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Keywords: ferroelectric oxids; synchrotron x-ray powder diffraction; size-strain

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Structural Phase Transitions in Nanoscaled Systems with Jahn-Teller Ions. Sophia Petrova[c], Eugenia Vykhodets[d], Robert Zakharov[c], Mikhail Ivanov[b], Nikolai Tkachev[a], Anatolii Fishman[c]. [a]*Institute of High-Temperature Electrochemistry UD RAS.* [b]*Institute of Metallophysics NAS of Ukraine.* [c]*Institute of Metallurgy UD RAS.* [d]*Urals' State Technical University (USTU-UPI).*
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Specific features of the structural phase transitions of the first order were investigated in nanosized crystals with Jahn-Teller (JT) ions. As an example the phase transitions of martensite type, with changes in symmetry from a cubic (S) to a tetragonal (H) one, have been considered. It was shown the temperature and the latent heat of the transition decrease significantly for the nanoscaled grains. A possibility of multi-phase state with a coexistence of low-symmetry (H) and high-symmetry (S) JT-phases was predicted for the nanocrystalline materials [1] and proved for the nanoscaled Mn-O system (figure). With a certain ratio among parameters of cooperative interactions and random crystal fields at JT ions the structural phase transition can be reduced or suppressed totally. To explain the results the Kanamori model taking into account the size of nanocrystallites, the distribution of cations over non-equivalent crystallographic sublattices as well as the presence of random crystal fields in such systems was used. Figure. Temperature dependence of crystal lattice parameters and a subsequence of phase transitions during heat treatment of the course-grained (closed marks) and nanoscaled (open marks) oxide Mn_2O_3.

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Keywords: structural phase transitions; X-ray high-temperature powder diffraction; nanocrystalline materials

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Structure Determination on Asthmatic Drugs by Synchrotron Powder Diffraction. Jey-Jau Lee[a], S. Thamotharan[b], J. Jeyakanthan[a], R. Bansal[c], R. Yadav[c]. [a]*National Synchrotron Radiation Research Center, Taiwan.R.O.C.* [b]*Institute of Bioinformatics and Structural Biology, Department of Life science, National Tsing Hua University, Taiwan.R.O.C.* [c]*University Institute of Pharmaceutical Sciences, Panjab University, India.*
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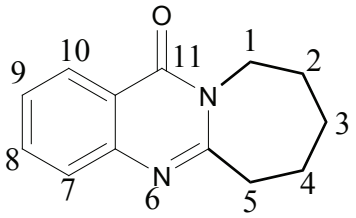
Asthma is a popular disease nowadays. There are many factors which are responsible for inducing symptoms of asthma. Many classes of drugs namely bronchodilators and anti-inflammatory agents have resulted in substantial improvement in survival and quality of life of asthmatic patients. Here we aim to search for a new chemical entity possessing better bronchodilatory effects and find out the structure solution by mean of synchrotron powder diffraction.
2,3,4,5-tetrahydroazepino[2,1-*b*]quinazolin-11(1*H*)-one(*1)* has been studied as a template. In addition, a number of nitrogenous functions were introduced at position 8, 9. The synthesized compounds were studied for their bronchodilatory activity using isolated guinea pig tracheal chain. The 3-D structure is also a key feature to understand their function. In this report, three series asthmatic drug targets structures are successfully solved by synchrotron powder diffraction data and combined simulated annealing method.



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Keywords: structure-aided drug design; structure from powder diffraction; quinazoline

FA5-MS01-P20

Study of the Molecular and Crystalline Structure of Three Nitrogen-Sulphur Pro-Ligands by X-Ray Powder Diffraction and Solid State Dftb Calculations. Asiloé J. Mora[a], Edward E. Ávila[a], Gerzon E. Delgado[a], Andrew N. Fitch[b], Michela Brunelli[c], Ricardo R. Contrera[a], Luis Rincón[a]. [a]*Departamento de Química, Facultad de Ciencias, Universidad de Los Andes, Mérida, Venezuela.* [b]*European Synchrotron Radiation Facility, BP220, F-38043 Grenoble CEDEX, France.* [c]*ILL Institut Laue-Langevin, BP 156, 38042 Grenoble cedex 9, France.*
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In the last decades, inorganic chemist has faced the need to mimic the properties of metal sites in metalloproteins to synthesize new catalytic materials with advantageous