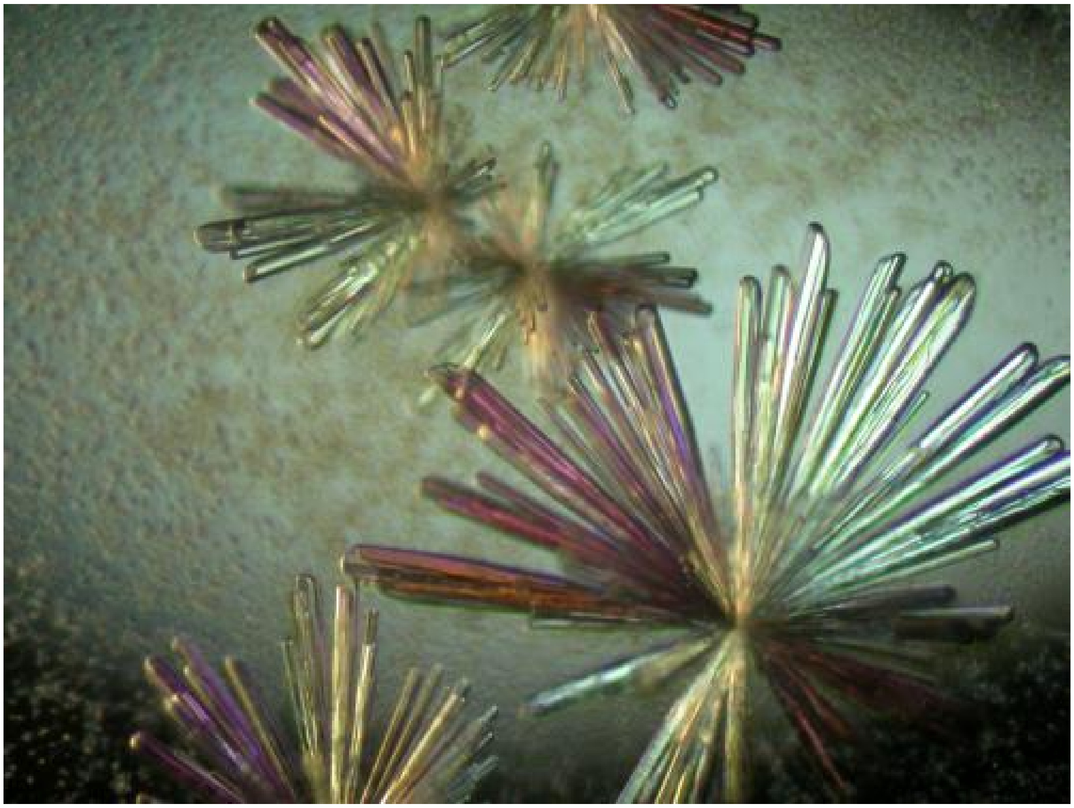
X-rays shine light on atoms at work in a chemical reaction

June 19 2014, by Timothy Prior



Not your standard protein. Credit: orinoco14, CC BY-NC

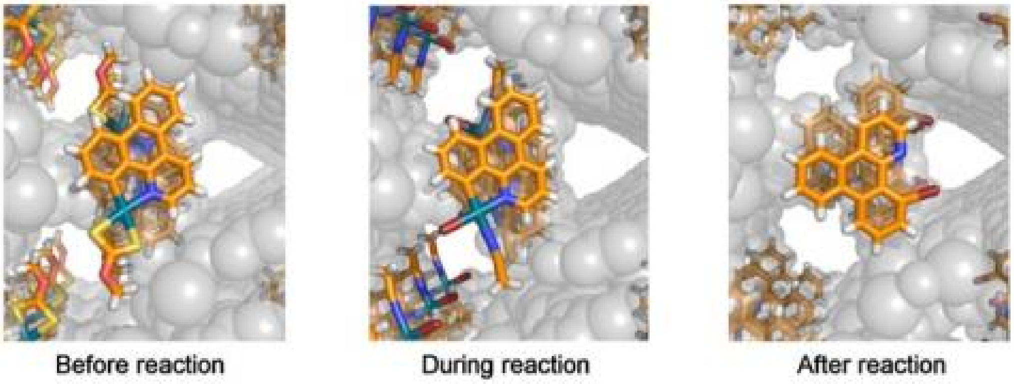
For more than 100 years, scientists have "peered" at atoms in a crystal by analysing the way they scatter X-rays. This process, known as crystallography, reveals the chemical structure of compounds in the crystal and has applications so wide-ranging – from drugs to new materials – that it has become central to how science is done.

But almost all of these advances have depended on revealing the chemical structure of unchanging compounds. However, if Makoto Fujita at the University of Tokyo and his colleagues are proved correct, this may all change. For they have developed a method to capture "images" as chemical reactions happen. The difference is in someways as big as that when cameras went from capturing still images to shooting film.

