

Spectroscopy

Chemistry is in the world all around us! As you've explored AP Chemistry, you've gradually learned that we can explain and even manipulate our surroundings just by understanding the fundamental principles that dictate chemicals.

But have you ever wondered, how do scientists even know what molecules they're working with? If there's no obvious change like a color shift or bubbling, how do they know a chemical reaction has happened? Even if those signs happened, how do chemists know they've synthesized the product they wanted to?

This is where the concept of spectroscopy comes into play. **Spectroscopy** helps scientists to figure out what an unknown substance is by analyzing specific properties that give clues to what a molecule could be.

Definition

In chemistry, spectroscopy is the science of identifying a substance based on characterizing spectra.

There are many different types of spectroscopy that detect all sorts of molecular properties. Things can get complex very quickly! This article, however, will explain the basics of the most common types of spectroscopy and the identifying properties they detect. The four types of spectroscopy covered in this lesson are the ones that are most likely to show up on the AP Chemistry exam.

Overview

- In this lesson, you'll get a refresher on the **electromagnetic spectrum** and how it relates to spectroscopy.
- Then, you'll learn about **photoelectron spectroscopy**, and the types of graphs it produces.
- You'll learn about how **IR spectroscopy** works, and what the spectra it produces look like.
- After, we'll cover **UV-vis spectroscopy** and the type of spectra it produces.
- Finally, we'll cover **mass spectroscopy**, and what the resultant graphs look like.

The Electromagnetic Spectrum

To understand what the electromagnetic spectrum is, you first have to understand the concept of radiation. You've probably heard the word radiation before. It could be from somebody describing their cancer treatment, or from your mother reminding you to wear sunscreen to not get hurt from the sun's radiation. As it turns out, radiation is all around you... all the time. All radiation is just a type of energy that moves and spreads as it travels.

Definition

Radiation is just energy that moves (typically in waves) and spreads as it travels.

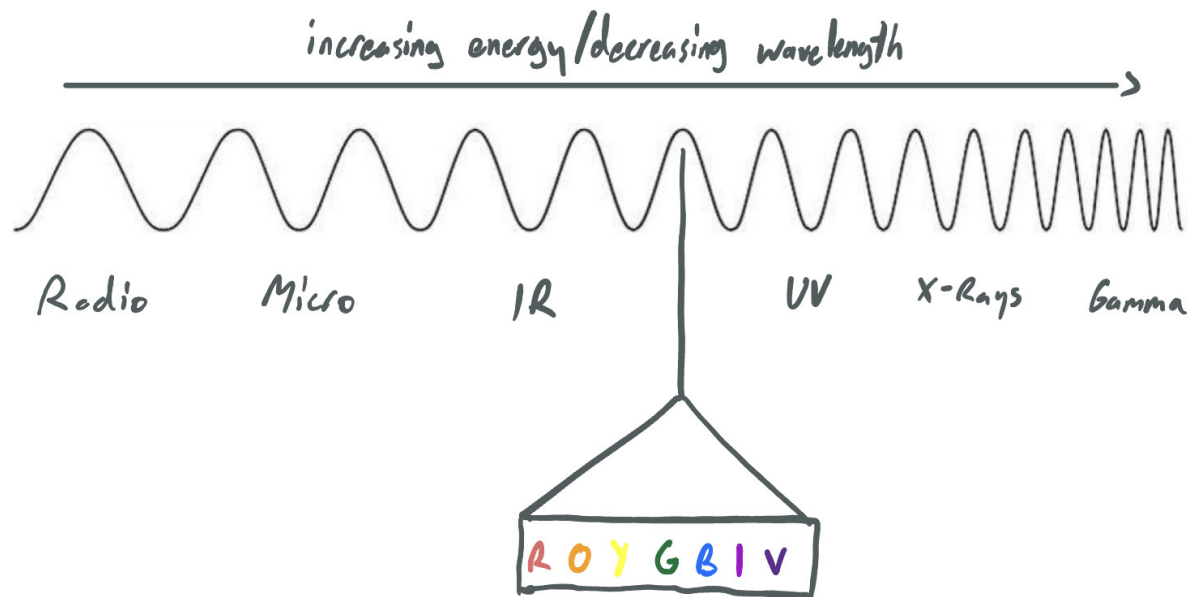
That might sound easy enough, but what types of radiation are there? Did you know that all visible light is radiation? What about when you're in the car and turn on the radio? That's radiation too! These are both forms of electromagnetic radiation.



Different types of EM radiation are characterized and organized in the electromagnetic spectrum based on their wavelength.

Definition

The electromagnetic spectrum characterizes and organizes different forms of electromagnetic radiation based on their different wavelengths.



A basic diagram of the electromagnetic spectrum.

