APPLICATION OF NEUTRON POWDER-DIFFRACTION TO MINERAL STRUCTURES KARSTEN KNORR, WULF DEPMEIER pdf

1: Forschung in der FakultÃ¤t fÃ¼r Chemie

The application of neutrons to study the crystal structures of powdered minerals is of growing popularity among earth scientists. This has just recently been demonstrated at a workshop on Neutrons at the Frontiers of Earth Sciences and Environments (NESE) (Rinaldi and Schober).

IUCr sponsorship and support of meetings Meetings supported since A full list of meetings that have been supported since may be found here. Such meetings will also be eligible for support through the Visiting Professorship Scheme , where appropriate. The IUCr Visiting Professorship Scheme will pay the travel and insurance costs for up to three eminent scientists to enable them to present a short course at a workshop or school. It is the policy of the IUCr that strong emphasis should be given to provide a programme that is balanced with respect to gender and nationality. Application procedure Requests for IUCr sponsorship and nominal financial support for meetings are received and considered by the Sub-committee on the Union Calendar, which makes recommendations to the Executive Committee. The Application Form may be downloaded here. Completed Forms should be returned to the Chair of the Sub-committee via email: Rules The IUCr sponsors symposia and workshops on topics relevant to crystallography. There is a well defined procedure that should be followed when applying for sponsorship. The main rules are as follows: Applications for sponsorship are considered if they are submitted at least nine months in advance of the date of the meeting. Applications will be considered by the Committee three times a year at the end of February, June and October. Applications for sponsorship should be timed accordingly. For example, for a meeting to be held in June an application should be submitted by September of the previous year at the latest. Requests from satellite meetings may be submitted, and possible financial support requested, separately or through the Organising Committee of the main meeting. Meetings other than satellite meetings scheduled to be held within one month before or after an IUCr Congress will not be considered for sponsorship. For any meetings scheduled to be held between one and two months before or after a Congress, the application for sponsorship requires the approval of the Chair of the Congress Programme Committee. For meetings other than satellite meetings scheduled to be held, in the respective region, within one month before or after a meeting of a Regional Associate American Crystallographic Association, Asian Crystallographic Association, European Crystallographic Association, Latin-American Crystallographic Association , the applicants for sponsorship must seek the approval of the Chair of the Regional Associate Organizing Committee. IUCr sponsorship can only be given to meetings that are international in character and open to participants from all countries. For international meetings the membership of the Programme Committee is a good indication of this. National meetings are only supported if held in developing countries. IUCr sponsorship should only be given to meetings that include a speaker policy and statistics relating to gender balance on the conference website. Active crystallographers should be involved in the organization of the conference and one or more sessions should deal with specific crystallographic topics. This does not automatically include any session on condensed matter physics, materials science or symmetry not related to crystallography. According to these criteria all meetings organized by IUCr Commissions automatically qualify. Organizers of any meeting seeking IUCr sponsorship and support must assure the Sub-committee on the Union Calendar that the authorities of the country in which the meeting is to take place guarantee free entrance of bona fide scientists from all countries. Explicit support from the Chairs of the relevant IUCr Commission s is required for any international meeting except for the meetings of Regional Associates and from the Commission on Crystallographic Teaching for any international schools except for those organized by an IUCr Commission. Email addresses for the Chairs may be found here. Travel support for young scientists is available for all meetings including schools. This money should not be used for waiver of registration fees or for any purposes other than travel, accommodation and subsistence for the sponsored scientists. It is recommended that the presentations of young scientists supported by the IUCr should be in English. Consideration should be given

as to whether the proposed meeting is appropriate in subject, form and timing with respect to other related meetings. Except in special cases, IUCr funds should not be used to sponsor more than one event per year in the same location. Registration fees should be the same for both local and non-local participants. The International Union of Crystallography is a non-profit scientific union serving the world-wide interests of crystallographers and other scientists employing crystallographic methods.

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2: Publications - RWTH AACHEN UNIVERSITY Institute of Crystallography - English

We have presented a broad range of examples demonstrating the power of neutron powder diffraction for tackling problems in mineral structures related to weak X-ray scattering, neighboring elements.

