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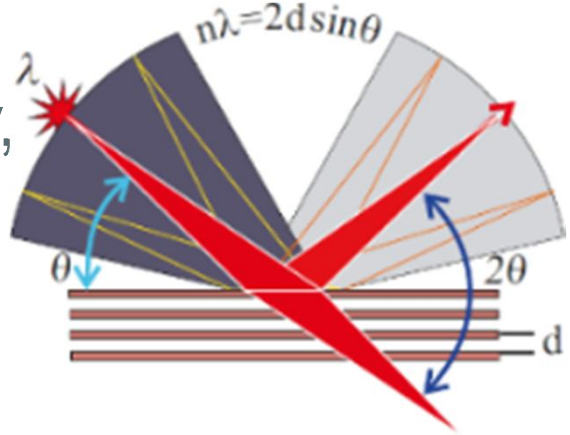
X-Ray Diffraction Research Centre of St.Petersburg State University

Andrey Zolotarev, Vladislav Gurzhiy,
Maria Krzhizhanovskaya



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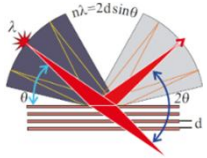

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Research Park SPbSU

Analytical centers

- Interdisciplinary Resource Centre for Nanotechnology
- Magnetic resonance methods of research
- Research Centre for X-ray Diffraction Studies
- Methods of matter content analysis*
- Optical and laser methods of research
- Physical methods of surface research
- Thermogravimetric and calorimetric methods of research
- Diagnostics of materials for medicine, pharmacology and nanoelectronics
- Development of molecular and cell technologies*
- Cultivation of microorganism
- «Chromas» Core Facility
- Computation Center

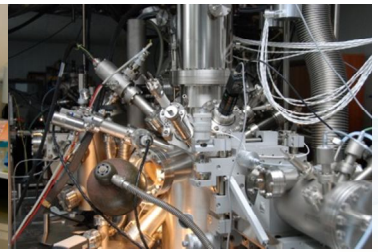
Technological centers

- Nanoconstruction of photoactive materials
- Innovative technologies of composite nanomaterials*
- Center for Sociological and Internet Research
- Observatory for Environmental Safety*
- Remote sensing of the Earth and applied geoinformatics
- Research and modelling of geoecological processes and systems (Geomodel)

Educational centers

- Educational Center for Physics
- Resource Centre for Microscopy and Microanalysis
- Educational Resource Centre for Chemistry*



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Research Centre for X-ray Diffraction Studies

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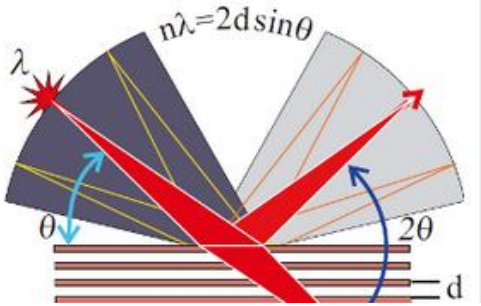
English version

We are pleased to welcome You on the website of the "Center of X-ray diffraction studies" at St.Petersburg State University.

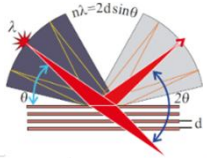
The Center of X-ray diffraction studies at St.Petersburg State University (XRD Center SPbSU) provides methodological and practical support for broad research community, including affiliates of SPbSU, national and international groups. It serves the purpose of ensuring the most efficient use of leading-edge scientific instrumentation for educational and research activities in various fields related to development of advanced materials, including biologically active systems, drugs, and nano-scale functional materials.

The main tasks of XRD Center are:

- methodological and practical support of scientific work done by researchers, post-graduates, trainees and graduate students at SPbSU;
- providing educational services and support of practical courses related to X-ray diffraction techniques in all branches of material science offered by SPbSU according to established plans;
- lecturing, consultation and other forms of distribution of information concerning advanced techniques of research using the equipment available at XRD Center.



X-ray diffraction is the scattering of X-rays by crystals (or molecules in liquids and gases), during which the secondary deflected beam of the same wavelength appear from the primary radiation beam, resulting from the interaction of primary X-rays and electrons of the substance. The direction and intensity of the secondary beams depend on the structure of the scattering object.



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Research

- Single crystal X-ray diffraction analysis
- Powder X-ray diffraction analysis
- Thermal X-ray analysis
- High-resolution X-ray diffraction and defectoscopy
- Spectroscopy. IR spectroscopy, DSC, TGA

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Research

Single crystal X-ray diffraction analysis. Refinement of the crystal structure.

Determination of linear and angular unit cell parameters, symmetry and space group of crystals, atomic coordinates and its thermal displacement parameters, interatomic distances and angular characteristics for the chemical bonding, calculation of the theoretical powder patterns according to the single-crystal X-ray diffraction data. Refinement of the site occupancy factors (e.g. in the case of solid solutions). Description of the coordination polyhedra geometric characteristics and ways of their arrangement in the structure. Подробнее →

Powder X-ray diffraction analysis. Crystalline phase qualitative and / or quantitative analysis.

