

## **Explainer: What is X-ray crystallography?**

February 4 2014, by Mark Lorch



Crystallography: from a handheld experiment in 1912 to the size of many football fields today. Credit: Diamond Light Source

Around 100 years ago a father and his son in north England conducted an experiment that would revolutionise the way scientists study molecules. A refined version of their method still remains one of the most important tools for scientists.

To achieve this feat, William Henry Bragg and his son William Lawrence Bragg used table salt (sodium chloride). They prepared a clean



crystal of salt and shone X-rays on it, which created a beautiful geometric pattern on a photographic paper placed behind it.

Others had done similar things before, but the Braggs made an intuitive leap. They realised that tucked away in the layout of the dots was information about salt's molecular structure. Lawrence Bragg then came up with a formula, now known as Bragg's law, that could be used to extracted this information allowing him to work out how the atoms of sodium and chlorine are arranged in a salt crystal.

Today we know that inside crystals there are atoms arranged in regular patterns. Each of these atoms has a dense core containing neutrons and protons, and less dense outer shells containing electrons. X-rays that hit these obstacles interact with other X-rays that cause a phenomenon called diffraction, something all waves (light or sound) undergo whenever they hit obstacles. The result of this diffraction is what was captured on the photographic plate by the Bragg team.

Even if you never paid attention in a chemistry lesson, you may recognise the ball-and-stick representation of chemical structures, where balls are the atoms and sticks the bonds that hold them together. But this was not known to the Braggs. Their work not only confirmed the existence of atoms but also showed how they come together to form compounds.





X-ray diffraction pattern of an enzyme crystal. Credit: Jeff Dahl

From that moment on, the mysterious way that atoms interact with each other was within the grasp of scientists. They could begin to unravel the structures of molecules. In the last century, <u>27 Nobel prizes</u> have been awarded for discoveries directly resulting from the use X-ray crystallography. The impact of the Yorkshire-born family's work can be put no better than by Max Perutz, a recipient of one of those 27 Nobels:

Why water boils at 100°C and methane at -161°C, why blood is red and



grass is green, why diamond is hard and wax is soft, why glaciers flow and iron gets hard when you hammer it, how muscles contract, how sunlight makes plants grow and how living organisms have been able to evolve into ever more complex forms ... the answers to all these problems have come from structural analysis.

In 1953 Rosalind Franklin used X-ray crystallography to produce images from a crystal of DNA. One of those images, called photograph 51, eventually led James Watson, Francis Crick and Maurice Wilkins to describe the helical structure of DNA is dubbed the <u>most important</u> <u>"photograph"</u> ever taken.





The famous photograph 51. Credit: Raymond Gosling/King's College London

These images taken by crystallographers are known as diffraction patterns, and now we can create such patterns <u>using laser pointers</u>. When the light from a laser passes through a helical spring it produces a characteristic "X" mark on the wall behind.

To most, and without an understanding of Bragg's Law, it is difficult to make the leap from a spotty cross to underlying structure of invisible atoms. But the result bears a striking similarity to Franklin's famous image. The angle of the cross and the distance between the spots contains information about the thickness of the wire and tightness of the spring, compressing the spring, for instance, changes the pattern produce. Similarly photo 51 contains all the data required to unlock the structure of DNA.

DNA is probably the most famous structure determined by X-ray crystallography, but it is just one among thousands: from table salt to drugs and from materials to massive intricate proteins the structure of which drives our understanding of the process that makes life possible. X-ray crystallography's impact is one reason why the UN has called 2014 the International Year of Crystallography.





A ball-and-stick model of proline. Credit: Peter Murray-Rust

## The future is bright

But chemists have a love-hate relationship with X-ray crystallography, because it still has one major limitation. As its name suggests, the method requires crystals and they need to be of certain quality and size. Growing good salt crystals is easy, but producing a crystal of a complex molecule like a protein is often met with failure. Many scientists have built their careers by just learning how to build good quality crystals of a particular protein.

That is why today's advances in X-ray crystallography are driven, in part, by attempts to circumvent the crystal problem. One way to do this is to use more powerful X-rays. Just as a bright torch is more revealing than a candle, the more energy in an X-ray beam the smaller the crystal



required to get a good diffraction pattern.

The X-ray source used by the Braggs was a small glass tube resembling a light bulb. It produced X-rays just strong enough to reveal the structure of a simple salt crystal. In contrast modern light sources are vast particle accelerators called synchrotrons, like the <u>Diamond Light Source</u>. These instruments can be hundreds of meters across and produce beams tens of thousands of times more powerful than the Sun itself. And with these incredible beams scientists can extract structures from smaller and smaller crystals, until it become possible to do away with crystals.

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