You've probably seen an electromagnetic spectrum graph like the one shown above. As we move from the right to the left, wavelengths get shorter, and in turn, frequency increases. As it turns out, this simple rule can be used to help scientists deduce what molecules they're working with using a few principles.

Molecules, depending on their structure, absorb a certain amount of energy that corresponds with a specific frequency. If we can figure out this frequency- we can figure out the energy it is proportional to and then figure out the actual molecular structure. This rule is fundamental to almost all types of spectroscopy. While the specifics won't be tested on the AP exam, knowing when to use what kind of spectroscopy will be. To know which spectroscopy to use, a rudimentary understanding of what each type of experiment detects.

As you most likely have guessed by now, IR spectroscopy has to do with substances that absorb radiation within the IR electromagnetic range. UV-Vis deals with absorption within the UV and visible range, and so on. However, each type of spectroscopy that we'll cover has different primary usages and reveals different characteristics about atoms and molecules- so types of spectroscopy are NOT interchangeable. (You can't use IR spectroscopy instead of UV-Vis spectroscopy and expect to get the same information or results, and so on.)



 Deep dive

There are other types of spectroscopy you might be interested in, such as NMR spectroscopy and fluorescence spectroscopy. However, these won't be covered on the AP Chemistry exam! So for now, get these other types of spectroscopy under your belt.

Photoelectron Spectroscopy

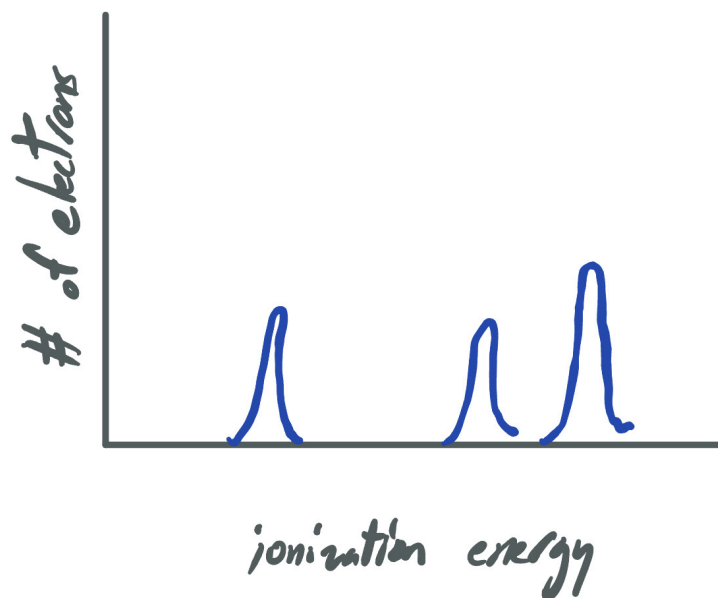
Photoelectron spectroscopy manipulates the fact that atoms and molecules within a sample will have differing amounts of relative energies to determine what the structure of a sample looks like. When we think about electrons, where do we most commonly associate them? We know that certain elements tend to have a certain amount of electrons. We also know that bonds involve sharing electrons or donating them. Therefore, because we know the energy from these electrons is going to be indicative of present elements and the bonding associated with them, we can determine both of these with PES.

Focusing on the elements involved, we can use PES to essentially "zoom in" on atoms in a sample to see unique electron shells, discrete energy levels, and atomic orbitals. This is done by 'plucking off' electrons from the sample using high-energy EM radiation like X-Rays or UV. By doing this, we can measure what the ionization energy is for each of these 'plucks,' ending up with a graph that looks something like the following. (*Ionization energy is also known as binding energy.*)

Definition

Photoelectron spectroscopy detects the ionization energy from removing electrons one by one with X-ray or UV radiation. This reveals information about individual atoms and their orbitals in samples that are gaseous or solid.





Drawn example of nitrogen under Photoelectron Spectroscopy.

Above, there is a PES spectrum of a pure, idealized sample of nitrogen. We know that nitrogen has an electron configuration of $1s^2 2s^2 2p$ in its ground state. Analyzing the PES of our nitrogen gas sample, we can see that we have three peaks that correspond with the three discrete levels of energy. We can also see that the height of the peaks is relative to how many electrons are in each subshell. For example, the first two peaks are equal in height because $1s^2$ and $2s^2$ both have 2 electrons. The third peak, which represents $2p$ is half in height because there is only one electron in its subshell. This technique can be applied to the PES spectrum to determine what element is being analyzed.

Now that we understand the basics of how it works, what does PES usage look like in an experimental design?

Example

We could use photoelectron spectroscopy to

- Determine what specific element we're working with
- Learn more information about individual atoms
- Visualize the difference between orbitals

Photoelectron spectroscopy is typically used with samples in a gaseous or solid phase.

