Study of atomic movement may influence design of pharmaceuticals

February 16 2007

Chemists at the University of Liverpool have designed a unique structure to capture the movement of atoms which may impact on future designs of pharmaceuticals.

The research, funded by the Engineering and Physical Sciences Research Council, will further understanding of how to control chemical reactions and will influence improvements in a range of important processes from the design of biopharmaceuticals to the engineering of new catalysts, enabling scientists, for example, to develop products in more environmentally friendly ways.

The Liverpool team created a porous crystal which has 'walls' of atoms and cavities which act as containers for molecules. They used this crystal to accommodate a set of molecules as they took part in a chemical reaction similar to reactions by enzymes and proteins to regulate and keep alive living systems.

The crystal was put into a powerful X-ray diffraction machine at Daresbury laboratory, Warrington. This allowed scientists to pinpoint precisely the positions of individual atoms, providing snapshots of their movement. Because the reaction was carried out within the cavities of the crystal, the team was able to locate the positions of the atoms both before and after the reaction. This is the first time that the positions of atoms both at the beginning and the end of a chemical process have been seen.

Professor Matthew Rosseinsky explains: “To design more efficient processes which run with less waste and less energy input, scientists need a better understanding of the way in which atoms move during chemical reactions. We designed a robust structure that remained stable when a chemical reaction occurred inside its walls – a structure with an opening the same size as a single molecule of aspirin. The X-ray experiment then allowed us to see how the entire structure changed during the chemical process.

“Chemical reactions are essential in key manufacturing methods and in maintaining life in living systems and so this new research could influence the understanding of a wide range of important processes. This includes the chemical reactions involved in the production of anti-cancer drugs as well as reactions which allow biological molecules in plants and animals to convert food into energy.”

The research is published in *Science* magazine.

Source: University of Liverpool