



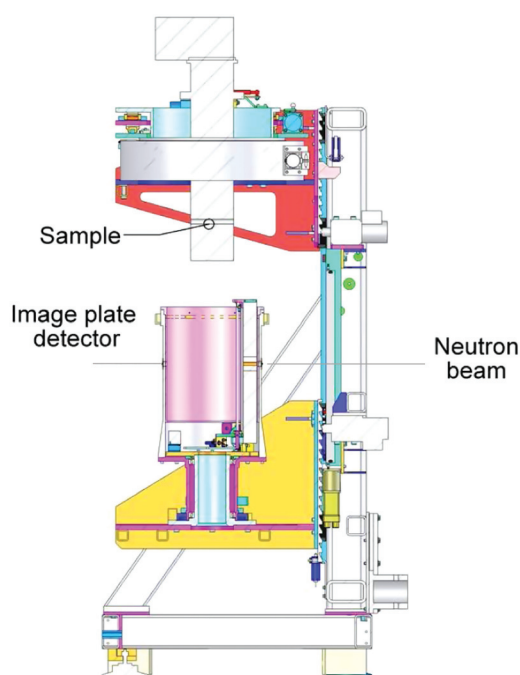
Australian Government

# Ansto

### For more information contact:

Dr Alison Edwards: +61 2 9717 7247  
alison.edwards@ansto.gov.au

Dr Ross Piltz: +61 2 9717 3607  
ross.piltz@ansto.gov.au



### Instrument specifications:

**Koala is located on the thermal neutron guide TG3 and uses a 'white beam' – that is a spectrum or range of wavelengths – facilitating efficient use of a large proportion of the available neutron beam.**

- Fast data collection: one structure per day for large samples
- Small samples: ~ 0.1 mm<sup>3</sup> or less with slower data collection
- Solid angle for quasi-Laue diffractometer at least 2 $\pi$
- Neutron wavelength is peaked as 1.3 Å
- Suitable for crystals with d-spacings up to 40 Å
- Q-range ~ 10 ( $\sin\theta/\lambda \sim 0.9 \text{ \AA}^{-1}$ )
- Sample environment: 6 K to 800 K (standard), gas-environment (hydrogen, oxygen, inert), electric fields

# KOALA

## Quasi-Laue diffractometer

Koala will be one of the leading small-molecule crystallography instruments in the world and will be used for determining the complex crystal structure of a wide range of chemicals and minerals.

### What makes Koala special?

The diffraction patterns created when neutrons hit a sample in Koala, will allow scientists to determine the location of atoms within the crystal and provide them with information about the crystal's structure and its properties. Single-crystal neutron diffraction studies complement X-ray crystallography by revealing the precise positions of light atoms such as hydrogen, which cannot be determined by X-ray. The highly accurate structural data produced by these techniques have revolutionised many areas of science.

### Applications

Koala will be useful for:

- Development and study of new pharmaceuticals - through diffraction studies of potential drug candidates
- Modern synthetic chemistry research - using diffraction studies to fully determine specific interatomic interactions of new chemicals
- Advanced materials research - to identify materials and to examine subtly different formulations at the interatomic scale
- Minerals research - understanding of the structure of new phases and the effect of the different phases on processing conditions
- Distinguishing between iso-electronic species (eg. K<sup>+</sup>, Cl<sup>-</sup> or elements near each other in the periodic table).

**Relevant fields include:** chemistry, physics, materials science, geology and biology.

### Case Study 1:

#### Unravelling complex compounds

Neutron diffraction has been used to study one of the most important steps in catalytic processes, the oxidative addition of dihydrogen to a transition metal.

The compound [Os<sub>2</sub>ClH<sub>2</sub>(PPh<sub>3</sub>)<sub>3</sub>] was first made 30 years ago but was wrongly formulated as [Os<sub>2</sub>ClH(PPh<sub>3</sub>)<sub>3</sub>]. Subsequent proton-NMR studies identified an additional di-hydrogen ligand and further NMR and isotopic studies (using deuterium) revealed two types of hydrogen bonding.

Recent neutron diffraction studies using the quasi-Laue instrument VIVALDI at ILL conducted on a small single crystal of the compound revealed the stereochemistry of the complex and allowed the nature of the bonds from the metal to the three hydrogen atoms to be fully determined.

