The Australian Nuclear Science and Technology Organisation (ANSTO) is one of Australia’s largest public research organisations and custodian of much of the country’s important science infrastructure including the OPAL nuclear research reactor, the Australian Synchrotron, accelerators, cyclotrons and neutron beam instruments. ANSTO is a valued partner for industry, government, and universities and, as a primary producer of nuclear medicine, is a vital part of the Australian medical system.

**Crystallography at ANSTO**

The Bragg Institute at ANSTO’s Lucas Heights Sydney campus is named in tribute to Nobel Prize winners William Henry and William Lawrence Bragg. It leads Australia in the use of neutron scattering in crystallography.

At the centre of the research institute is the OPAL research reactor, along with state-of-the-art neutron beam instruments used for diffraction, affectionately named after Australian fauna including:

- **Wombat** a high-intensity powder diffractometer
- **Echidna** a high-resolution powder diffractometer
- **Koala** a Laue single-crystal diffractometer.

In addition, ANSTO operates the Australian Synchrotron in Melbourne, which produces extremely intense X-ray beams. Synchrotron light sources have revolutionised X-ray crystallography since the 1980s, and the Australian Synchrotron is now the centrepiece of X-ray crystallography in Australia. Three of the Synchrotron’s nine beamlines are dedicated to crystallography. These are the:

- Macromolecular and micro-crystallography beamlines (MX1 and MX2)
- Powder diffraction beamline (PD).

The Bragg Institute offers two proposal rounds per year with the Australian Synchrotron offering three rounds.
Case studies

Helping to understand hydrogen

Crystallography was the key which unlocked the remarkable secrets of the Chinese puzzle molecule. The molecule was made by scientists at National Dong-Hwa University in Taiwan. Their initial X-ray crystallographic measurements provided a partial model but major questions remained for which neutron crystallography was the key. The full detail of the structure was revealed by a Bragg Institute researcher using the Koala Laue neutron diffractometer to locate the 15 hydrides (single hydrogen atoms bearing a negative charge) present in the twenty-eight copper fifteen hydride core of the molecule which has alternating layers of hydride (depicted in red) and copper (shown in cyan) wrapped in an outer shell of molecules in the remarkable structure shown below.

The study revealed a new binding mode of hydride which adds to the growing body of knowledge about hydrogen – the smallest molecule – which lies at the centre of one of our great technological challenges. While the Chinese puzzle molecule can never be the way to store hydrogen for use in a car, the knowledge this puzzle has revealed to us strengthens our understanding of the chemistry of hydrogen which is required if hydrogen cars are ever to become a reality.

Powder diffraction goes to the planets

Australian Synchrotron researchers have successfully investigated some of the simple materials which form the extraordinarily complex geological features of Jupiter and Saturn’s icy moons.

From the Chaos Terrain on Europa (a moon of Jupiter) to the Tiger Stripes of Enceladus (one of Saturn’s companions) it seems that these simple structures can produce just as diverse features as their terrestrial silicate counterparts.

Australian Synchrotron researchers are recreating moon-like conditions at the powder diffraction (PD) beamline, and using the beamline’s high-resolution diffraction capacity to probe the interior of these materials.

They have re-evaluated the structure of the most water-rich sulphuric acid hydrate (an octahydrate) yet discovered and measured its thermal expansion.

The results show that sulphuric acid octahydrate’s response to heat is strongly influenced by how the water molecules are coupled together through the structure. The relatively strong bonding of the water molecules restricts the structure from expanding in two directions, so that practically all the thermal expansion happens in only one crystallographic direction.

Sulphuric acid octahydrate also has high overall negative thermal expansion, exceeding that of water ice below 140K (below -133°C). Since typical daily temperatures on Europa peak at 125K or -148°C, models that only account for water ice would underestimate the material expansions that could occur in this temperature range.