Identification of different crystalline phases and the determination of their relative concentrations in mixtures according to the powder X-ray diffraction. Precise determination of the known substance unit cell parameters to detect and determine the concentrations of isomorphic impurities. Diffraction patterns indexing, determination of the unit cell parameters and a possible space group for the new compounds. Full analysis of the powder X-ray diffraction pattern, which includes refinement of the crystal structure and determination of some characteristics of the defect substructure for the new material. Подробнее →

Thermal X-ray analysis. Crystalline phase qualitative and / or quantitative analysis in the temperature range of -180 – 1600 ° C.

Provides information on the phase transition temperature, the most reliable way to interpret a variety of transformations, "solid-to-solid" (polymorphic transitions, decay and formation of chemical compounds and solid solutions, amorphization), "solid-to-liquid" (congruent, eutectic and peritectic melting, melting of the solid solutions, and crystallization from the melt), "solid-to-gas" (hydration, dehydration, loss of other volatile components except H2O and OH). Подробнее →

High-resolution X-ray diffraction and defectoscopy with D8 DISCOVER diffractometer

The study of ultrafine (nano-) materials, bulk single crystals, thin films and alloys by analyzing reflections profile by the means of wide angle scattering, small-angle scattering and diffraction at grazing angles. Studying of surface and interface structures between the substrates and thin films, determination of layer thickness and tracking of structural changes into the sample. NDT quality (excellence) control of massive industrial crystals for electronics and optics; determination of stress and textural studis of ceramic and metal samples. Investigation of "microstructures": characterization of crystalline materials micro structure and microstrain, characterization of the defect substructure in bulk samples and in catalysts nanoscale crystals. Подробнее →

Spectroscopy. IR spectroscopy, DSC, TGA

Auxiliary methods to obtain additional information for proper interpretation of the single-crystal and powder X-ray diffraction data include UV-, IR- and visible light spectroscopy, differential scanning calorimetry and thermogravimetric analysis. Подробнее →

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Education

For the formation of SPSU students practical research skills in disciplines related to the X-ray diffraction and X-ray analysis two training laboratories were organized in the "Center of X-ray diffraction studies". Training laboratories are working in the open mode, i.e. all the resources without exception available to studying in school hours, according to the schedule in individual departmental courses. Based on training labs facilities, students and graduates of SPbSU can also conduct their own research involves the identification of crystal phases, and determination of their relative concentrations in mixtures, precise determination of the lattice parameters of a known substance to detect and determine the concentrations of isomorphic impurities, and characterization the unit cell and possible space group of new compounds.

On the basis of educational laboratories it is planned to hold thematic training courses for employees as from SPbSU as from external organizations.

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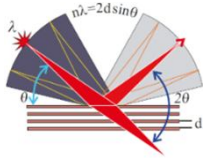

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Equipment

The "Center of X-ray diffraction studies" is built on a network principle - for the convenience of users two sites of equipment location with a total staff of employees have been organized.

Equipment located in the Vasilyevsky Island training and research Complex of SPbSU:

- The research facility **Rigaku «R-AXIS RAPID»**
- Single crystal diffractometer **Bruker «Kappa APEX DUO»**
- High resolution diffractometer **Rigaku «Ultima IV»**
- The research facility with low- and high-temperature cameras based on **Rigaku «Ultima IV»**
- Desktop powder diffractometer **Bruker «D2 Phaser»**
- The training and research facility based on three desktop powder diffractometers **Rigaku «MiniFlex II»**

Equipment located in the Petrodvorets training and research Complex of SPbSU:

- The research facility **Bruker «D8 DISCOVER»**
- Single crystal diffractometer **Oxford Diffraction «Supernova»**
- Single crystal diffractometer **Oxford Diffraction «Xcalibur»**
- Desktop powder diffractometer **Bruker «D2 Phaser»**
- The training and research facility based on three desktop powder diffractometers **Rigaku «MiniFlex II»**

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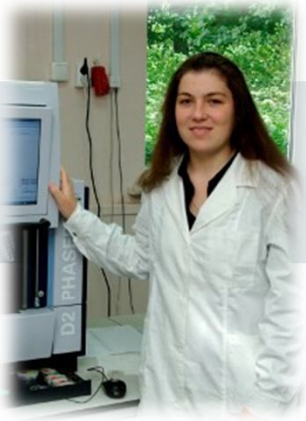






