Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie

Sektion für Kristallwachstum und Kristalltechnologie
Section de Croissance et Technologie des Cristaux

sc | nat

Member of
the Swiss Academy of Sciences

EPDIC 10

European Powder Diffraction Conference
Geneva, September 1 - 4, 2006

UNIVERSITÉ DE GENÈVE

Swiss Society for Crystallography

No. 67

SGK/SSCr NEWSLETTER

March 2006

SGK/SSCr Newsletter No. 67

On the Cover:

EPDIC is the only European conference completely dedicated to all aspects of the analysis of polycrystalline material by diffraction methods. Started in Munich in 1991, **EPDIC** s have rapidly become the focal point for all researchers in the field and are now regarded to be ideal places for the presentation and diffusion of new developments in powder diffraction instrumentation, analysis, and applications. **EPDIC** conferences are the place where all powder diffractionists, can meet and exchange ideas and experiences. **EPDIC-10** will be organized by the **University of Geneva** and **SGK/SSCr** and supported by **SCNAT.** It will take place in **Geneva, Sept. 1-4, 2006** (http://www.sgk-sscr.ch/EPDIC10/EPDIC10.html).

Letter from the President

It is really a pleasure how crystallography is flourishing. Life sciences are more and more operating on molecular level, materials science goes to smaller and smaller structures down to the nanometer scale. This is the scale of crystallography and structure/property-relationships are a core business of crystallography since almost a century. So, a lot of all that fashionable nano/bio stuff could be seen as crystallography. Could be but is not, not at all. Well, this really our problem and not that of politicians or academic bureaucracy.

Let us stop mourning that crystallography is not recognized as it should be. It does not matter that our nice colleagues do a lot of our core business without accepting or even knowing that they could be called crystallographers. We also did not recognize that they were doing crystallography. Today the term 'crystallography' is used synonymously with 'structure determination and description'. It does not really matter if we will be able to fill this term with a new meaning. We should not waste our time to convince the others that our meaning of crystallography is the right one. Let us better use our time to do the right crystallography. If we are at the frontiers of structural science then we will have our place in academic research and education anyway, no matter how we will be called in future.

In 2006, there is an important jubilee not only for the Swiss crystallographic community. On February 27th, we celebrate the 100th birthday of Fritz Laves (27.2.1906-12.8.1978), who was from 1954 to 1976 professor for crystallography and petrography at ETH Zurich. A detailed article on Laves' life and scientific contributions appeared in *Zeitschrift für Kristallographie* **151** (1980) 1-20, and a special issue of the same journal dedicated to Laves will appear in May this year. In recognition of his pioneering work, the recent progress in understanding intermetallic phases will be reviewed. It is now fifty years ago, when Fritz Laves presented his ideas on the factors governing the structure of metals at a seminar on the Theory of Alloy Phases during the 37th National Metal Congress and Exposition, Philadelphia, 1955 (F. Laves: Crystal structure and atomic size. In *Theory of Alloy Phases,* pp. 124-198, Cleveland, ASM 1956). He came to the conclusion that „as a consequence of these principles (space-, symmetry- and connection-principle) the stoichiometric formulae of intermetallic compounds are frequently fixed rather by the geometrical properties ... than by the formal valencies of the components". By Laves's principles some peculiarities of structures could be explained that were not covered by „the three factors considered by Hume-Rothery (a) size factor, (b) electrochemical factor, (c) valence electron concentration".

The 100th anniversary of Laves's birthday coincides with the first year of activity of the *European Network of Excellence* dedicated to the study of complex metallic alloys (*CMA*)[1]. Crystallography should play a major role in it.

Walter Steurer
President of the SSCr

[1] http://www.cma-ecnoe.org/

Annual Report of the President of the SGK/SSCr for 2005

Work of the committee:

The committee met two times in 2005; in between the committee members stayed in contact by e-mail. The committee dealt mainly with managing the society, with its relation with the ECA, prepared this annual meeting, and two international meetings held in Switzerland, the 3rd International Workshop on Crystal Growth Technology in Beatenberg in 2005, and the EPDIC-10 conference 2006 in Geneva.

