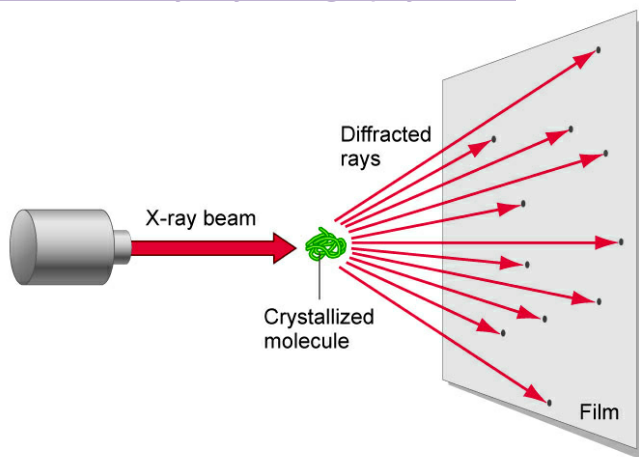


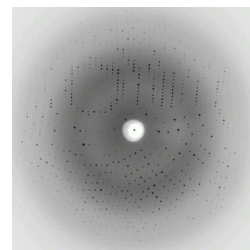
Guide to Understanding X-ray Crystallography

What is X-ray Crystallography and why do I need to learn it? X-ray Crystallography is a scientific method of determining the precise positions/arrangements of atoms in a crystal where beams of X-ray strikes a crystal and causes the beam of light to diffract into many specific directions.

How does X-ray Crystallography work?



1. X-ray beams are shot through a crystal of the atom. (Note: The crystal is mounted to a Goniometer to keep it in place during the process).
2. The crystal causes the beam of X-Ray to diffract in a predictable pattern based on their crystal lattice structure.
3. The result is a diffraction pattern generally seen as the picture on the right.

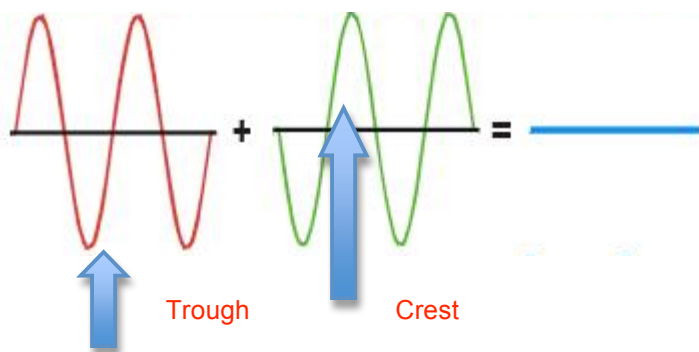


What is the Significance of the Diffracted Pattern and why should I care?

First we need to understand how the diffracted pattern is actually constructed and what figure out what it tells us. Only then will we fully understand how and why it is a valuable tool to understanding the molecular arrangements of atoms.

1. Diffracted photons can add and subtract, giving different areas of photon intensities.

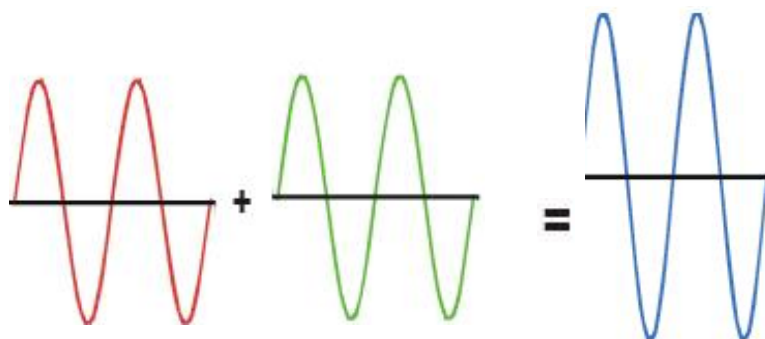
DESTRUCTIVE INTERFERENCE



Destructive interference occurs when there is a collision of photons in such a way that their intensities cancel out.

How do I remember this? Think of destructive interference as adding and subtracting. When you add (-1) and (1), you get 0. The same concept applies. You're adding a "function" with its "inverse function"; therefore they both cancel out.

CONSTRUCTIVE INTERFERENCE



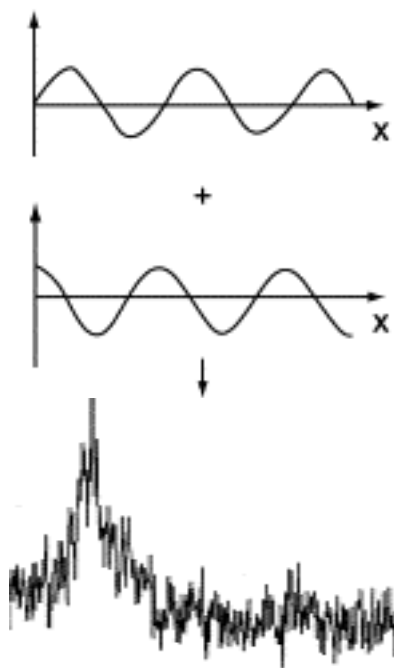
Constructive interference occurs when there is a collision of protons in a way that their intensities combine.

Trough

Trough

How do I remember this? Think of constructive interference as adding and subtracting, similar to the destructive interference. If you add (1) and (1), you will obviously get 2. The same concept applies here. You are adding a function with another function that is identical. When combined, they create a bigger function.

