In this issue

Scientific anniversaries

The special section in this issue of *Current Science* marks two anniversaries. The first is the centenary of Roentgen's discovery of X-rays. The second is the fiftieth year following the discovery of nuclear magnetic resonance (NMR) by Felix Bloch and Edward Purcell. One could hardly have imagined at the turn of the century that Roentgen's discovery was to spawn a whole host of techniques, which were to change the face of twentieth century science. While the uses of X-rays in medicine are widely appreciated, Roentgen's rays have also had a dramatic impact on diverse scientific disciplines. X-ray crystallography begun by Max von Laue and the Braggs (father and son), has established itself as the most powerful method for the determination of the three-dimensional structures of molecules and is central to the practice of chemistry and biology. X-ray diffraction from fibers yielded the critical experimental data that proved so important in the model-building studies that led Linus Pauling to the α-helical and β-sheet structures of polypeptides, James Watson and Francis Crick to the DNA double helix and G. N. Ramachandran to the collagen triple helix. X-ray diffraction from single crystals transformed the field of chemical structure determination which for years had been dominated by degradative strategies. Dorothy Hodgkin's spectacular successes with penicillin and vitamin B_{12} in the 1940s and 1950s firmly established X-ray diffraction as an essential tool in chemistry. Protein structure determinations, haemoglobin and myoglobin, by Max Perutz and John Kendrew in the late 1950s set the stage for the explosive growth of X-ray crystallography over the last two decades. Much of the recent advances have been fuelled by enormous improvements in X-ray sources, data collection methodologies, computational resources and strategies for structure determinations, which provide solutions to the 'phase problem'. Several spectacular successes in the last year are testimony to the power of crystallography. These include the structures of bovine mitochondrial F-1 ATPase (molecular mass ~300000 Da) and the membrane-bound enzyme cytochrome oxidase. Crystallography has provided the most detailed view of complex structures with a near-atomic resolution. Details of molecular interactions which are at the heart of almost all biological phenomena have been revealed by many studies of complexes. The pace of research in the area of structural biology today is breathtaking, with crystallography being the preeminent technique.

Nuclear magnetic resonance is not far behind. When NMR was first developed in the mid-1940s as a technique to measure nuclear magnetic moments accurately, few would have predicted that an esoteric activity in physics departments would one day become a central technique in chemistry, biology and medicine. An inkling of what was to come was apparent when the Larmor frequencies determined for hydrogen nuclei (protons) by the discoverers of NMR, Bloch and Purcell, were different in the samples of water and mineral oil. Chemistry was soon to snatch the technique from physics. The NMR spectrum of ethyl alcohol (CH_3CH_2OH) recorded in 1951 revealed three groups of 'resonances' clearly establishing that nuclear resonance frequencies depend to a measurable extent on chemical environment. The dam broke shortly thereafter with NMR quickly becoming the method of choice for chemical structure determination, particularly in organic chemistry. Initially hampered by sensitivity problems, NMR was essentially a chemist's technique. The advent of Fourier transform spectroscopy in the late 1960s and two-dimensional NMR in the 1970s have propelled NMR to the realm of biology, with macromolecular structure determinations becoming a reality. NMR has another dimension. Magnetic resonance imaging (MRI) has become the method of choice for visualizing soft tissues. Radiology departments in medical institutions today boast of MRI facilities. The pace of change in NMR methodology is extremely rapid, rivalling crystallography in the area of structure determination. NMR has the major advantage that single crystals are not required; solutions will do. However, there are significant limitations on the sizes of molecules that can be studied – a disadvantage not shared by crystallography.

In marking the anniversaries of X-rays and NMR, *Current Science* presents a series of articles (**page 878**) which focus on historical development and current status of these techniques, with special reference to their practice in India.

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