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# SOFIA INITIATIVE "MINERAL DIVERSITY PRESERVATION"

VIII International Symposium
MINERAL DIVERSITY
RESEARCH AND PRESERVATION

#### СОФИЙСКАЯ ИНИЦИАТИВА "СОХРАНЕНИЕ МИНЕРАЛЬНОГО РАЗНООБРАЗИЯ"

VIII Международный симпозиум МИНЕРАЛЬНОЕ РАЗНООБРАЗИЕ ИССЛЕДОВАНИЕ И СОХРАНЕНИЕ

EARTH AND MAN NATIONAL MUSEUM 4, Cherny vruh Blvd., 1421 Sofia, Bulgaria 9-12 OCTOBER 2015

НАЦИОНАЛЬНЫЙ МУЗЕЙ "ЗЕМЛЯ И ЛЮДИ" бул. "Черии връх" 4, София 1421, Болгария 9-12 ОКТЯБРЬ 2015

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MINERAL DIVERSITY RESEARCH AND PRESERVATION VIII МЕЖДУНАРОДНЫЙ СИМПОЗИУМ

МИНЕРАЛЬНОЕ РАЗНООБРАЗИЕ ИССЛЕДОВАНИЕ И СОХРАНЕНИЕ

**ABSTRACTS** 

ТЕЗИСЫ



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ФОНДАЦИЯ "АСАРЕЛ"

## WWW-MINCRYST: NEW STAGES OF DEVELOPMENT OF INFORMATION-CALCULATION SYSTEM OF MINERAL'S CRYSTALLOCHEMISTRY

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In this article the Internet-oriented WWW-MINCRYST information-calculation system (ICS) intended for work with crystal structures of minerals, their synthetic analogs and elements is described. The ICS main components are actually a database (about 9300 records for almost 4000 unique phases), supplied with a complex of tools of search and information choice, means of multimedia representation of information (interactive polyhedral- and sphere-drawn crystal structures, different types of spectral drawing, etc.), opportunities of processing of spectral information, system of dynamic cross-references to mineralogical databases. The ICS is available at http://database.iem.ac.ru/mincryst or http://mincryst.iem.ac.ru without any restrictions.

The primary local crystallochemistry database MINCRYST has been created in 1985 under leadership of Anatoly Chichagov, and, thus, authors collect and proceed crystallographic data to database and ICS already more than 30 years. Anatoly Chichagov became the main initiator of creation of ICS and its ideological "locomotive". More than 18 years ago, in end 1997, Internet-oriented variant of database WWW-MINCRYST has been created and till now the successfully develops. The ICS became one of the first both in Russia, and in world practice of Earth's sciences.

The information fund of WWW-MINCRYST contains now about 9300 records, including more than 3700 unique mineral (IMA approved) and synthetic analogues names. About 400 records are added to system annually. Each record contains "monocrystal" and "polycrystal" characteristics of a crystal phase. The database supports powerful system of complex search of phases on many parameters, including names, chemical composition, structural characteristics, sources of information etc. The built-in program WWW-Crystpic give an effective interactive graphic representation of model of crystal structure both in balls and in polyhedrons. A wide change of parameters of demonstration of structure, direct calculation of interatomic distances, angles and cell parameters are possible. The module WWW-Mixipol allows users to get graphic representations of quasi-real full profiles of calculated polycrystals-roentgenograms including a mode of mixture of different minerals (up to 6 kinds of minerals). The ICS supports dynamic cross-references with the leading world mineralogical and crystallographic databases.

In recent time classifications by Georg Bokii is added. Now the system of calculation of maintenance of elements according to ideal and real formulas of a mineral sample is created.

Annually ICS WWW-MINCRYST gives out more than to 48000 users nearby 77 gigabyte of the data. This work is supported by a Russian Fund of Basic Researches, grant 15 07-08399-a.