

dimensional diffractometer, including geometry convention, critical components, and configurations associated with various applications.

NEW STRUCTURAL PROTOTYPING SYSTEM USED BY THE LINUS PAULING FILE AND PROPOSED FOR THE POWDER DIFFRACTION FILE

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The PAULING FILE is a materials database project. It was launched in 1995 and is a long-term project and will comprehensively cover all non-organic compounds (no C-H bonds) including Alloys, Intermetallics and Inorganics and consists of four interconnected parts: Constitution, Structure, Diffraction, and Physical Properties. The linkage of the four different groups of data was considered as most important, therefore the PAULING FILE was designed as phases oriented materials database.

The structural prototyping is a well-known concept in inorganic chemistry where often a large number of compounds crystallize with very similar atom arrangements. The compilation Strukturbericht started to catalogue crystal structures into prototypes named by codes such as A1, B1 or A15. These notations are still in use, however, nowadays prototypes are generally referred to by the name of the compound for which this particular kind of atom arrangement was first identified, i.e. for the prototypes enumerated above: Cu, NaCl, Cr₃Si. The PAULING FILE uses a longer notation, which includes also the Pearson symbol and the space group number: Cu,cF4,225, NaCl,cF8,225, Cr₃ Si,cP8,223. All data sets with published coordinates in the PAULING FILE are classified into prototypes, following criteria defined in TYPIX.¹ According to this definition, isotypic compounds must crystallize in the same space group, have similar cell parameter ratios, and occupy the same Wyckoff positions in the standardized description with same or similar values of the atom coordinates. If all these criteria are fulfilled, the atomic environments should be similar. No distinction is made between structures with fully and partly occupied atom

sites. When possible, a prototype has been assigned also to data sets without atom coordinates. The prototype is often stated in the publication, in other cases it has been assigned by the editors. The assigned prototype may in some cases be an approximation of the real structure, ignoring for instance a certain disorder.

One of the most challenging tasks in material science is the design and identification of new materials with beforehand-defined physical and/or chemical properties. In order to reach this objective in general materials scientists use two different approaches:

1. The first approach is to simulate the motion of the atoms in the material as well as their electronic interactions as close to reality as possible by using quantum-mechanical calculations. In theory there is no input other than the laws of quantum mechanics, so using these calculations the material properties can be understood from first principles. Based on this understanding it should be possible to design new materials with defined properties just by computer simulations, resulting in calculated data.
2. The second approach seems to be less challenging at first glance, since it does not ask for the really fundamental principles but it is based on a more pragmatic level. Most of our current knowledge in chemistry and material science has been collected empirically, just by searching for patterns and rules in experimental results published in the literature. Certainly the part of the calculated data and knowledge based on fundamental principles is steadily increasing and the derived data automatically will become part of the second approach.

In both cases the new structural prototyping system is an essential part for its potential success in future. We will try to demonstrate its potential with the help of several practical examples.

¹E. Parthe, L. Gelato, B. Chabot, M. Penzo, K. Cenzual, and R. Gladyshevskii, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, 8th Ed. TYPIX - Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types, 4 volumes, Heidelberg: Springer 1993, 1994.

Calendar of Meetings

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1–4 September 2004

QENS2004 Seventh International Conference on Quasi-elastic Neutron Scattering. Arcachon-Bordeaux, France. [Contact: A. Desmedt, QENS2004, Laboratoire de Physico-Chimie Moléculaire, UMR5803–CNRS, Université Bordeaux I, 351 Cours de la Libération, F-33405 Talence cedex, France. Fax: 33 540 008 402; E-mail: info@qens2004.org; Info: <http://www.qens2004.org>].

2–5 September 2004

EPDIC 9 Ninth European Powder Diffraction Conference. Prague, Czech Republic. Held at Charles University. Includes a full-day session on phase analysis and size/strain software. [Contact: Radomir Kuzel, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16 Praha 2, Czech Republic. Tel: 420 (2) 2191 1394; Fax: 420 (2) 2491 1061; E-mail: epdic-9@post.cz; Info: <http://www.xray.cz/epdic>].

4–8 September 2004

5th European Conference on Mineralogy and Spectroscopy (ECMS). Vienna, Austria. [Contact: ECMS 2004 Organising Committee, Institute of Mineralogy and Crystallography, University of Vienna-Geocentre, Althanstrasse 14, A-1090 Wien, Austria. Fax: 43 (1) 4277 9532; E-mail: mineralogy@univie.ac.at; Info: <http://www.univie.ac.at/Mineralogie/ECMS2004>].

6–10 September 2004

E-MRS 2004 Fall Meeting of the European Materials Research Society. Warsaw, Poland. Held at the Warsaw University of Technology. Preceded by a workshop on Intergranular and Interphase Boundaries—Experimental Techniques of Investigation and Computer Simulation Methods, 1–4 September in Warsaw. [Contact: Conference Secretariat, Warsaw University of Technology, Faculty of Materials Science and Engineering, ul. Woloska 14, 02-507 Warsaw, Poland. Tel: 48 (22) 660 8794; Fax: 48 (22) 660 8794; E-mail: fall2004@e-mrs.org; Info: <http://www.e-mrs.org/meetings/fall2004>].