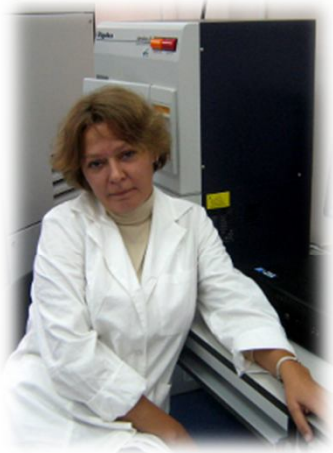

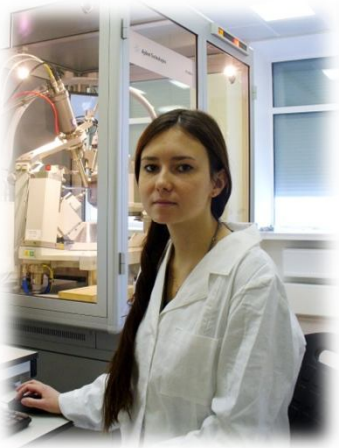


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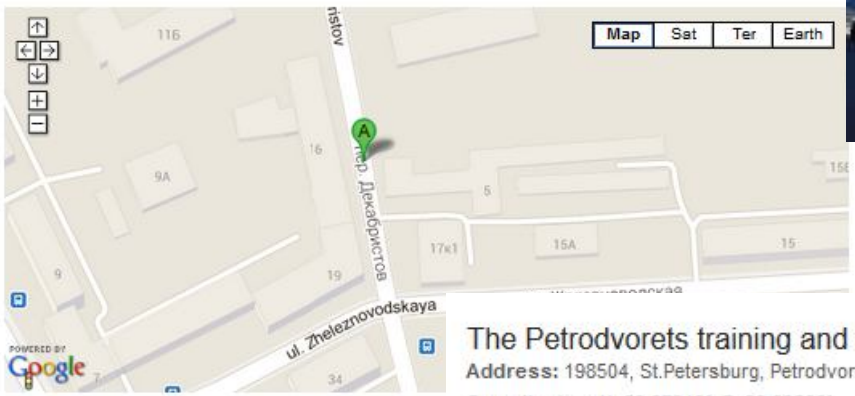
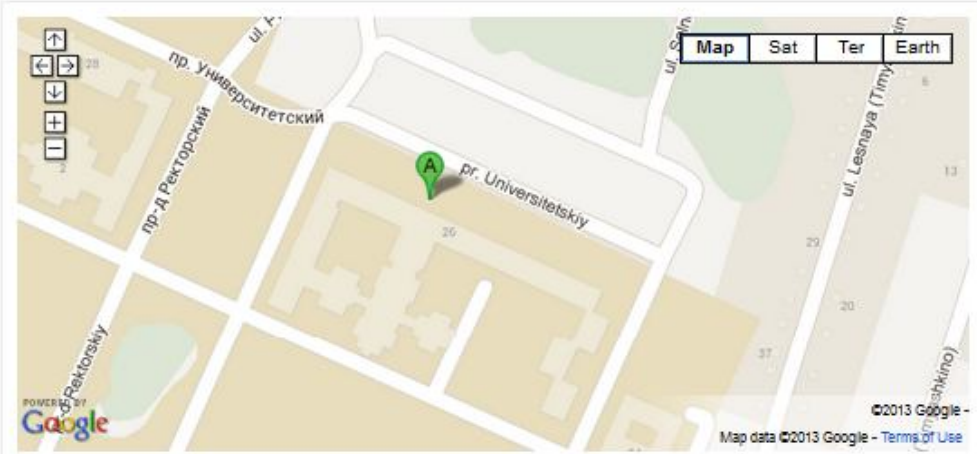
The Vasilyevsky Island training and research Complex of SPbSU

Address: 199155, St.Petersburg, Decabristov lane 16
Coordinates: N=59.95296°, E= 30.24854°
Phone number: +7 (812) 363-6883
E-mail: xrd@spbu.ru



The Petrodvorets training and research Complex of SPbSU

Address: 198504, St.Petersburg, Petrodvorets, Universitetskiy pr. 26
Coordinates: N=59.87913°, E=29.83586°
Phone number: +7 (812) 363-6883
E-mail: xrd@spbu.ru



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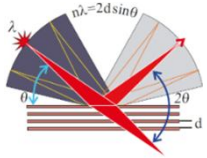

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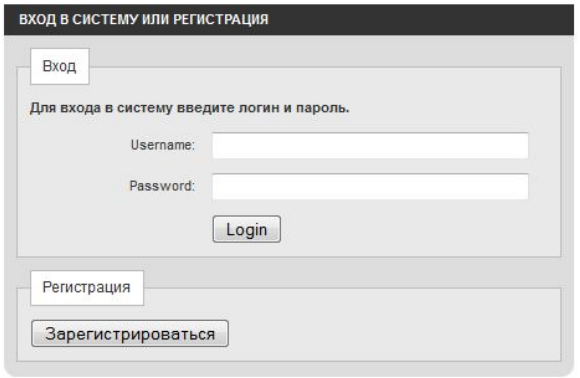
Санкт-Петербургский государственный университет
РЦ «Рентгенодифракционные методы исследования»



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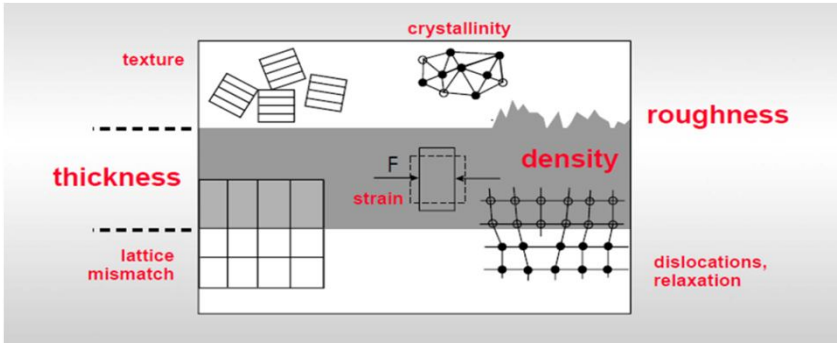
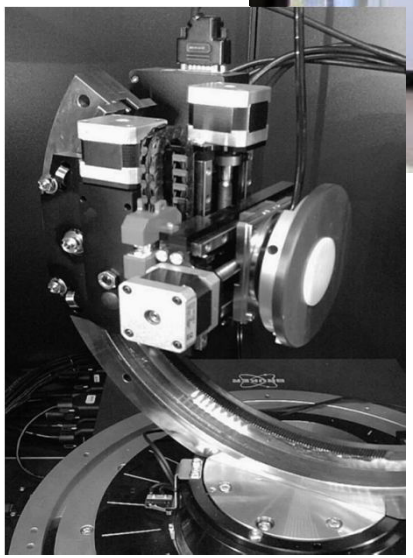
High-resolution X-ray diffraction and defectoscopy