Dark magic

At this very moment, there are billions of chemical reactions taking place in your body. And yet each of these chemical reaction is special, because for it to occur two or more molecules have come in close contact under the right conditions. These "right conditions" are mostly dependent on the energy available in the system. Without enough energy, the necessary movement of electrons will not occur and the reaction will fail.

In nature, the required amount of energy has always been a tricky thing to achieve. To overcome this situation, many biological reactions make use of a catalyst, which does not react with the substances but accelerates the reaction. For instance, your body contains small amounts of manganese, zinc, and copper that are all required as catalysts for key reactions in the body.



The X-ray snapshots in the figure show the atomic arrangement of the molecule being brominated before, during, and after the reaction. All contained within the crystalline host, which has been greyed out. Red is the bromine atom. Credit: Fujita et al/JACS

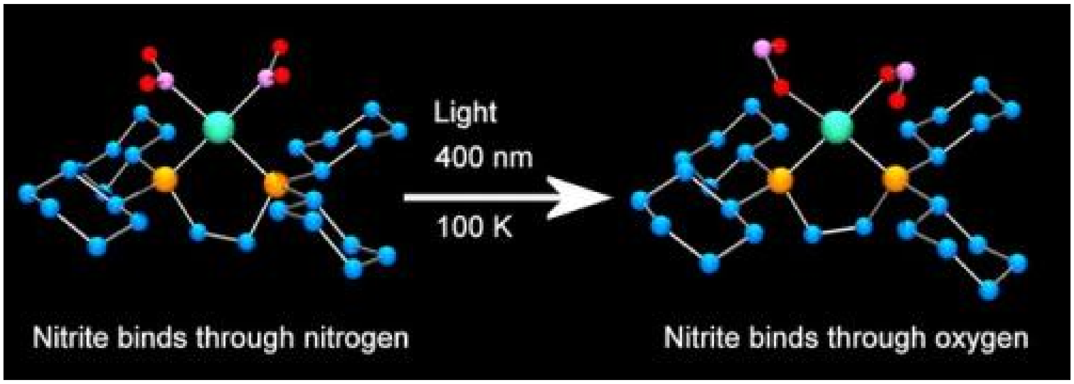
Although chemists have known about catalysts for nearly 200 years, we still don't always understand how they work. Fujita and his colleagues looked at palladium as a catalyst in a reaction where it accelerates the attachment of a bromine atom to a larger molecule. This chemical reaction is quite important commercially, because many useful chemicals, including key drugs and pesticides, contain bromine.

Just as most reactions in your body occur in water, most industrial reactions are carried out in solutions. However, crystallography cannot provide a snapshot of molecules moving in solution. So Fujita trapped the catalyst and reacting molecules in a cage, before taking X-ray snapshots during the reaction. This allowed him to have the molecules "immobile" for enough time to capture in X-ray image.

Using these images Fujuta was able to understand the workings of the catalyst, as he describes in the *Journal of American Chemical Society*. More importantly, this work marks a new dawn for crystallography.

The old experiments of "static" crystallography are now so routine that some modern instruments need almost no human input. Now scientists are looking for new challenges. Just as Fujita has shown that it is possible to probe the arrangement of atoms during a reaction, others are trying to monitor the response of a crystal to light, pressure, extremes of temperature, or even an atmosphere of reactive gas.

Matthew Warren at the University of Bath and colleagues use something called photocrystallography to show light causes changes in chemical structure. Some of the best chemicals to study this phenomenon are called "coordination compounds". They consist of a large metal atom surrounded by small molecules, called ligands. Shining light on these can cause a change in the arrangement of the ligands. In this case the ligand was a nitrite ion – a negatively charged molecule that contains nitrogen atom attached to two oxygen atoms (NO_2^-).



Light of wavelength 400 nm causes the nitrite ligand to flip and bind through oxygen. (Nitrogen atoms are colours pink, oxygen atoms are red, and the nickel atom is coloured green) Credit: Tim Prior

Normally nitrite binds to a metal, in this case nickel, via the nitrogen atom. But, as they report in [*Chemistry – A European Journal*](), when light of the right wavelength shines upon the crystal, the binding of nitrite changes. The nitrite flips round and binds via one of the oxygen atoms. This changes happens within the crystal. Without new developments in crystallography, we would never have been able to find out about the flip.

This is important because, before the flip, certain types of light pass through the crystal but afterwards these are absorbed. In the future, compounds like this may be incredibly useful as light operated-switches in optical computing.

This year is the International Year of Crystallography, and with such developments we seem to be approaching a golden age. X-ray sources are becoming brighter than ever before which means experiments that were once impossible are becoming routine. Crystallography played a pivotal role in technological advances in the last 100 years. New experiments should keep it at the forefront of discovery in the next 100.

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