7–10 September 2004

X-TOP 2004 7th Biennial Conference on High Resolution X-ray Diffraction and Imaging. Prague, Czech Republic. Held at Prague Honice Castle (near Prague.) [Info: <http://www.physics.muni.cz/kfpx/top>].

15–17 September 2004

15th European Conference on Diamond, Diamond-like Materials, Carbon Nanotubes, Nitrides, and Silicon Carbide. Riva del Garda, Italy. [Contact: April Williams, Elsevier, The Boulevard, Langford Lane, Kidlington, Oxford OX5 1GB, United Kingdom. Tel: 44 (1865) 843089; Fax: 44 (1865) 843958; E-mail: a.williams@elsevier.com; Info: <http://www.diamond-conference.elsevier.com>].

3–7 October 2004

31st Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Portland, Oregon, USA. [Contact: FACSS, Post Office Box 24379, Santa Fe, NM 87502, USA. Tel: 1 (505) 820 1648; Fax: 1 (505) 989 1073; E-mail: facss@facss.org; Info: <http://www.facss.org>].

16–17 November 2004

Crystallographic Society of Japan Annual Meeting. Osaka, Japan. [Contact: Crystallographic Society of Japan, Nissei Otuka3-chome, Bldg. Otuka 3-11- 6, Bunkyo-ku, Tokyo 112-0012, Japan. Tel: 81 (3) 5940 7640; Fax: 81 (3) 5940 7980; E-mail: cr-info@riz.co.jp; Info: <http://www.soc.nii.ac.jp/crsj/index-e.html>].

6–7 December 2004

Micro- and Mesoporous Mineral Phases. Rome, Italy. Organized by the IUCr Commission on Inorganic and Mineral Structures and the Accademia Nazionale dei Lincei. To include mineralogical, crystallographic, and technological aspects of these materials. [Contact: Info: <http://lcm3b.uhp-nancy.fr/cims/micromesoporous.htm>].

13–17 February 2005

Neutron Diffraction Characterization of Mechanical Behavior. San Francisco, California, USA. A symposium to be held during the 134th TMS Annual Meeting & Exhibition. [Contact: TMS Meeting Services, 184 Thorn Hill Road, Warrendale, PA 15086, USA. Tel: 1 (764) 776 9000 ext 243; Fax: 1 (764) 776 3700; E-mail: mtgserv@tms.org; Info: <http://www.tms.org/Meetings/Annual-05/AnnMtg05Home.html>].

14–18 February 2005

Australian X-ray Analytical Association 2005 Conference and Exhibition. Perth, Western Australia, Australia. [Contact: Dr. Brian O'Connor, Curtin University, GPO Box U1987, Perth, WA 6001, Australia, toconnorb@cc.cutin.edu.au or Tulips Meeting Management, Post Office Box 116, Salamander Bay, NSW 2317, Australia. Tel: 61 (2) 4984 2554; Fax: 61 (2) 4984 2755; E-mail: axaa@pco.com.au; Info: <http://www.pco.com.au/axaa2005>].

21–23 February 2005

4th Pharmaceutical Powder X-ray Diffraction Symposium, Barcelona, Spain. Sponsored by the International Centre for Diffraction Data, Newtown Square, Pennsylvania, USA. PPRD is a forum for discussion among scientists working in the fields of X-ray diffraction and pharmaceuticals. Topics of the symposium include regulatory and patent issues, acquisition and use of XRPD data, powder pattern indexing, as well as other topics surrounding these combined fields of interest. [Contact: Leah Mooney, e-mail: ppxrd@icdd.com].

14–18 March 2005

International Centre for Diffraction Data, Spring Meeting. Newtown Square, Pennsylvania, USA. [Contact: Linda Shertz, International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. Tel: 1 (610) 325 9814; Fax: 1 (610) 325 9823; E-mail: shertz@icdd.com; Info: <http://www.icdd.com>].

12–14 April 2005

British Crystallographic Association Annual Spring Meeting. Loughborough, England, United Kingdom.

28 May–2 June 2005

American Crystallographic Association Annual Meeting. Orlando, Florida, USA. [Contact: Khalil Abboud at abboud@chem.ufl.edu; Ed Collins at edward_collins@med.unc.edu; Info: <http://www.hwi.buffalo.edu/ACA>].

27 June–1 July 2005

Joint 20th AIRAPT - 43rd EHPRG International Conference on High Pressure Science and Technology. Karlsruhe, Germany. Associated with the 7th EMU School in Mineral Behaviour at Extreme Conditions in Heidelberg, 19–28 June. [Contact: Prof. Dr. Eckhard Dinjus, Forschungszentrum Karlsruhe (ITC-CPV), PO Box 3640, D-76021 Karlsruhe, Germany. Tel: 49 (7247) 82 24 00; Fax: 49 (7247) 82 24 44; Info: <http://hikwww2.fzk.de/ehprg>].