Bruker «D8 DISCOVER»

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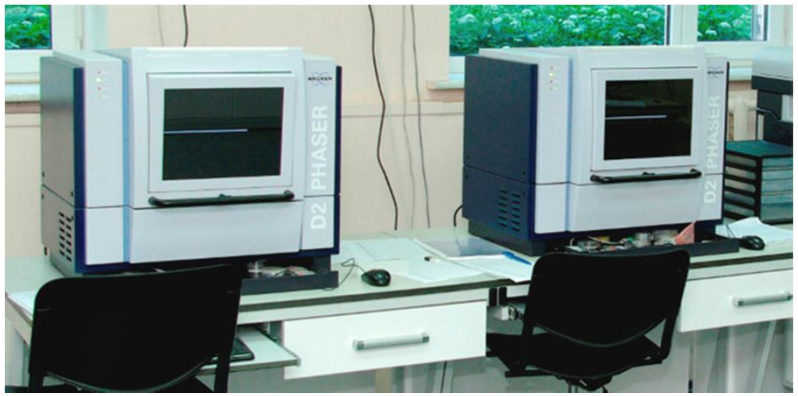
Powder X-ray diffraction analysis.
Crystalline phase qualitative and / or quantitative analysis.



Bruker «D2 Phaser»

Rigaku «MiniFlex II»

Rigaku «Ultima IV

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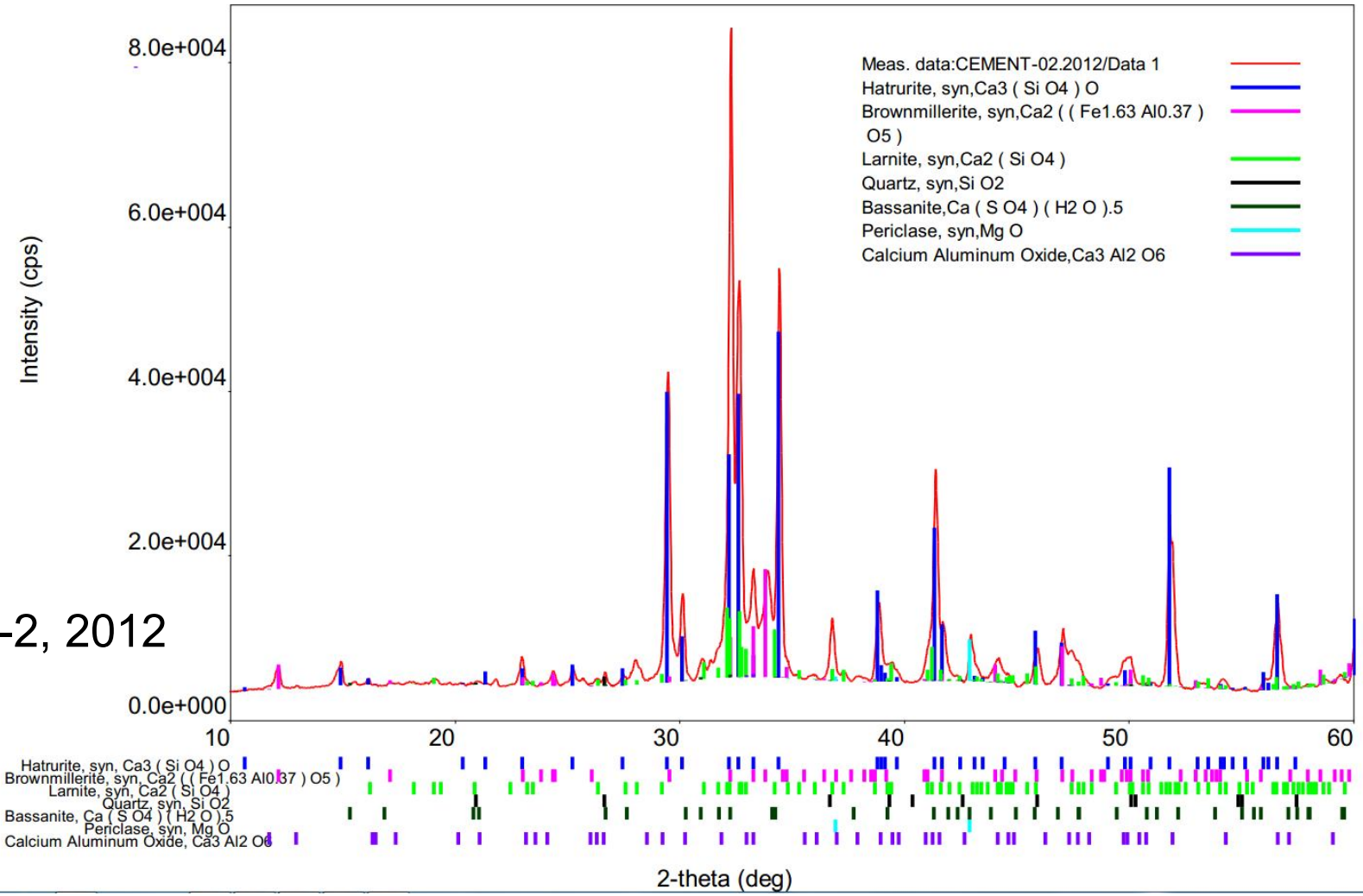
Powder X-ray diffraction analysis.
Crystalline phase qualitative analysis of cements.

