Centre of collective usage

Center for provision of multiple-access highly specialized equipment

Center head, Academician

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Founded in 2008 and reorganized in 2014, the Center for provision of multiple-access highly specialized equipment gets together the unique equipment available at the Institute of Bioorganic Chemistry, Uzbekistan Academy of Sciences, and supplies concerned academic institutions of all ministries and agencies with the equipment.

Research directions

The Center aims at accumulation of highly specialized equipment making possible significant improvement of experiments and intensification of their conduction, as well as at efficient use of the equipment in experimental and applied studies, technical and methodical assistance for the equipment to be used in the academic activity.

The Center’s activity is focused on

- the execution of orders from research institutions of Uzbekistan Academy of Sciences and other agencies for governmentally run basic, applied and innovation studies, as well as those from the user-organizations for contract-based research
- the provision of services for use of multiple-access highly specialized equipment, organization of experiments, conduct of measurements, sample preparation, analysis of results, etc. to the organizations using the equipment in question
- the support of research in the sphere of knowledge intensive technologies

- the generation of prepositions for the competitive grants and the participation in their fulfilment
- the participation in the qualifying of Bachelors and Masters for higher educational institutions by training on the highly specialized equipment

Today, the Center for provision of multiple-access highly specialized equipment possesses

- Xcalibur-1 Oxford Diffraction diffractometer equipped with a CCD (charge couple device detector) (Kappa-geometry, graphite-151 monochromatised Mo-Kα radiation) for comprehensive reconstruction analysis of monocrystals of both organic and inorganic compounds. Annually, nearly 95 complete and 100 preliminary experiments are conducted. The device is mainly used for the routine determinations of crystal structures from the compounds synthesized or isolated at the Institute of Bioorganic Chemistry, Institute of the Chemistry of Plant Substances, Institute of General and Inorganic Chemistry, Uzbekistan Academy of Sciences, as well as the National University of Uzbekistan, Bukhara State University and Tashkent Chemical Technological Institute

- Agilent Technologies 6520 QTOF mass spectrometer (Tandberg Instruments LLC, Norway) combined with a nano-flow liquid chromatograph. Annually, nearly 80 experiments are conducted. The Institute of Bioorganic Chemistry, Institute of the Chemistry of Plant Substances and National University of Uzbekistan are among the main ordering customers

- Leica binocular microscope (Switzerland) for observation of bioorganic microscopic objects. The observations are performed by request of the ordering customer. The Institute of Bioorganic Chemistry is the main ordering customer
- XRD -6100 Shimadzu X-ray Diffractometer (Japan) for qualitative and quantitative X-ray analysis of organic and inorganic compounds. Annually, nearly 300 experiments are conducted. The Institute of Bioorganic Chemistry, Institute of General and Inorganic Chemistry, Institute of Nuclear Physics, Uzbekistan Academy of Sciences; Karakalpkstan subsidiary of Uzbekistan Academy of Sciences, Samarkand State University and others are among the main ordering customers

- Agilent 6400 Series Triple Quadrupole LC/MS Systems for determinations of crystal structures from the compounds synthesized or isolated at the Institute of the Chemistry of Plant Substances, the Institute of Bioorganic Chemistry, Uzbekistan Academy of Sciences, as well as at the National University of Uzbekistan.

The Center is financed by the public funds as well as by non-budgetary sources from the ordering customers and sponsors, and from the grants the Center participates to.

Principle achievements include

Comprehensive X-ray structural analysis of 300 compounds consisting of single-crystal growing, visual selection, identification of the elementary unit parameters, selections of images, determination of crystal structure, search for analogues in the Cambridge Structural Database, three-dimensional graphics and reporting.

More than 3000 determinations were performed on the XRD -6100 Shimadzu X-ray Diffractometer for the Institute of Bioorganic Chemistry, the Institute of General and Inorganic Chemistry and other institutions of Uzbekistan Academy of Sciences. The results made possible solution of problems associated with the composition, crystallinity and other parameters of the polycrystalline samples.

The center performed nearly 350 thermal analysis measurements. The literature data on methods for the chromatography-mass-spectrometry of natural, synthesized and complex compounds were examined. More than 100 compounds of various origins were studied. The methods for study on the structures of complex compounds by mass spectrometry were generated.

The training courses in crystallography and chromatography-mass-spectrometry facilitates qualification of novel generation specialists having a good command of the base crystallographic knowledge which can be used in the research and practice of the specialized academic and higher education institutions of Uzbekistan.

The Center’s workers provide functional condition, trouble-free operation and safety of the highly specialized equipment they are responsible for. The Center permanently

participates in the qualifying of Bachelors and Masters for higher educational institutions by training on the highly specialized equipment by requests from the academic institutions of Uzbekistan Academy of Sciences, the equipment of which was transferred to the Center.

Xcalibur-1 Oxford Diffraction diffractometer equipped with a CCD is intended for

- production of monocrystals suitable for Z-ray structural analysis
- selections of images
- determination of crystal structure, coordinates of atoms, anisotropic displacement parameters, bond distances, valency an dihedral angles
- determination of a crystalline structure, packing of molecules and intermolecular contacts

XRD -6100 Shimadzu X-ray Diffractometer is intended for

- imaging of the specimen powder (crystalline, polymeric, etc)
- qualitative phase analysis
- quantitative phase analysis based on Rietveld structure
- determination of crystallinity, sized of nano-particles, etc.

Agilent Technologies 6520 QTOF mass spectrometer is intended for

- highly efficient qualitative analysis
- identification of structure of unknown compounds
- determination of precise mass of molecular ion and fragments to unequivocally identify structure of unknown compounds
- automatic screening of complex mixtures and search for in the libraries of mass-spectra

- identification of a protein by databases
- analysis of posttranslational modification of proteins
- determination of amino acid sequence of peptides

Leica binocular microscope is intended for

- observation of microscopic objects both statically and automatically with 10x-100x magnification
- capacity of the image digitization
- analysis and the storing of the data by means of computer programs

NETZSCH STA-409 PG Simultaneous Thermal Analyzer is intended for

- simultaneous thermogravimetric and differential scanning measures in the temperature range of 120-600°C
- thermal analysis with registration of the specimen mass by temperature
- registration of heat flow characterizing changes taking place as a result of warming or cooling
- determination of thermal stability and specimen composition

Problems of commercialization

Today, search for and analysis of natural minerals is strongly associated with the method of X-ray phase analysis and X-ray structural analysis. The X-ray phase analysis is a current method for identification of phase condition of crystalline bodies. The method is based on the X-ray diffraction on the lattice. Based on the Institute of Bioorganic Chemistry, Uzbekistan Academy of Sciences, a group dealing with the identification of compositions of mineral rocks, clays, soils, slags, construction materials, ores, etc (qualitative and quantitative analysis) successfully functions. Crystal powders should serve as the specimens. There are methods for identification of amorphous component in the specimens. To perform a qualitative and a quantitative phase analysis, up-to-date X-ray equipment is used, such as XRD -6100 Shimadzu X-ray

Diffractometer, as well as *Crystallography Open Database (COD)* and *American Mineralogist Crystal Structure Database (AMCSD)* to perform the analysis quickly and accurately. The equipment of thermal analysis, to name, NETZSCH STA-409 PG, and IR-spectrometer may serve for comprehensive and all-sided study on minerals and clays.

The options may serve as a basis for conduct of contract-based research jointly conducted by the Institute of Bioorganic Chemistry and other organizations.

Services

The Center delivers services for collection of experimental data, sometimes conducting research by the request of an ordering customer by means of the highly specialized equipment of foreign origin.