Ten new members joined (Kazimierz Conder, Vladimir Dmitriev, Jozsef Donat, Deborah Gonzales Mantero, Miroslav Kobas, Philippe Kocian, Lucile Pernot, Ekaterina Pomjakushina, Jean-Philippe Rapin, Oksana Zaharko), and four individual and one collective member (Siemens Building Technologies AG) left the society during the year, so that the number of members increased to 167 (150 full, 9 students, 7 collective and 1 honorary).

In 2005 three SGK/SSCr Newsletters (64-66), and 5 IUCr. Newsletters (Vol. 12 no. 2-4, Vol. 13 no. 1-2) have been distributed to the members. Also our society web page (http://www.sgk-sscr.ch/) and membership database have regularly been updated.

The committee awarded travel grant of 650 CHF per person to Eric Germaneau (PhD student at EPF Lausanne) who presented a poster "Monte-Carlo Simulation of the Incommensurate Structure of 4,4'-Diethoxyazoxybenzene**"** and to Deborah Gonzales Mantero (PhD student at the University of Neuchâtel) who presented a poster "2-D and 3-D Metal-Organic Frameworks: A Crystal Engineering Approach" on XX Congress of the IUCr. in Florence.

Annual meeting of the SGK/SSCr:

The annual meeting 2005 of the SGK/SSCr was held at the EPF Lausanne, October 13, under the theme "Crystallography and Physics". Four lectures were invited:
- Edgar Weckert (DESY, Hamburg): *The new radiation sources, PETRA III and the European XFEL at DESY.*
- Andras Sütő (Hungarian Academy of Science, Budapest): *Ab initio structure determination by charge flipping.*
- Jean-Louis Hodeau (CNRS Grenoble): *Resonant diffraction*.
- Franz Pfeifer (PSI, Villigen): *Coherent x-ray diffraction*.

Other 3 oral and 19 poster presentations gave an overview of crystallographic research in Switzerland.
Information on the activity of the Swiss Steering Committee of the SNBL (Swiss-Norwegian Beamline) at the ESRF, Grenoble, was given during the SGK/SSCr annual meeting.

Relation with the ECA and IUCr:

ECA Council Meeting was held in Florence on the 25th and 28th August 2005. The report of the SSCr delegate, Prof. Helen Stoeckli-Evans and of the delegate for Individual Members, Prof. Hans Grimmer, is given separately.
General Assembly of the IUCr. was held in Florence on the 24th, 25th, 28th and 29th August 2005. The report of the Swiss delegates, Dr. Radovan Cerny (replaced on 24th August by Prof. Walter Steurer) and Prof. Hans Grimmer, is given separately.

Relation with the SCNAT:

Hans Grimmer represents the SGK/SSCr in the Senate and Radovan Černý in Section I of the SCNAT, which contributed in the year 2005 1000,- CHF to the travel grants for young scientists, 2000.- CHF for the organization of the annual meeting, and 1000.- CHF for our delegation to IUCr congress 2005 in Florence and to the council meeting of the ECA.
Annual Meeting of the SCNAT was held in Bern, July 14-15, under the title "Einstein today".
Meeting of the SCNAT Senate was held in Bern, Mai 13, with following conclusions important for the SSCr:

- New SCNAT president for 2007-2012 is Prof. Denis Monard, *Friedrich Miescher Institut in Basel.*
- Annual Meeting 2006 of the SCNAT will be held at the University of Zurich, October 12- 13, with a topic "Chemistry on the border with Biology and Medicine".
- Annual Meeting 2007 of the SCNAT will be held with a topic related to Mathematics.
- Reform of the SCNAT has started with following milestones:

May - November 2005	General concept, discussion within the societies.
November 2005 - May 2006	Revised concept and project of new status of the SCNAT.
May 2006 - End 2007	New organization.