PDF-2, 2012



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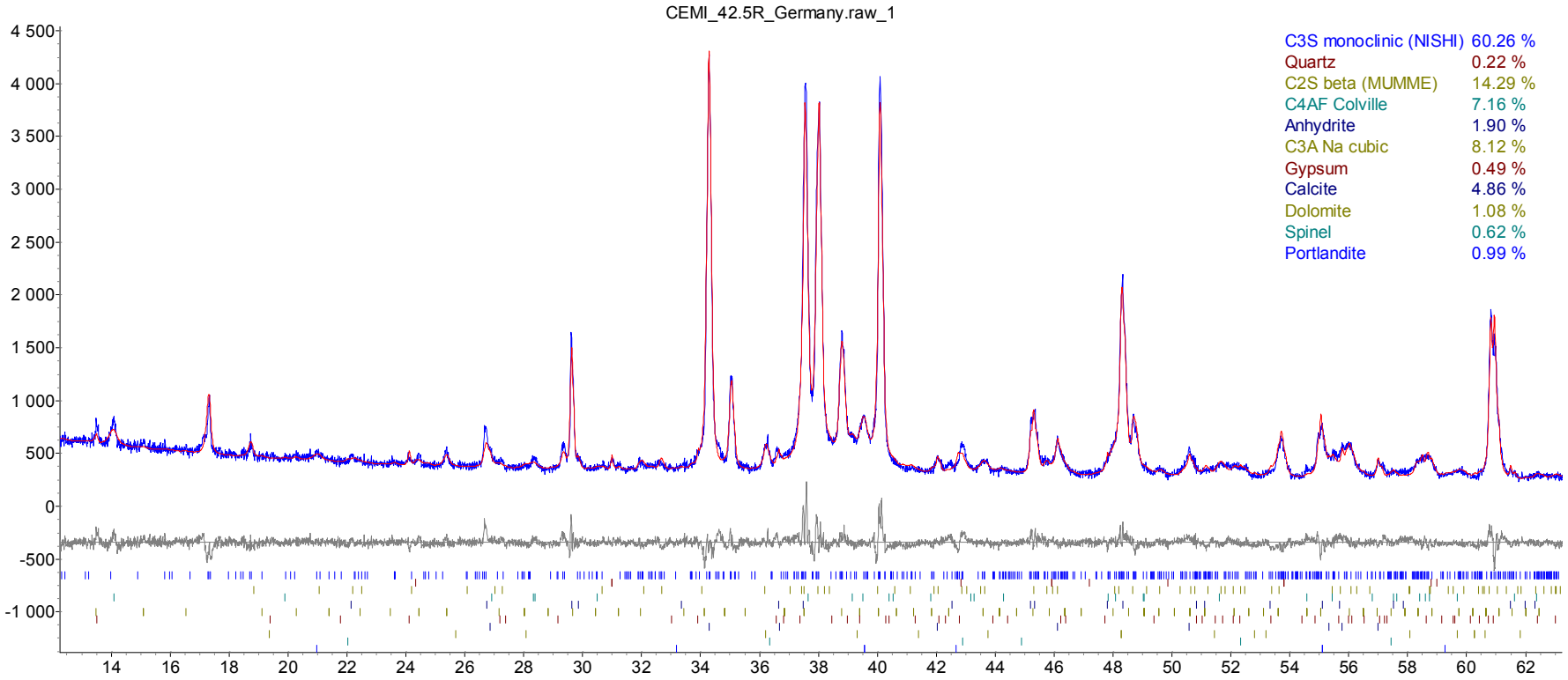
Powder X-ray diffraction analysis.
Crystalline phase quantitative analysis of cements.



