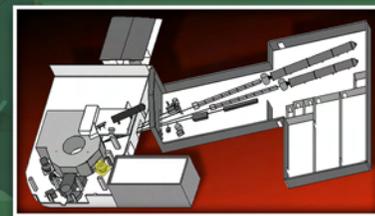


# INSTRUMENT

# HB-3A

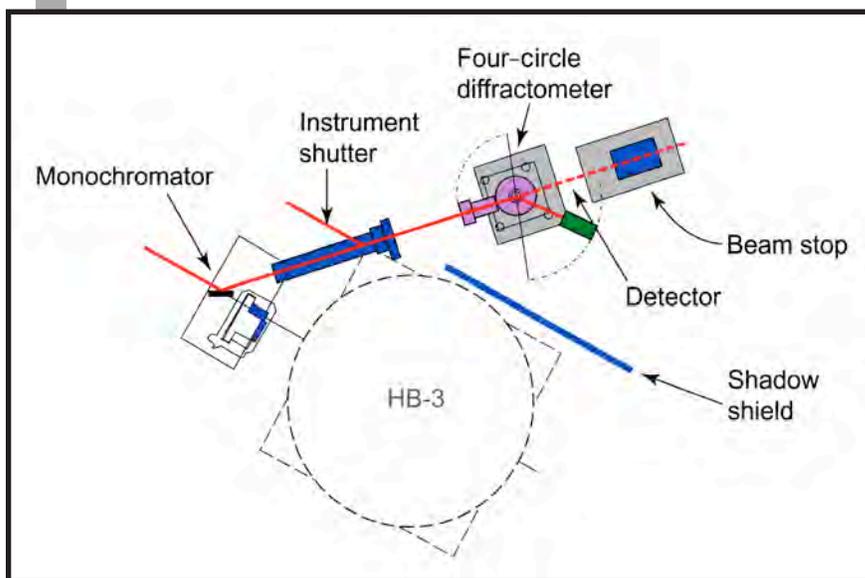
HIGH FLUX ISOTOPE REACTOR

## FOUR-CIRCLE DIFFRACTOMETER



The Four-Circle Diffractometer goniometer has a full  $\chi$  circle with a 10-K closed-cycle helium refrigerator. The detector is  $^3\text{He}$  with a 7-anode array in a honeycomb pattern. The upper  $2\theta$  limit is  $100^\circ$ . A multilayer-[110]-wafer silicon monochromator with the reflection from planes of the  $\langle 011 \rangle$  zone ensures sharp diffraction peaks in specified ranges of detector angles by control of the horizontal radius of curvature. Any plane from the  $\langle 011 \rangle$  zone can be set in Bragg position, but only the (155), (133), (022) with (044), and (111) with (333) reflections are of practical interest. For the fixed monochromator angle of  $48^\circ$ , these reflections provide principal incident wavelengths of 0.618, 1.01, 1.56, and 2.55 Å, respectively. A PC-based LabView system provides

user-friendly diffractometer control and data acquisition. The beam size is  $5 \times 5 \text{ mm}^2$ , and the minimum crystal size is  $1 \text{ mm}^3$ . The maximum crystal dimension is about 4 mm. The flux on the sample is estimated to be greater than  $5 \times 10^6 \text{ n/cm}^2/\text{s}$ .



### SPECIFICATIONS

Beam spectrum	Thermal
Monochromators	Vertically focusing silicon
Monochromator angle	$48^\circ$
Incident wavelength	0.618 Å (155), 1.01 Å (133), 1.56 Å (022), 2.55 Å (111)
Goniometer	Huber, full chi circle, with 10 K CCR
Scattering angle	$-110^\circ < 2\theta < 110^\circ$
Detector	7 anode $^3\text{He}$ (honeycomb pattern)
Crystal size requirement	$> 1 \text{ mm}^3$
Unit-cell size	$< 15,000 \text{ Å}^3$
Flux at sample	$> 5 \times 10^6 \text{ n cm}^{-1} \text{ s}^{-1}$ (est.)

Status:  
To be commissioned in 2008

### APPLICATIONS

This instrument is suitable for a wide range of small-unit-cell crystallography studies, from structure refinement and solution to charge and nuclear density mapping. Problems from chemistry, physics, materials science, and mineralogy have been addressed. Specific areas of study include hydrogen bonding and weak interactions, organometallics, supramolecular chemistry and crystal engineering, metal hydrides, charge density, pharmaceuticals, and magnetic structures. More general solid-state physics problems in magnetism, diffuse scattering, and ordering phenomena can also be addressed.

FOR MORE INFORMATION, CONTACT

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[http://neutrons.ornl.gov/hfir\\_instrument\\_systems/HB-3A.shtml](http://neutrons.ornl.gov/hfir_instrument_systems/HB-3A.shtml)



May 2008