Przemyslaw Dera Z. Petersburg State University, University Emb. The existence of Abstract. The high-pressure room temperature behavior PbCO3-II sets lead carbonate apart from the other arago- of PbCO3 was investigated by angle-dispersive synchro- nite-type carbonates. It was suggested previously that the tron powder diffraction up to The cell parameters at earth-alkaline cations. The transformation lone-pair occupies an inert orbital in the ligand sphere and is supposed to be of 2nd order. The studies carried out by and PbCO3 with aragonite-type structure at ambient con- Rieger and Mudring suggest that cation-anion inter- ditions De Villiers, ; Chevrier et al. Accord- actions are the true driving forces responsible for lone pair ing to the pressure homologue rule, stoichiometric com- distortions. This implies, fraction experiments were performed and their results are that all carbonates with aragonite structure should have reported in this work. High-pressure powder X- et al. Lin and ray diffraction patterns were taken up to The exposure time per image was about 10 s. The sample and three ruby chips 5 mm in size for pressure calibration were loaded into the sample cham- ber. The pressure was determined by the ruby fluorescence method Mao et al. Two DACs were used in the experiments. In the first cell argon was used as a pressure transmitting medium. A trace amount of Pt was mixed with the sample in an agate mortar, to act as an absorber for laser radiation for possi- ble annealing of the sample, which, however, was not rea- lized. Nitrogen was used as pressure transmitting medium in the second cell. Geometry parameters for the radial integration of the two-dimensional data and the sample to detector distance Pressure dependence of diffraction patterns of PbCO3 from Lattice and structural parameters were derived using 0. Nitrogen was used as pres- sure transmitting medium in the experiments up to The suite of programs Coelho, The background was measurements at 9. Tick marks denote reflection positions for Re upper row , Pt middle row and Ar lower row and pertain only to measurements at to add to this function an anisotropic broadening term to 9. In our analysis we found that the convolution with a suitable fourth-order spherical harmonic function repro- Results duced this anisotropic broadening well. To partly com- At ambient conditions, lead carbonate is orthorhombic, pensate for the low scattering power of oxygen and car- space group Pmcn standard setting: The cell para- bon compared to lead restraints were introduced for meters reported by Chevrier et al. In addition, the z-parameters of the atoms are nine-fold coordinated by oxygen and occupy oxygen and carbon atoms were constrained to keep car- Wyckoff position 4c. According to Chevrier et al. The isotropic displacement parameters were along the c-axis. Carbon is at Wyckoff position 4c and constrained for all atoms to have identical values oxygens are at 4c O1 and 8d O2 Fig. The evolution of the diffraction patterns as function of The strong preferred orientation of the gasket material pressure up to 16 GPa at room temperature is presented in Rhenium was accounted for by using a March-Dollase ap- Fig. Measurements up to Three additional diffraction patterns taken at used to determine the unit cell volume V0 at a pressure of 9. Refined unit cell parameters for PbCO3 as function of pres- sure. Standard deviations in parentheses were corrected by an esti- mated SCOR value of 3. Observed circles and calculated solid line diffraction pat- The difference and the tick marks for Data taken from Chevrier et al. Figure 3 showed small, but significant differences between ob- shows a plot of the structure refinement of lead carbo- served and calculated patterns. From Raman spectroscopic nate at 0. All fits up to data evidence for a phase transition to a phase II at about 7. The fit to the experimental data 7. In order to demonstrate the symmetry breaking from orthorhombic to monoclinic, the results of structure refinements of the Table 1 lists the refined unit cell parameters at dif- ferent pressures. All c2 values are in the order of magni- tude around 1. Errors obtained by the refinement proce- dure were multiplied by an estimated SCOR value of 3 Berar and Lelann, , because of the well-known fact of systematically too small e. The critical pressure pc of the phase transition was esti- mated from the dependence of sin b vs. The slope of 0. The symmetry relationship al- lows the development