International meetings in Switzerland:

The 3rd International Workshop on Crystal Growth Technology (the IWCGT-3) was be organized by H. J. Scheel, S. Uda and D. Witter from September 10 to 18, 2005, in Beatenberg, Switzerland. 38 speakers presented one-hour lectures on research and numerical simulation of crystal growth processes, crystal growth industry, crystal machining and crystal characterization. Approximately 90 crystal growers and technologists from 12 different nations, some of them with their families, attended the workshop. The detailed report is given separately.
The European Powder Diffraction Conference (EPDIC-10) will be held in Geneva, 1-4 September 2006, Uni Mail, organized by the SSCr and the University of Geneva (http://www.sgk-sscr.ch/EPDIC10/EPDIC10.html) and supported by the SCNAT.

Radovan Černý
President of the SSCr, 2005

Minutes of the General Assembly, 2005

Place: Auditoire 410, Collège Propédeutique 2, Université de Lausanne, Dorigny,
October 13, 2005, 17^{25} - 18^{15}
Presided over the meeting: R. Černý, President of the Society
Present: 19 Members and 1 Guest (Joanna Ropka)

1) The proposed **Agenda** of the meeting is accepted.
2) The **Minutes of the last General Assembly** in Neuchâtel on October 6, 2004 are accepted.
3) **Report of the President** (R. Černý)

Work of the committee

The committee met twice in 2005; in between the committee members stayed in contact by e-mail. In addition to preparing this annual meeting, the committee dealt mainly with managing the society, with its relation with the ECA, and with two international meetings held in Switzerland, the Third International Workshop on Crystal Growth Technology in Beatenberg in September 2005, and the EPDIC conference in Geneva in September 2006.

Ten new members joined (Donat Jozsef Adams, Kazimierz Conder, Vladimir Dmitriev, Deborah Gonzalez Mantero, Miroslav Kobas, Philippe Kocian, Lucile Pernot, Ekaterina Pomjakushina, Jean-Philippe Rapin, Oksana Zaharko), and four individual and one collective member (Siemens Building Technologies AG) left the society during the year, so that the number of members increased to 167 (150 full, 9 students, 7 collective and 1 honorary).

Since last year's annual meeting 3 SGK/SSCr Newsletters (64-66), and 5 IUCr Newsletters (Vol. 12 no. 2-4, Vol. 13 no. 1-2) have been distributed to the members. Also our society web page (http://www.sgk-sscr.ch/) and membership database have regularly been updated.

Relationship with the Swiss Academy of Sciences (SCNAT)

Hans Grimmer represented the SSCr in the Senate and Radovan Černý in Section I of the SCNAT, which contributed in the year 2005 1000,- CHF to the travel grants for young scientists, 2000.- CHF for the organization of the annual meeting, and 1000.- CHF for our delegation to the IUCr congress 2005 in Florence and to the council meeting of the ECA.

The meeting of the SCNAT Senate was held in Bern on May 13; the following conclusions are of importance for the SSCr:

- New SCNAT president for 2007-2012 is Prof. Denis Monard, Friedrich Miescher Institut in Basel.
- The Annual Meeting SCNAT 2005 was held in Bern, 14. - 15. July, with the title "Einstein today".
- The Annual Meeting SCNAT 2006 will be held at the University of Zurich, 12. - 13. October, with a topic
- on Chemistry at the border with Biology and Medicine.
- The Annual Meeting SCNAT 2007 will be held in Basel with a mathematical topic related to the birthday
- of Leonhard Euler in 1707.

- Reform of the SCNAT:

May - November 2005:	General concept, currently discussed within the societies.
November 2005 - May 2006:	Revised concept and project of new statutes of the SCNAT.
May 2006 - End 2007:	New organization.