Ritveld, TOPAS

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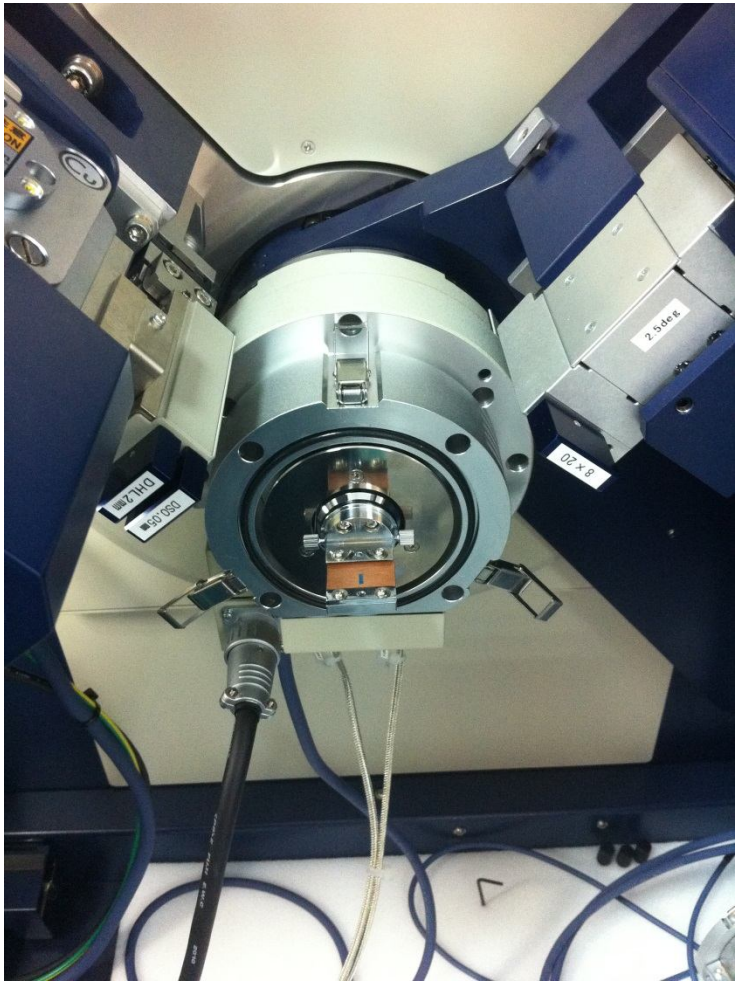
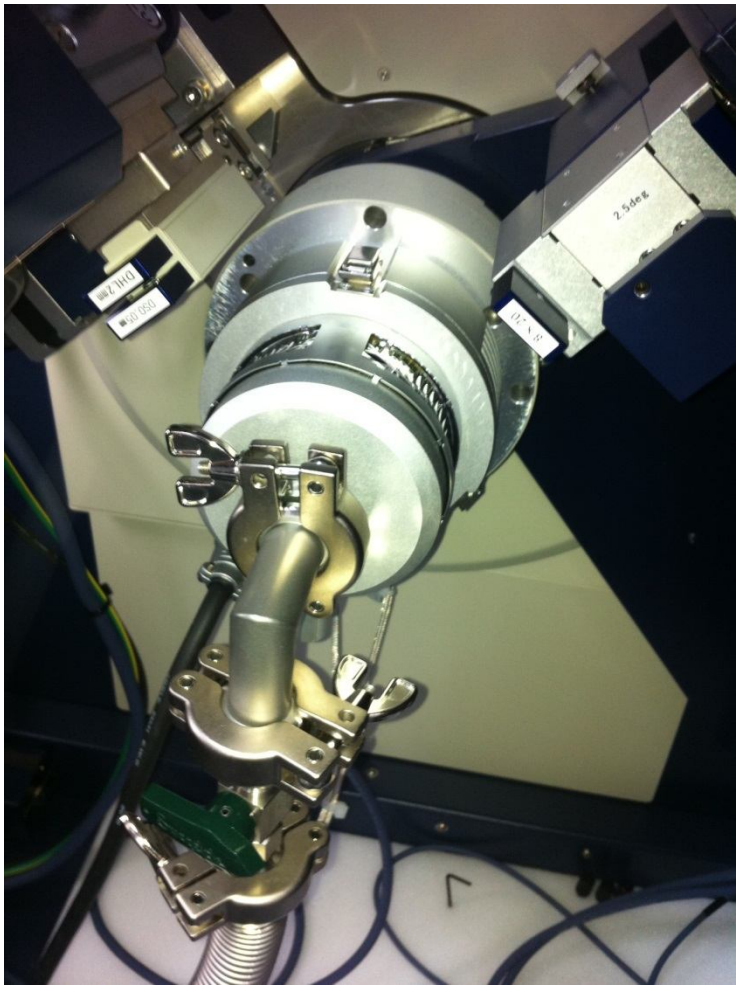
Thermal X-ray analysis. Crystalline phase qualitative and / or quantitative analysis in the temperature range of -180 – 1600 ° C.