1–5 August 2005

54th Annual Denver X-ray Conference. Colorado Springs, Colorado, USA. [Contact: Denise Flaherty, International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. Tel: 1 (610) 325 9814; Fax: 1 (610) 325 9823; E-mail: Flaherty @icdd.com; Info: <http://www.dxcicdd.com>].

23–31 August 2005

20th IUCr General Assembly and International Congress of Crystallography. Florence, Italy. [Contact: Congress Secretariat, XX Congress IUCr, Dipartimento di Energetica, Università di Firenze, via S. Marta 3, 50139 Firenze, Italy. Tel: 39 (055) 479 6240; Fax: 39 (055) 479 6342; E-mail: iucr@iucr2005.it; Info: <http://www.iucr2005.it>].

9–13 October 2005

32nd Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Quebec, Canada. [Contact: FACSS, Post Office Box 24379, Santa Fe, NM 87502, USA. Tel: 1 (505) 820 1648; Fax: 1 (505) 989 1073; E-mail: facss@facss.org; Info: <http://www.facss.org>].

28 November–2 December 2005

International Conference on Neutron Scattering. Sydney, Australia. [Contact: Brendan Kennedy, School of Chemistry, Building F11, University of Sydney, Sydney, NSW 2006, Australia. E-mail: b.kennedy@chem.usyd.edu.au; Info: <http://www.sct.gu.edu.au/icns2005>].

Summer 2006

23rd European Crystallographic Meeting. Leuven, Belgium.

16–23 July 2006

7th International Conference on the Occurrence, Properties, and Utilization of Natural Zeolites. Socorro, New Mexico, USA. [Contact: Robert Bowman, New Mexico Institute of Technology, Socorro, New Mexico, USA. E-mail: bowman@nmt.edu].

Summer 2008

21st IUCr General Assembly and International Congress of Crystallography. Osaka, Japan.

Short Courses & Workshops

30 August–8 September 2004

6th European Mineralogical Union School: Spectroscopic Methods in Mineralogy. Vienna, Austria. Note that the School is concurrent with the 5th European Conference on Mineralogy and Spectroscopy, 4–8 September, also held in Vienna. [Contact: Prof. Dr. Anton Beran *or* Prof. Dr. Eugen Libowitzky, Institute of Mineralogy and Crystallography, University of Vienna-Geocentre, Althanstrasse 14, A-1090 Vienna, Austria. E-mail: mineralogie@univie.ac.at; Info: http://www.univie.ac.at/Mineralogie/EMU_School].

31 August–2 September 2004

Fourth Size-Strain Workshop. Prague, Czech Republic. Held at Charles University, immediately preceding EPDIC 9 Ninth European Powder Diffraction Conference. [Contact: Radomir Kuzel, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16 Praha 2, Czech Republic. Tel: 420 (2) 2191 1394; Fax: 420 (2) 2491 1061; E-mail: epdic-9@post.cz; Info: <http://www.xray.cz/s-s4>].

1–4 September 2004

Workshop on Intergranular and Interphase Boundaries—Experimental Techniques of Investigation and Computer Simulation Methods, Warsaw, Poland. Precedes the 2004 Fall Meeting of the European Materials Research Society. [Contact: Conference Secretariat, Warsaw University of Technology, Faculty of Materials Science and Engineering, ul. Woloska 14, 02-507 Warsaw, Poland. Tel: 48 (22) 660 8794; Fax: 48 (22) 660 8794; E-mail:

fall2004@e-mrs.org; Info: <http://www.e-mrs.org/meetings/fall2004>].

13–14 September 2004

FaME38 Joint ILL/ESRF Workshop on Engineering Applications of Neutrons and Synchrotron Radiation. Grenoble, France. [Contact: E-mail: FaME@ill.fr; Info: <http://www.ill.fr/FaME38/workshop>].

14 September 2004

Pores and Surface Area Measurement in Particle Systems. London, England, United Kingdom. Held at Imperial College. [Contact: Ron Buxton, Particle Technology Ltd., Station Yard Ind Estate, Hatton, Derbyshire DE65 5DU, United Kingdom. Tel: 44 (1283) 810091; Fax: 44 (1283) 520412; E-mail: particle@rsc.org; Info: <http://www.rsc.org/lap/rsccom/dab/ana010.htm>].

15–18 September 2004

N2M2 Second Neutrons and Numerical Methods Workshop. Grenoble, France. [Contact: E-mail: n2m2@ill.fr; Info: <http://www.ill.fr/Events/N2M2>].

21 September–2 October 2004

School of Small and Ultra-Small Angle Neutron Scattering: Structural and Dynamical Studies. Palau, Sardinia, Italy. The School of Neutron Scattering “Francesco Paolo Ricci.” [Contact: Carla Andreani; E-mail: carla.andreani@roma2.infn.it; Info: <http://www.delphina.it/orso.htm>].