of a ferroelastic spontaneous strain. Observed circles and calculated solid line diffraction pat- across the phase transition the components of the corre- tern for PbCO3 at Tick marks denote reflection positions for rows from up to monoclinic setting as described by Ohashi et al. This points at a possible additional sym- the low pressure regime contributes significantly to the metry change in the pressure range between 13 and scalar spontaneous strain es Fig. The changes of the 16 GPa. According to Raman spectroscopic data Minch other three e11, e22, e33 are non-significant and around et al. Therefore, our evaluation Refined atomic coordinates and bond lengths with an- of the dataset at Hence, the are given in Table 2 and 3, respectively. The pressure dependence of the normalized lattice para- Table 2. Bov shown in Fig. Note, the incompressibility of the a and b is 0. Standard deviations in parentheses were corrected by an lattice parameters, in contrast with the continuously com- estimated SCOR value of 3. Standard deviations in parentheses were corrected by an estimated SCOR value of 3. The same observation is valid for the Câ€”â€”O bond lengths. They are varying from 1. This is consistent within 3s with the reported Câ€”â€”O 1. Hence, the changes reported here, if real, should be understood as a trend, rather than a statistically confirmed fact. The parallel carbonate groups, the structure of PbCO3-II was error bars for both, pressure and lattice parameters, correspond to the size of the symbols. The lines are curve fits of second-order Birch- re-refined with constraints to keep the carbonate groups Murnaghan equation-of-states to the data. Results of two experiments parallel as described in the experimental part. This did not are presented. Therefore, in Tables 2 and 3 we give the structural parameters resulting from this Discussion constrained refinement. At ambient conditions phase transition. Anti-parallel arrows in phase I symbo- three atoms are at special positions 4c Pb, C, O1 and lize the strong compression of PbCO3-I along the c-axis one O2 is at general position 8d of space group Pmcn. The slightly C atom and three sites for oxygen atoms Table 1. The canted anti-parallel arrows in PbCO3-II indicate that O2 oxygen site 8d splits into two 4e general positions further compression of the c-axis results in a shear along designated O2. As can be seen the b-axis, thus preserving the minimum Câ€”â€”C-distance. The oxygen atoms are strongly apparently shows further shortening of the Câ€”â€”C distances. However, in Minch et al. However, some Pbâ€”â€”O bonds become noticeably shorter Fig. Thus the coordination changes only slightly, with Pbâ€”â€”O bond distances varying from 2. However, all changes of the bond lengths Pbâ€”â€”O are Fig. The evaluation of refined Câ€”â€”C distances with pressure. The 0 GPa Chevrier et al. For the nated as O2. The size of the symbols corresponds to errors tively. GeoSoil- As can be seen from Fig. Department of Energy, Office of second order nature of the phase transition. RF programme state contract Special thanks go to anonymous reviewer for very helpful comments. Finite strain isotherm and velocities for single-crystal and polycrystalline NaCl at high pressure and K. A high pressure infrared spec- order Birch-Murnaghan equation-of-state to the unit cell troscopic study of PbCO3-cerussite: Neutron single-crystal refinement of cerussite, PbCO3, lattice compression is highly anisotropic, namely more and comparison with other aragonite-type carbonates. Kristal- than five times stronger along the c axis than along a or b. This behavior is found for other aragonite-type carbonates Coelho, A. General profile and structure analysis as well, e. Crystal structures of aragonite, strontianite, and exceeds that along a and b even by a factor 10 Holl witherite. Note that in the aragonite-type structures Dollase, W. Is cerussite an Aragonite?

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3: CiNii å›³æ›¸ - Neutron scattering in earth sciences

Karsten Knorr. Bruker AXS mc, No.) were refined based on the results of neutron powder diffraction for a synthetic sample with the composition of x = (2) and simulated as functions of.

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4: Minerals as advanced material I

Important applications have been in crystallography (e.g. atomic positions of hydrogen and Al-Si ordering in feldspars and zeolites, Mn-Fe-Ti distribution in oxides), magnetic structures, mineral physics at non-ambient conditions and investigations of anisotropy and residual strain in structural geology and rock mechanics.

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Swiss Journal of Geosciences 1 , Geological Magazine, , â€" Nature Geoscience 4 3 , Geochimica et Cosmochimica Acta 75, Physics and Chemistry of Minerals 38 8 , A ureilite with an extremely high degree of shock melting; Meteoritics and Planetary Science, 46, â€" Hydrometallurgy , Janots, E. Geochimica et Cosmochimica Acta 75, Keiter, M. Geological Society of America Special Paper 48, 43 p. Implications for the reaction mechanism and acid neutralization. American Mineralogist 96, The Kadavur anorthosite complex, southern India: Journal of Applied Crystallography 44, Implications for sources, histories and large impacts. Geochimica et Cosmochimica Acta 75 8 ,

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5: Authors Contributions

Read Volume 63 Issue 1 of Reviews in Mineralogy and Geochemistry.

