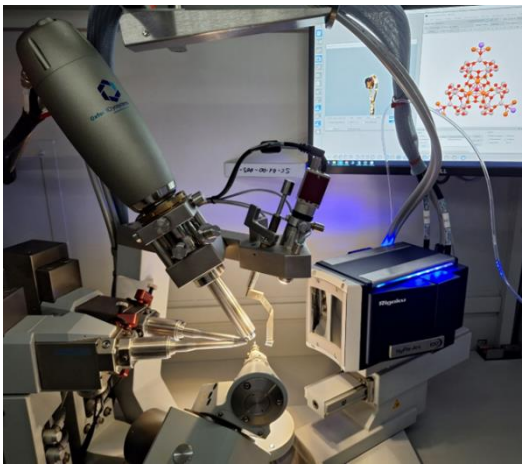
Ben-Gurion University of the Negev

IKI

Ilse-Katz Institute of Nanoscale Science & Technology

Single crystal X-ray diffraction

Equipment:



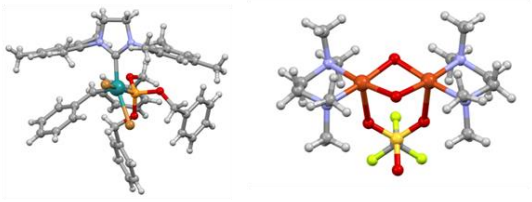
Rigaku Synergy-S - The Rigaku Synergy-S is a high-performance single-crystal X-ray diffractometer designed for precision structural determination.

- **HyPix-Arc 100°**: A curved hybrid photon detector for comprehensive data collection.
- **Kappa multi-axis goniometer**: Allowing flexible crystal orientation and improved data acquisition.
- **Dual radiation sources (Cu, Mo)**: Enabling versatile analysis across a wide range of sample types.
- **Cryo-system**: Facilitates low-temperature measurements for sensitive or temperature-dependent structures.
- Capable of analyzing very small crystals (20 µm and above), making it suitable for challenging samples.

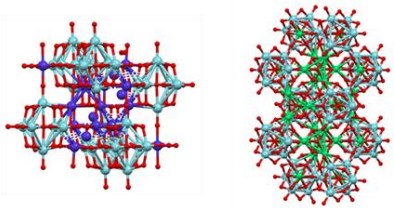
Services:

1. **Crystal screening & data collection** - establishing the presence of a single crystal (screening), pre-experiment to determine initial data collection strategy, collection of dataset according to crystal system and symmetry.
2. **Advanced structural analysis** - identification of twinning, commensurate/incommensurate modulation, and absolute structure (molecular chirality).
3. **Structure solution & electron density mapping** - generation of electron density maps and solving the crystal structure for publication or computational studies.
4. **Hirshfeld atom refinement (HAR)** - quantum-level refinement for precise determination of hydrogen atom positions and anisotropic displacement parameters.
5. **Preparation of crystal structure for publication** - deposition of crystal structure in databases (CCDC, CSD, ICSD etc.).
6. **High resolution powder diffraction** - X-ray diffraction analysis of sub-milligram amounts of powder samples. Contact for demonstration and details.

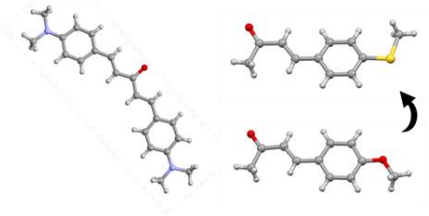
Examples of in-house solved structures:



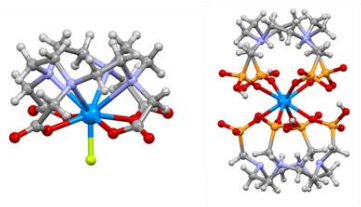
Organometallic catalysts



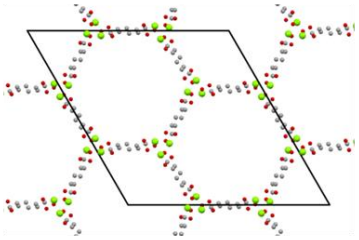
Polyoxometalate catalysts



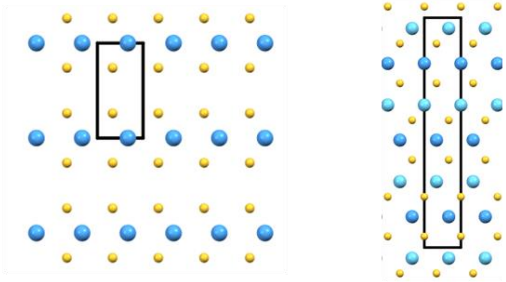
Organic molecules



Chelation complexes



Metal-organic frameworks (MOFs)



Transition metal dichalcogenides (TMDs)

For more details please contact:

Dr. Mark Baranov

Mail: markbara@post.bgu.ac.il

Phone: 08-6461236

Building 51, Floor 1, Room 105