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
Instrument: Bruker-Nonius KappaCCD, equipped with a CCD detector and a liquid-nitrogen low-temperature device.

Capabilities: The KappaCCD, acquired in 2001, embodies the state-of-the-art technologies for rapid, precise, and accurate X-ray diffraction. This instrument is particularly useful for investigating 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.

Capabilities: A serial diffractometer collects one diffraction spot at a time. This CAD4 is an excellent instrument for small molecules and crystals where slow data collection is not a concern. The serial diffractometer is also excellent for teaching and research, as it can illustrate, display, and apply the principles of crystallography. A CAD4 diffractometer requires little maintenance.

Instrument: Nonius CAD4 serial diffractometer, equipped with a scintillation detector, liquid-nitrogen low-temperature device, and a long 2theta-detector arm.

Capabilities: The long 2theta-detector arm allows better resolution of diffraction spots for crystals with long unit-cell dimensions. The increase in resolution is particularly evident in the signal-to-noise ratio, which 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, the solvent can be removed, and the crystal mass can be reduced.

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