds — explain how a breathalyzer uses IR spectroscopy to detect alcohol."*

Final takeaway table (show on screen / read aloud):

You learned...	Household Example
Spectrophotometer = light source → monochromator → sample → detector	Measures how much light is absorbed
Beer's Law: A = εbc	Absorbance ∝ concentration (double concentration = double A)
UV-Vis spectroscopy = measures UV/visible absorption	Sunscreen (blocks UV), pregnancy test (color line)
IR spectroscopy = measures bond vibrations	Breathalyzer (detects ethanol by C-H bond)
Fluorescence = absorbs high-energy light, emits lower-energy	Glow sticks, black light posters, forensic UV
Mass spectrometry = measures molecular weight	Drug testing, identifying unknown powders
NMR spectroscopy = measures hydrogen environments	MRI medical imaging (sees inside your body)
Beer's Law equation	A = εbc (A = absorbance, ε = molar absorptivity, b = path length, c = concentration)

Final line (preview of wrap-up): "That's the full Level 2 curriculum — 13 lectures on the math and deeper science behind the chemistry in your home."

SUPPLEMENTARY MATERIALS FOR L2-12 (No Grade)

Resource	Household Connection	Description	How to Find It
PhET "Beer's Law Lab" simulation	Interactive Beer's Law	Change concentration, see absorbance change	Search "PhET Beer's law"
IR spectroscopy tutorial	Breathalyzer	Interactive bond vibrations	Search "IR spectroscopy interactive"
Mass spectrometry simulation	Drug testing	Virtual mass spectrometer	Search "mass spectrometry simulation"
MRI animation	Medical imaging	How MRI works (simplified)	Search "MRI animation physics"

"This week, look at a glow stick (if you have one) or watch a video of someone cracking one. Notice that the light is fluorescence — the chemical reaction produces energy that excites the dye, which then emits light. Next time, tell us what color glow stick you saw."