

"The story of Spectroscopy"

Let's start at the end: we take our photons for a walk and then ask them what they have seen.

Our story have two parts: In the first part we meet our explorers, the photons. In the second part we meet the "*Terra incognita*", our unknown land- the molecules.

Chapter one, where we meet our explorers

As you might know the light we see has a split personality: on the one hand- it acts like a wave, and on the other hand the light is carried by particles- the photons.

To get some intuition about the wavy nature of the light imagine yourself standing on the beach watching the water waves of the sea. The distance between successive waves is called the "wavelength", and the number of waves rushing towards you every minute is called the "frequency" of the waves. The frequency and the wavelength are related via the speed of the waves. Like the water waves of the sea, the light has also wavelength and frequency which are related via the speed of light. The nice thing is that the wavelength and frequency of light are manifested as colors. For example, a blue light has shorter wavelength than that of a red light.

The light however, is not exactly a wave, as it is carried by particles, the photons. The wavy properties of the light have very interesting relations to the photons' properties. One important feature is the relation between the energy of the photon and the wavelength (or frequency) of the wave. The photon's energy is proportional to the frequency, or alternatively, proportional to the inverse of the wavelength. If the wavelength is λ and the frequency of the wave is ν , then the energy of the photons is: $E = h\nu = hc/\lambda$, where c is the speed of light and the constant h is called "Planck constant" (the constant is named after the physicist Max Planck who discovered it in 1900).

To summarize the last two paragraphs- think about it in the following way: when a wave of light is propagating with wavelength λ , it is carried by many photons, each of them has exactly the same energy, $= hc/\lambda$.

The photons are quite nasty, and they have some strange properties (for example, they have no mass). One of the bizarre properties of the photon which we are going to use later, is their ability to be created out of nowhere, and in the same way to disappear. Notice that due to the conservation of energy, creating a photon "costs" you an energy $E = hc/\lambda$ and similarly, when a photon is disappeared someone must gain its energy.

Chapter two, where we meet the *Terra incognita*

We want to use photons to study the structure of different materials, so let's spend a few minutes to discuss the building blocks of materials- the molecules. Molecules are groups of atoms held together by chemical bonds, you can picture them in your mind as groups of balls connected by springs. The balls represent the different atoms, and they can have different sizes and masses according to the atoms' properties, and the springs (also with different spring constants) represent the chemical bonds that hold the atoms together. Now, have in your mind such a group of balls connected by springs, give it a little hit and watch it vibrate. These vibrations are determined by the masses of the balls, the strengths of the springs and the arrangement of the entire structure. The important thing is: the way it vibrates is a specific property of a molecule, in other words – the vibrations are the molecule's fingerprints. Those fingerprints of molecules are exactly what we are looking for!

Some words on quantum mechanics

The simple model of springs and balls to describe molecules is quite useful to get some intuition about the vibrations of the molecules. There are, however, differences between molecules and the daily life springs and balls. Maybe the most striking difference is the quantum nature of the molecules vibrations. Let's pause for the moment, and discuss a few insights that quantum mechanics gives us and turn out to be very useful for us when sending our photons to their mission.

Quantum mechanics describes the physics of ultra-small systems, typically nano-scale systems such as molecules, atoms and elementary particles like electrons and photons. While the classical physics in general and classical mechanics in particular describes quite well the daily life physics, many phenomena that appear in small systems contradict the classical picture. A stunning phenomena, which gave quantum mechanics its name, is the observation that many physical quantities can change only in discrete amounts (in Latin - *quanta*), and not in a continuous way like in classical physics. This observation plays a crucial role in spectroscopy.

In physics, vibrations are typically treated in the framework of harmonic oscillator. In classical physics, harmonic oscillators are systems which are subjected to a force when they are shifted from their equilibrium, where the force is proportional to the displacement from the equilibrium point. Simple examples of such systems are a mass attached to a spring, and a swinging pendulum. The vibrations of molecules, however, cannot be described by the classical harmonic oscillator. Instead, they are described by the quantum version of harmonic oscillator, the "quantum harmonic oscillator". Unlike harmonic oscillators, which change their energy continuously, quantum harmonic oscillators change their energy only in discrete amounts. The classical picture of masses and springs with certain possible vibrations for each molecule, manifest in the quantum case of real molecules vibrations as a certain set of discrete energy changes. To be more specific, each molecule can change its energy by a discrete set of energies, this discrete set is unique for each molecule. If you want – this set of energies is the quantum fingerprint of the molecule.

These are great news for us, since the discrete nature of molecules vibrations fits exactly the properties of our explorers, the photons. As mentioned above, photons have the weird ability to disappear, however, they can only disappear if they deliver their entire energy. So if we want to identify a

molecule, we can throw photons towards it and see if they disappear. If a photon is disappeared – then the molecule have changed its energy according to the photon's wavelength. By sending more and more photons in many wavelengths we can reveal the molecule quantum fingerprint, the energy set of its vibrations.

Chapter three – how does it work in practice?

We have now all the knowledge that we need in order to send our spies to their mission. Having a light source that shine broadband light (that is, light in many wavelengths) gives us the ability to emit photons in various energies. Sending our explorers away is done by lighting the sample in study.

When the light shines on the sample, the photons penetrates into it, meeting in their way the molecules that compose the sample. Each of the molecules has its own specific set of energy, and if a photon with the correct energy hits it, there is a chance that the photon will simply disappear. The light source sends billions of photons, some of them will disappear – those with energy that matches the sample's vibrations.

After the photons penetrate into the sample, hitting its molecules again and again, some of them will leave the sample. What we need to do now, is simply to "ask" these photons, what they have seen. This is done by analyzing the color of the light that comes out of the sample. Some wavelengths will be missing, or more precisely in some wavelengths, the light will be attenuated relative to the others. These are the wavelengths that match the vibrations energy – these are the fingerprints of the sample components!

To conclude, in spectroscopy we shine a sample with a broadband light source. We then collect the light that comes out of the sample and analyze its wavelength content. By comparing the light we've sent and the light we collect we can analyze the molecular content of the sample.