The experimental team on instrument D1B

Animal magnetism

Developing polarised neutrons to reveal the magnetic side of proteins

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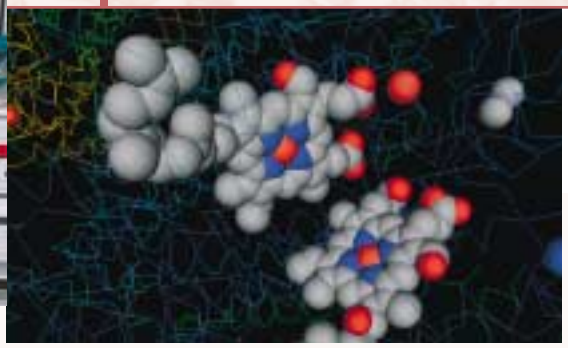

The active site of cytochrome *c* oxidase

Reactions in biological systems, such as energy-producing respiration, rely on a helping hand from enzymes containing metal atoms. These metallo-proteins catalyse the transfer of electrons in a reduction-oxidation (redox) mechanism. A typical example is cytochrome *c* oxidase (above). Such molecular assemblies are large and complex, and the details of the redox process are still uncertain; conventional studies using X-ray scattering, resonance or spectroscopic techniques are complicated by the presence of the many atoms in the enzyme's framework and the ambiguity of the data.

Polarised neutrons, however, have the potential to provide the information to unravel these mechanisms. Most enzyme-catalysed redox reactions involve the transfer of single electrons (each with a magnetic moment). They can therefore be located and followed, via the accompanying magnetic changes in the molecular system, using polarised neutron diffraction (p.6), without the interfering effects of the multitude of framework atoms.

In fact, the main obstacle in using neutron diffraction is that proteins such as cytochrome *c* oxidase are difficult to prepare in the required single-crystal form. For this polarised neutron technique to be used, it must first be modified to deal with powder and polycrystalline samples.

Powder diffraction is a well-established method of studying such materials. Instead of measuring individual reflections in three dimensions, as happens in single-crystal diffraction, the data are obtained as a one-dimensional set of complex, overlapping peaks from which information has to be extricated by a computer. In proteins, the complexity and large size of the protein structure amplifies the overlapping peak problem, so requires an optimised powder diffractometer.

A polarisation filter

The main technical difficulty to overcome is providing an intense-enough source of polarised neutrons over a wide wavelength range. Traditionally, ferromagnetic single crystals (p.6) are used, which produce polarised beams only at specific wavelengths. A new polarisation technique has recently been developed at ILL, which has a broader application and can be used with 'white' beams of pulsed neutrons (as provided by spallation neutron sources), as well as the continuous neutron source from a nuclear reactor such as ILL's.

The method is based on spin-polarised helium-3 which absorbs neutrons of one spin type, effectively acting as a spin filter. The device is compact (only a few centimetres long) and convenient. It is ideal for using with powder diffractometers, and will be suitable for experiments using the next generation of spallation sources that aim to follow the path of redox reactions with timed neutron pulses.

In June 2003, we carried out the first experiment to determine the applicability of this approach using the powder diffractometer D1B at the ILL. Data collected from a variety of organometallic and intermetallic materials clearly indicate that experiments can be designed to detect unpaired electrons in biological systems, thus heralding a new way of probing fundamental questions in biology – using magnetism. Chemists should also be able to apply the same technique to design novel redox catalysts. ■

The helium-3 cell used as a source of polarised neutrons

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