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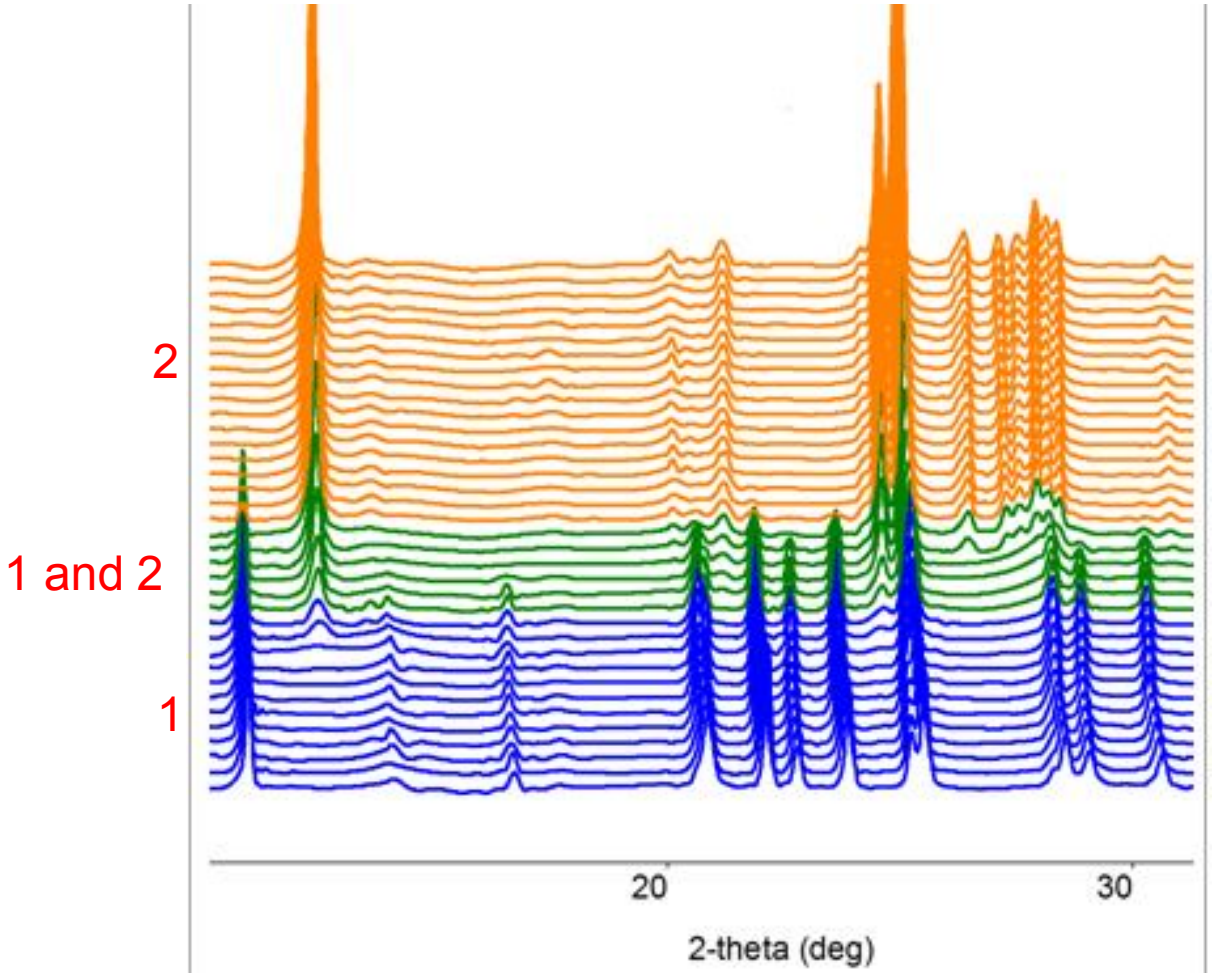

1 $Cs_2(UO)_2(Cr^{6+}O_4)_3 \rightarrow Cs_2((UO_2)_2Cr^{5+}{}_2O_8)$ 2

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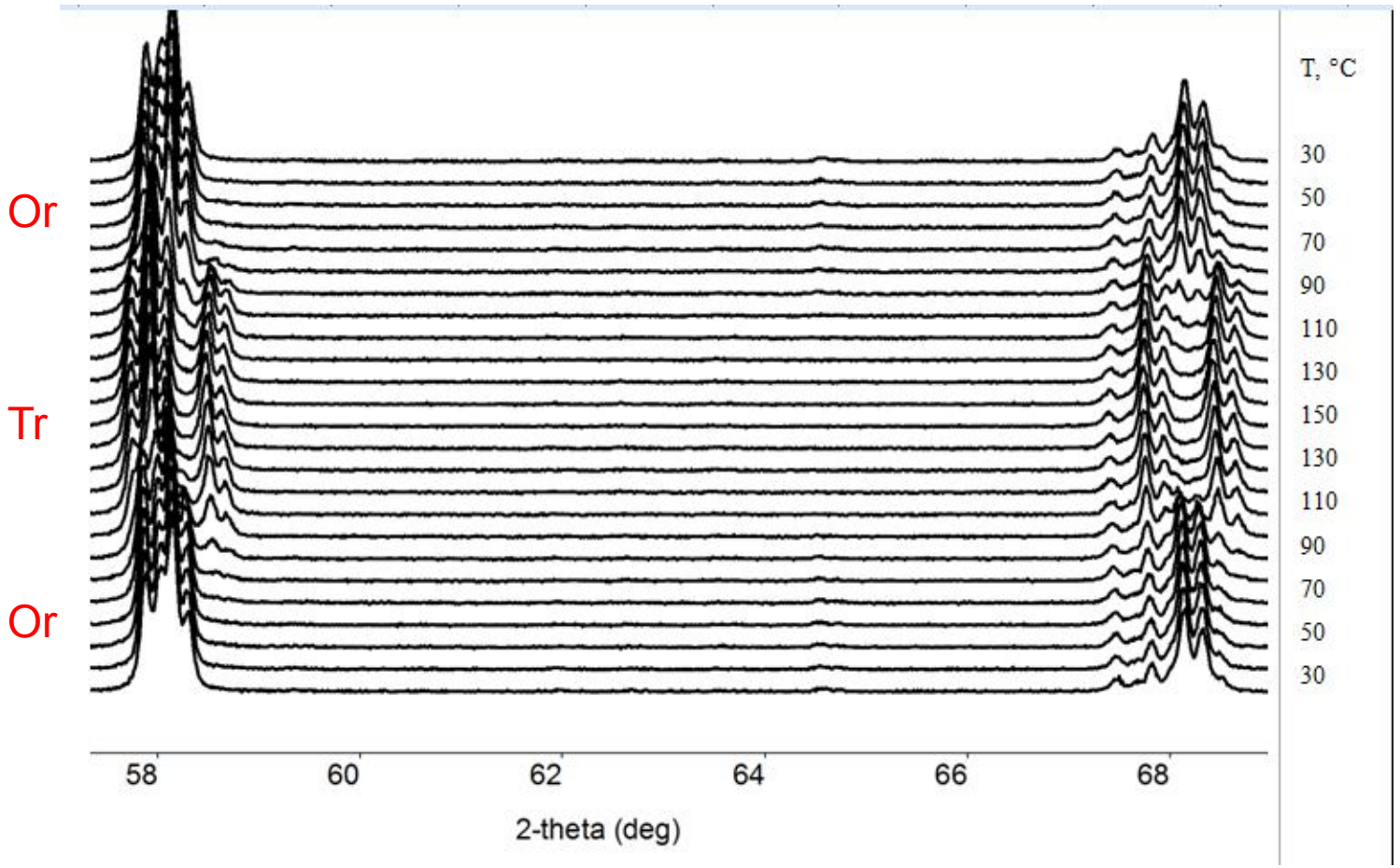
Thermal X-ray analysis. Crystalline phase qualitative and / or quantitative analysis in the temperature range of -180 – 1600 ° C.