IR Spectroscopy

Now, let's move a little further outwards. Rather than analyzing a sample atom-by-atom, what if we want to figure out what molecule we're working with? Infrared spectroscopy helps us to do this by experimentally determining how our substance interacts with IR light.

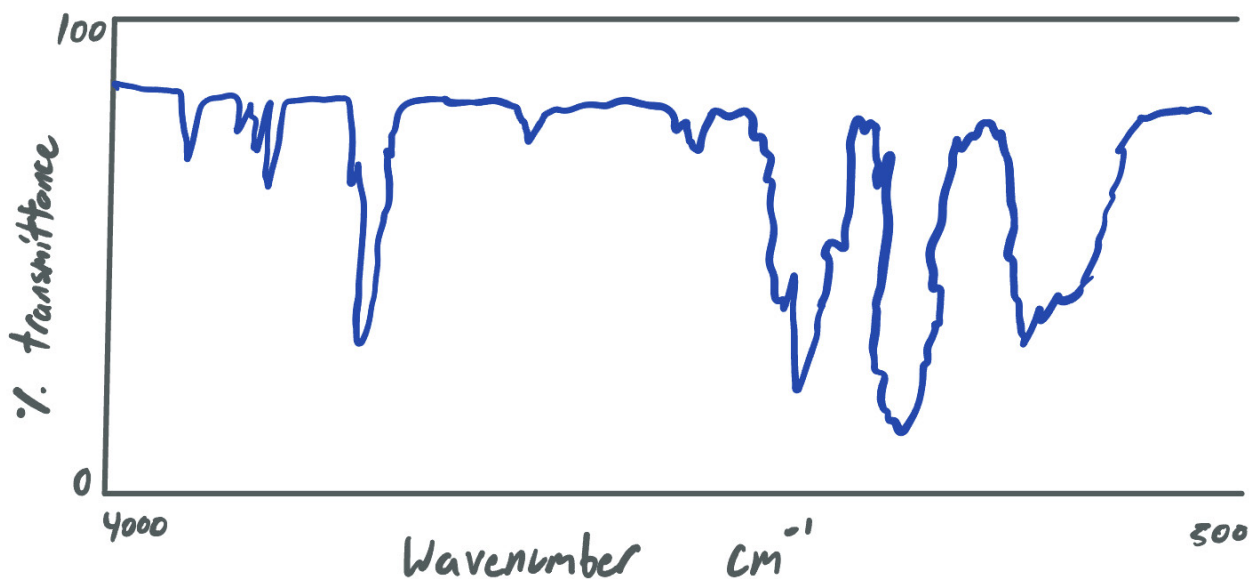


Definition

Infrared spectroscopy detects energy from bond vibrations to reveal information about functional groups and bond connectivity in solutions and solid samples.

We can do this in a few different ways. Sometimes chemists will look at absorption spectra to find in what unique manner the sample will absorb IR radiation. Emission spectra also tell the opposite: what pattern does our sample make as it emits IR radiation? In rare cases, IR reflection spectra are used to see how the sample reflects IR radiation.

IR spectra can quickly become complicated, but for the sake of the AP Chemistry exam, you'll need to know that IR spectra look something like the following:



Drawn example of an Infrared Spectroscopy graph.

IR spectra are usually measured in wavenumbers, which is just the reciprocal of the wavelength. The peaks on this graph represent different groups of characteristic atoms, otherwise known as functional groups. These peaks appear on different portions of the graph due to the different bond vibrations in reaction to IR radiation across the molecule. Because we can deduce what functional groups are in the molecule, we can also deduce the connectivity of the sample's bonds.

Now, what does IR spectroscopy look like in an experimental design?

Example

We could use IR spectroscopy to

- Determine what functional groups make up a molecule
- Figure out the bond connectivity within a molecule

IR spectroscopy is typically used with samples that are in a solid state or within a solution.



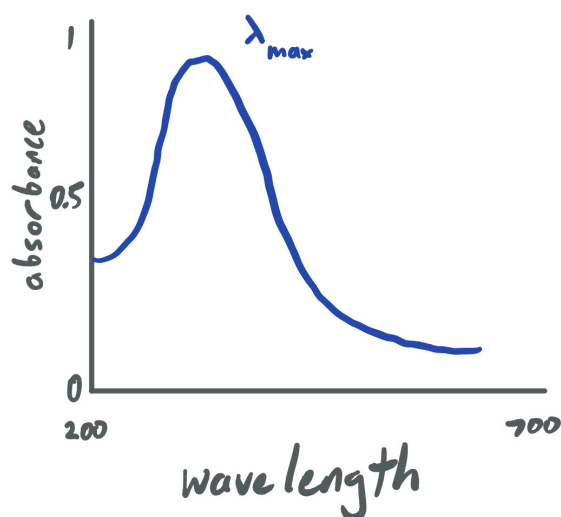
UV-Vis Spectroscopy

UV-Vis spectroscopy is similar in principle to IR spectroscopy. However, what is detected in UV-Vis spectroscopy is different from IR spectroscopy, the produced spectra look different, and there are different implications for the meaning behind what is detected. UV-Vis spectroscopy focuses on the ultraviolet and visible range of the EM radiation spectrum. As a result, UV-Vis spectroscopy primarily detects molecules that are rich in pi-bonds and metal cations.