ISBN ; ISBN13 For over half a century neutron scattering has added valuable information about the structure of materials. Unlike X-rays that have quickly become a standard laboratory technique and are available to all modern researchers in physics, chemistry, materials and earth sciences, neutrons have been elusive and reserved for specialists. A primary reason is that neutron beams, at least so far, are only produced at large dedicated facilities with nuclear reactors and accelerators and access to those has been limited. Yet there are a substantial number of experiments that use neutron scattering. While earth science users are still a small minority, neutron scattering has nevertheless contributed valuable information on geological materials for well over half a century. Important applications have been in crystallography e. Applications range from structure determinations of large single crystals, to powder refinements and short-range order determination in amorphous materials. Zeolites, feldspars, magnetite, carbonates, ice, clathrates are just some of the minerals where knowledge has greatly been augmented by neutron scattering experiments. Yet relatively few researchers in earth sciences are taking advantage of the unique opportunities provided by modern neutron facilities. As the following chapters will illustrate, neutron scattering offers unique opportunities to quantify properties of earth materials and processes. Focus of this volume is on scientific applications but issues of instrumental availabilities and methods of data processing are also covered to help scientists from such diverse fields as crystallography, mineral physics, geochemistry, rock mechanics, materials science, biomineralogy become familiar with neutron scattering. A few years ago European mineralogists spearheaded a similar initiative that resulted in a special issue of the European Journal of Mineralogy Volume 14, Since then the field has much advanced and a review volume that is widely available is highly desirable. The purpose of this volume is to provide an introduction for those not yet familiar with neutrons by describing basic features of neutrons and their interaction with matter as well illustrating important applications. The volume is divided into 17 Chapters. The first two chapters introduce properties of neutrons and neutron facilities, setting the stage for applications. Some applications rely on single crystals Chapter 3 but mostly powders Chapters and bulk polycrystals Chapters are analyzed, at ambient conditions as well as low and high temperature and high pressure Chapters Characterization of magnetic structures remains a core application of neutron scattering Chapter 6. The analysis of neutron data is not trivial and crystallographic methods have been modified to take account of the complexities, such as the Rietveld technique Chapter 4 and the pair distribution function Chapter Information is not only obtained about solids but about liquids, melts and aqueous solutions as well Chapters In fact this field, approached with inelastic scattering Chapter 10 and small angle scattering Chapter 13 is opening unprecedented opportunities for earth sciences. Small angle scattering also contributes information about microstructures Chapter Neutron diffraction has become a favorite method to quantify residual stresses in deformed materials Chapter 16 as well as preferred orientation patterns Chapter The volume concludes with a short introduction into neutron tomography and radiography that may well emerge as a principal application of neutron scattering in the future Chapter

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6: Mineralogical Society of America - Neutron Scattering in Earth Sciences

Note: Citations are based on reference standards. However, formatting rules can vary widely between applications and fields of interest or study. The specific requirements or preferences of your reviewing publisher, classroom teacher, institution or organization should be applied.