Reversible polymorphic transformation of Perovskite-like phase

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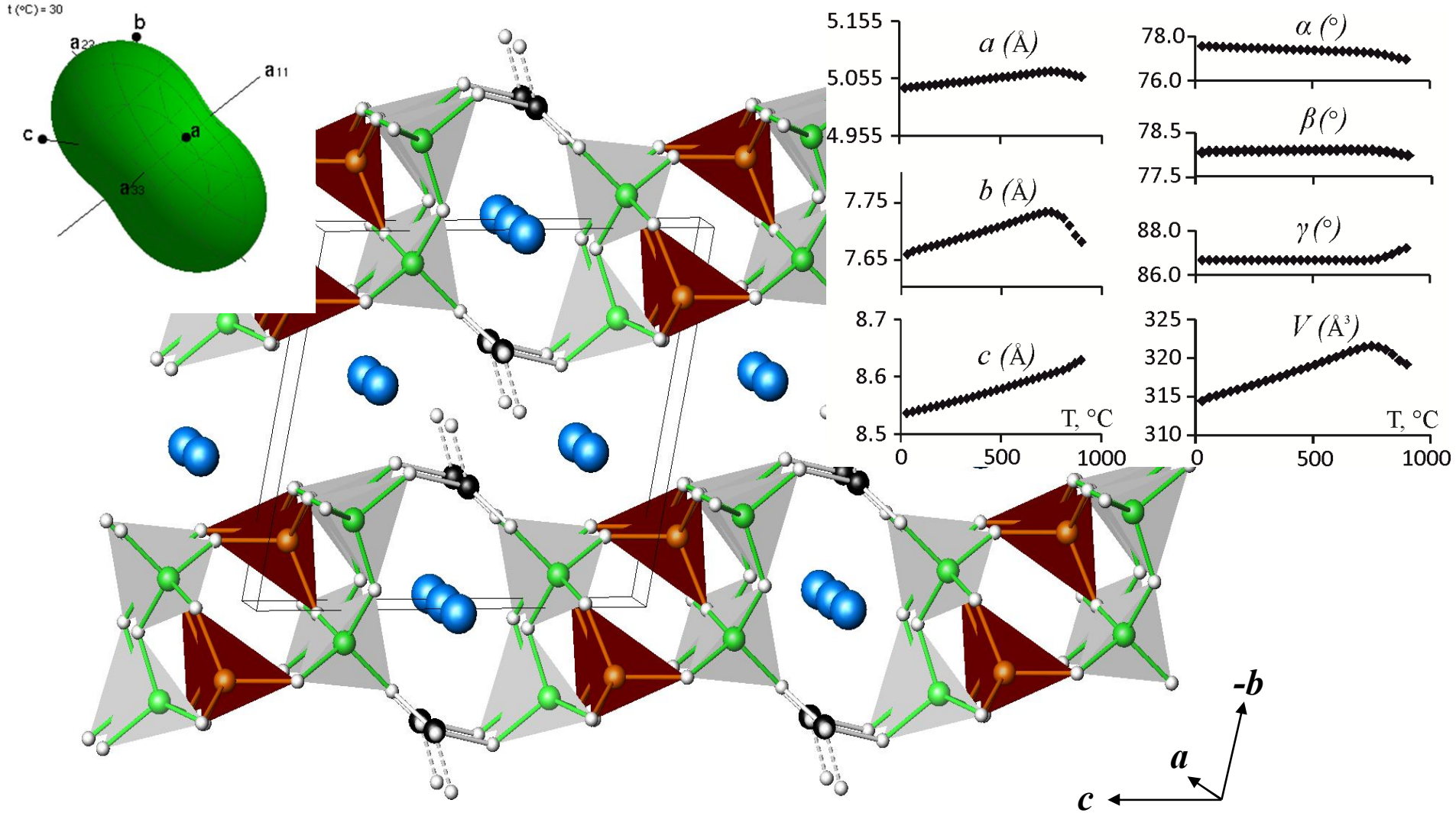
HTXRD of $Ba_3B_6Si_2O_{16}$



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Low-temperature polymorphic transformation