Definition

UV-Vis spectroscopy detects energy from the excitation of electrons at different wavelengths to determine where maximum absorbance occurs. Pi-bond-rich molecules or metal cations are typically used as samples in aqueous solutions.

A resulting UV-Vis spectrum might look something like the following:



Drawn example of a UV-Vis Spectroscopy graph.

Notice how our graph compares absorbance with wavelength. This spectrum shows the relative molecular absorbance at each specific wavelength and produces a curve that reveals the wavelength of maximum absorbance. This information might be important if you wanted to use this experimental data to find concentration, which could be done with Beer's Law.

Example

We could use UV-Vis spectroscopy to

- Determine the concentration of UV-absorbing molecules or metal ions
- Figure out the purity of a sample that absorbs UV light
- Apply Beer's Law to find relative concentrations within a sample

UV-Vis spectroscopy is typically used on samples that are within an aqueous solution.



Mass Spectroscopy

The last type of spectroscopy that could be mentioned is mass spectroscopy. Mass spectroscopy is quite different from the other types of spectroscopy mentioned. Mass spectrometry uses electrons with a high amount of energy to 'attack' a sample, which forces the ionization of the sample. This causes the sample to be 'split' into multiple ions.

Deep dive

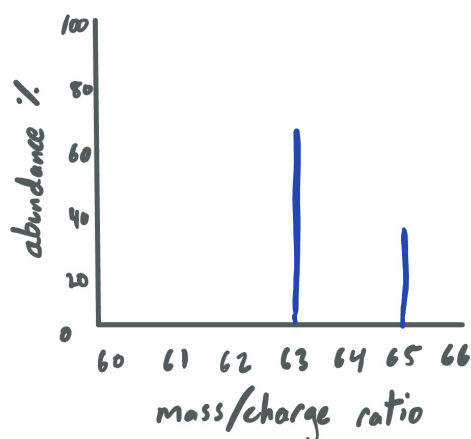
This means that if we were to take a molecule and run it through a mass spectrometer, it could be 'broken' into different ions at different points in the molecule, producing incredibly complex data.

For the sake of AP Chemistry, however, we care much more about what happens if we stick a sample of a pure element into a mass spectrometer. If we do this, it turns out that the sample splits into atoms with different masses. These are different **isotopes** of an element! (*Remember, isotopes are atoms with a differing amount of neutrons.*) **This means that mass spectroscopy can be used to prove the existence of the neutron.**

Definition

Mass spectroscopy uses electrons with high amounts of energy to 'attack' a sample and split it into multiple ions, or in the case of pure elemental samples, isotopes. It is used to find the relative abundance of these ions or isotopes.

A mass spectroscopy spectrum might look something like this:



Drawn example of copper under mass spectroscopy.

This graph means that ^{63}Cu is 69% abundant, while ^{65}Cu is 31% abundant. Be sure to note the mass to charge ratio as well, which can also be written as m/z .



Example

We could use mass spectroscopy to

- Find out the abundance of different elemental isotopes
- Prove the existence of the neutron

In AP Chemistry, typically only pure elemental samples are analyzed.

With that, you've now learned the four types of spectroscopy that are mentioned in the AP Chemistry exam. The exam emphasizes the *potential usages* of these different types of spectroscopy as opposed to how the actual equipment works, so be sure to understand which type of spectroscopy can be used for what!

Spectroscopy - Key takeaways

- The electromagnetic spectrum consists of different forms of EM radiation that exist in different wavelengths.
- Photoelectron spectroscopy detects the ionization energy from removing electrons one by one with X-ray or UV radiation. This reveals information about individual atoms and their orbitals in samples that are gaseous or solid.
- Infrared spectroscopy detects energy from bond vibrations to reveal information about functional groups and bond connectivity in solutions and solid samples.
- UV-Vis spectroscopy detects energy from the excitation of electrons at different wavelengths to determine where maximum absorbance occurs. Pi-bond-rich molecules or metal cations are typically used as samples in aqueous solutions.
- Mass spectroscopy uses electrons with high amounts of energy to 'attack' a sample and split it into multiple ions, or in the case of pure elemental samples, isotopes. It is used to find the relative abundance of these ions or isotopes.