PARTIAL INTERFERENCE



Partial interference occurs when the waves are only slightly unaligned. (Note: Most common)

How do I remember this? Think of partial interference as adding and subtracting, similar to both destructive and constructive interference. If you add (1) and (1.1), you get 2.1, which is slightly more complex than just adding (1) and (1) as you did before in constructive interference. The same concept applies here. You are adding a function that is VERY VERY similar to the other function, resulting in more complex patterns.

Note: the product is bit more exaggerated.

2. After we observe the reflections of the photons on the detector, we change the angle at which the x ray beam hits the crystal. The crystal should be as perfect as possible! Why does the crystal have to be perfect? Think of it this way. Atoms of the same type and that are in the same place within the structure will result in an additive diffraction, which would definitely be easier to detect! Therefore, the more perfect a crystal is, the more

atoms that will be present in the same places in the structure, which would be easier to detect. Imperfect crystals usually result in fuzzy patterns that are hard to interpret. We would then have to combine all the reflections together to find the three-dimensional diffraction pattern. **But why do we need to look at it at different angles?!** Well, think of it as a puzzle. One puzzle piece doesn't give you a clear picture of what the overall puzzle looks like. You need to gather all the pieces together and actually piece it together to get the final product.

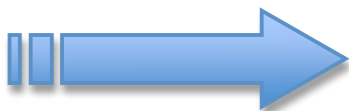


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Not enough information to figure out what the structure looks like!

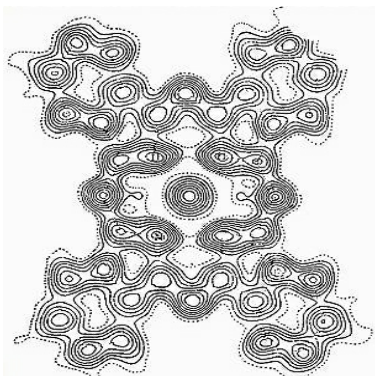
Gather all the pieces!

Put pieces together!



You have your final product!

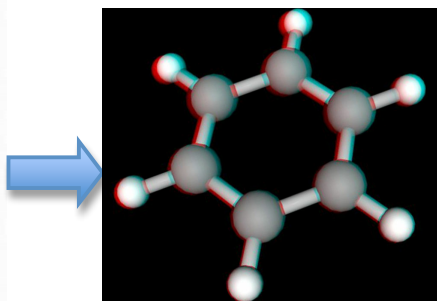
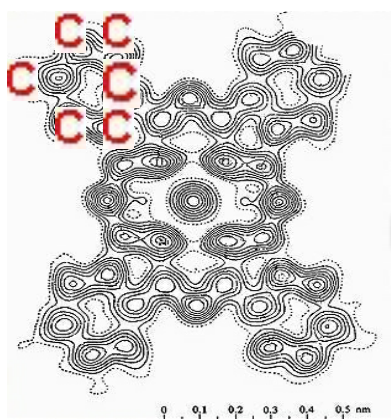
3. Well, where do we go from here after we have our diffraction pattern? Well the objective is to figure out the crystal structure from the diffraction pattern! So what allows us to go from the pattern to the structure? The **Electron Density Map!!!** This is an interpretation of the diffraction pattern as a plot of electron density versus the position in space. You can think of it as a two dimensional slice through the electron cloud.



The main thing to note about Electron Density Maps is that they depict the general structure of the crystal. Remember that diffraction is caused by electron clouds. That means that the higher the atomic number of an element, the larger its electron clouds are! This is really similar to the topographical maps they use on weather channels to show the height/size of mountains.

(Note: Hydrogen is VERY VERY HARD to locate because it has a very small electron cloud.)

4. Looking at the electron density map, you can tell which element falls where in the map by looking at the size of the electron densities! Assign the atoms (this often requires some idea of the structure before hand!). Then, connect the dots!

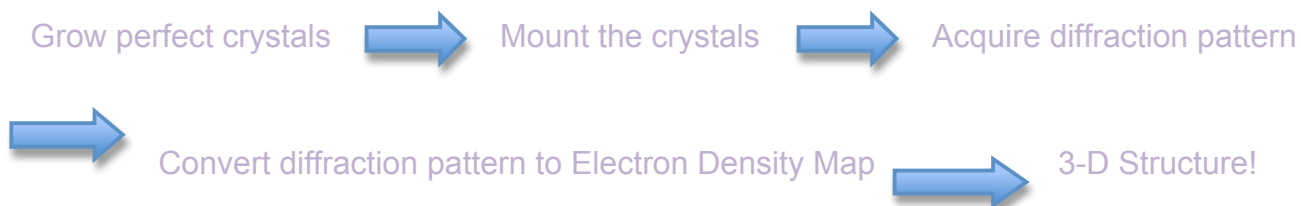


Note: This is only a portion of the structure)

What can X-ray Crystallography be used for?

1. **Molecular formula?** NOPE! X- ray diffraction only locates an atom in space and gives us some idea of the crystal structure, but it cannot directly reveal what elements are present.
2. **Stereochemistry?** YEP! X ray diffraction basically reveals the relative positions of the atoms in space so stereochemistry can absolutely be determined.
3. **Bond length?** YEP!
4. **Distance between atoms?** YEP!
5. **Electronegativity?** NOPE!
6. **Lone pairs?** NOPE!
7. **Formal charges?** NOPE!

Summary!



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