Journal of Physical Chemistry B. Enrique Abad, Judith B. Reaction mechanism of the bicopper enzyme peptidylglycine-alpha-hydroxylating monooxygenase. Journal of Biological Chemistry. National Research Center, Egypt Field of research: Non-metallic and organometallic chemistry Host: Synthesis and characterization of hydrazone ligand containing antipyrine moiety and its transition metal complexes. Monatsh Chemie Chemical Monthly. Synthesis and biological activity of ferrocenyl ligand derived from thiophenol and its coordination with some transition metals. Abd-Elzaher, and Khaled Mahmoud,: International Journal of Medicinal Chemistry Stefan Tampier, Sascha M. Heinemann, and Nicolai Burzlaff: Bis pyrazolyl acetic Acid Bearing Ferrocenyl Substituents. Organometallics 32 20 â€" Research on Chemical Intermediates. Mousa and Samia A. Synthesis, characterization and biological activity of some ferrocenyl complexes containing antipyrine moiety. Labib, and Mamdouh M. Egyptian Journal of Chemistry. EL Saied, Mohamad M. El Tabl, Mokhles M. Organometallics , , p. Research on Chemical Intermediates 40, , p. Egyptian Journal of Chemistry 57, , p. Main Group Chemistry 13, , p. Synthesis, anticancer activity and molecular docking study of Schiff base complexes containing thiazole moiety,. Youssef , Sheta M. Characterization of Eu III complex for determination of bumetanide in pharmaceutical preparations and in biological fluids, Egyptian Journal of Chemistry 59 5 Egyptian Journal of Chemistry 59, , p. El Saied, Mokhles M. El Tabl, Mohamad M. Synthesis, physicochemical studies and biological evaluation of unimetallic and heterobimetallic complexes of hexadentate dihydrazone ligands,. El-Sheikh and Mohkles M. Simple synthesis of novel copper metalâ€"organic framework nanoparticles: Natural products chemistry Host: Muna Ali Abdalla Mohamed Dr. El Fau Area, Eastern Sudan. Muna Ali Abdalla Mohamed and Dr. Endophytes as Producers of Peptides: Natural Products and Bioprospecting. Matasyoh, Marc Stadler, Roderich D. Journal of Natural Products. Medicinal Significance of Naturally Occurring Cyclotetrapeptides. Journal of Natural Medicines. Three New Cyclotetrapeptides Isolated from Streptomyces sp. Journal of Natural Products Research. Accepted, , [Streptomyces sp. Synthesis of some new thieno[2,3-d]pyrimidine derivatives. About the reaction of b-dimethylamino-a,b-enones with active methylene nitriles. Novel synthesis of N-arylpyrrole, pyrrolo[1,2-a]quinazoline, and pyrrolo[3,4-d]pyridazine derivatives. A novel synthesis of some 1,4-phenylene-bis-heterocyclic carboxamide derivatives. Sobhy , Peter Metz, Anna Jaeger: Sharaf, Peter Metz, Anna Jaeger: Synthetic applications of benzothiazole containing cyanoacetyl group. Synthesis of some novel pyridine and naphthyridine derivatives. Synthesis and reactions of some new selenolo[2,3-c]pyridazines. International Journal of Organic Chemistry. Sobhy, Peter Metz, Akram A. Synthetic Studies with 3-Oxo-N-[4-3-oxo- 3-phenylpropionylamino -phenyl]phenylpropionamide. Studies on the Reaction of Cycloalkanones with Malonodinitrile. Journal of Heterocyclic Chemistry. Synthesis of new functionalised derivatives of [1,2,4]triazolo[4,3-a]pyrimidine and pyrimido[2,1-b][1,3,5]thiadiazine as aromatase inhibitors. Journal of Chemical Research. Synthesis of some novel thiazole, thiadiazole and 1,4-phenylene-bis-thiazole derivatives as potent anti-tumor agents. Synthesis and some reactions of 1-arylacetylmethyl-1,2,3-triazoleDerivatives with anticonvulsant activity. Mini-Reviews in Medicinal Chemistry. Gomha, Peter Metz, Mohamed M. El Farargy, Fathy M. Design, synthesis and anticancer evaluation of novel pyrazole, pyrazolo[3,4-d]pyrimidine and their glycoside derivatives. Abdelrahman, Peter Metz, Mohsen A. Facile synthesis of some novel triazolo[3,4-b]thiadiazines and triazolo[4,3-b]tetrazines. Synthesis of some new pyridine-based heterocyclic compounds with anticipated anti-tumor activity. Ismail Abdelshafy Field of research: Abdelmoniem and Said A. Chemistry of 2-Arylhydrazonals 2I-Arylhysdrazonals. Abdel-Gallil and Daisy H. European Journal of Organic Chemistry. Optimizing scale up yield to Pyridazines and Fused Pyridazines. Recent Developments in Our

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Laboratories. Fathi and Ismail Abdelshafy Abdelhamid: Hassaneen and Ismail Abdelshafy Abdelhamid: Chalcones incorporated pyrazole ring inhibit proliferation, cell cycle progression, angiogenesis and induce apoptosis of MCF7 cell line. Anti-Cancer Agents in Medicinal Chemistry. Pawan Kumar Natural Product, Inc. Muniruddin Field of research: Name-Oshud Somporke Sacheton Houn. Dhaka, , pp. Assiut University, Egypt Field of research: Spectral studies of highly optically transparent polyblends of poly o-tuluidine doped with salicylidene-o-aminophenol. Scientific Research and Essay. Cecilia Olufunke Field of research: Macromolecular Chemistry and Physics. Foaming, water absorption properties of Kerstingiella geocarpa and Bambara groundnut as influenced by neutral salt. Preparation, composition and physico-chemical characteristics of native, oxidized and acetylated African yambean Sphenostylis Sternocarpa starches. Advances in Natural and applied Sciences. La Rivista Sostanze Grasse. Effect of salts on functional properties of Albizia lebbeck seed flour. Akintayo, Christine Fischer, Peter Langer:

7: WWU - Institut fÃ¼r Mineralogie - Publikationen - Archiv

FIGURE 2 Neutron powder diffraction pattern of a-NaN3/NaCI at about O.O6GPa, measured within 15 minutes utilising the Kiel/Berlin Cell K. KNORR AND W. DEPMEIER.

8: (IUCr) Sponsorship and support of meetings

The authors are, respectively, graduate assistant and associate professor of geochemistry, College of Mineral Industries, The Pennsylvania State University. Abstract Phase equilibria have been determined in the system CaO-Al 2 O 3 -H 2 O in the temperature range Â° to Â°C. under water pressures of up to atmospheres.

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