Description of the Facility

Mission
The mission of the CUNY X-ray Facility is to perform single-crystal analyses for the structure determination of molecules, which make up a crystal. This technique is called single-crystal X-ray crystallography. It is the ultimate method for definitive determination of molecular structures at the atomic level for both organic and inorganic compounds. Its uses range from simple identification of compounds to various exotic configuration and conformational studies.

Instruments

Bruker-Nonius KappaCCD System

Capabilities: The KappaCCD, acquired in 2001, embodies the state-of-the-art technologies for rapid, precise, and accurate diffraction data collection. It is particularly useful for biological crystalllography, as it can handle samples with high absorption coefficients, such as inorganic compounds containing heavy atoms, such as technetium and rhenium, to minimize absorption-correction errors.

Enraf-Nonius CAD4

Nonius CAD4 serial diffractometer, equipped with a scintillation detector and a liquid-nitrogen low-temperature device, on a Nonius Diffractis 586 X-ray generator with a copper sealed tube.

Capabilities: A serial diffractometer collects one diffraction spot at a time. This CAD4 is an excellent instrument for experiments requiring high-resolution crystallographic data. It is well-suited for projects that require detailed analysis, such as inorganic chemistry and material science.

Instrument: Nonius CAD4 serial diffractometer, equipped with a scintillation detector, liquid-nitrogen low-temperature device, and a long 2theta-detector arm, on a Nonius FR571 X-ray generator with a copper rotating anode.

Capabilities: The long 2theta-detector arm allows better resolution of diffraction spots for crystals with long unit-cell dimensions. The instrument's long-rotation capability also allows for longer data collection times, which can be beneficial for heavily absorbing samples. The high signal-to-noise ratio is higher than for data from a sealed tube; and thus smaller crystals may be used to collect data.

The low-temperature options immensely improve the flexibility of a diffractometer. When a crystal is cooled to cryogenic temperatures, the arrangement of molecules within the crystal lattice becomes more ordered, leading to better diffraction data. This is particularly useful for samples that are unstable at room temperature, such as those containing heavy atoms.