4) **Report of the Treasurer** (M. Hennig)
The Accounts for 2004 were published in SGK/SSCr Newsletter 64, the report of the auditors Ch. Bärlocher and K. Schenk in Newsletter 66. The accounts for 2004 are accepted by acclamation. Credits and Debits for 2005 are presented up to October 1. Also the budget for 2006 is presented. The annual membership fees remain unchanged.

5) **Report of Section Head** (H.J. Scheel)
The head and the secretary of the section SKT/SCT being both absent, this point of the agenda has to be dropped.

6) **Report of the Section Treasurer** (K. Fromm)
The Accounts for 2004 and the report of the auditor, M. Neuburger, were published in SGK/SSCr Newsletter 64. The accounts for 2004 are accepted by the assembly.

7) **Report of the delegates to the IUCr General Assembly** (H. Grimmer/R. Černý)
H. Grimmer reports on the 20th IUCr Congress of the IUCr, which was held in Florence, August 23-31, 2005. It was attended by 2800 participants from 62 countries (¼ of them students) and by 200 registered accompanying persons; 1600 posters and 527 lectures were presented. As usual, there was a large number of attendants from Switzerland, among them a member of the Scientific Program Committee (W. Steurer), two keynote lecturers (N. Ban and L. Mc Cusker) and four (Vice-)Chairmen of Microsymposia (Ch. Bärlocher, Ch. Brönnimann, A. Oganov and G. Kostorz).

The General Assembly admitted Greece as a new member, reinstated Argentina (after paying the fees for 1998-2005) and cancelled the membership of Ukraine, which had not paid its fees since 1996. A new IUCr Commission on "Mathematical and Theoretical Crystallography" was admitted, chaired by M. Nespolo (France); 2 of its 10 members are from Switzerland (H. Flack and H. Grimmer). In addition to continuing as editor of the "Journal of Applied Crystallography", G. Kostorz (Zürich) has been nominated as Editor-in-Chief of all IUCr Journals.

Osaka (Japan) has been confirmed as venue of the 21st congress of the IUCr in 2008, and Madrid (Spain) has preliminarily been chosen as venue of the 22nd congress.

A new Executive Committee of the IUCr has been elected, consisting of:

President:	Y. Ohashi (Japan)
Vice-President:	I. Torriani (Brazil)
General Secretary and Treasurer:	S. Lidin (Sweden)
Past President:	W.L. Duax (USA)

Ordinary members: P. Colman (Australia), G.R. Desiraju (India), C. Gilmore (UK)

G. Heger (Germany), C. Lecomte (France), D. Viterbo (Italy)

8) **Report of the delegate to the ECA Council Meeting** (H. Stoeckli-Evans)**:**
The ECA council meeting was held in Florence during the 20th IUCr Congress. Hans Grimmer represented individual members and H. Stoeckli-Evans acted as representative of the SGK/SSCr. Details are given in a separate report by H. Stoeckli-Evans.

9) **Award of travel grants** (R. Černý)
The two PhD students Eric Germaneau (EPFL) and Deborah Gonzalez Mantero (University of Neuchâtel), who presented posters at the XX Congress of the IUCr in Florence, receive travel grants of 650 CHF each.

10) **International conferences in Switzerland related to crystallography** (R. Černý)
The Third International Workshop on Crystal Growth Technology (IWCGT-3) was held in Beatenberg, September 10-18, 2005. It was successful not only scientifically but also financially, so that the deficit guarantee of the SSCr is not used.
Preparations for the tenth European Powder Diffraction Conference (EPDIC-10), which will be held in Geneva on September 1-4, 2006 are well underway. Persons willing to contribute to the organization of this event are encouraged to contact R. Černý.

11) **Election of the committee and the president of the SSCr for 2006-2008** (R. Černý)
R. Černý starts by thanking the retiring committee members H. Stoeckli-Evans and H. Grimmer; H. Stoeckli-Evans thanks the retiring president R. Černý. All three receive books in recognition for their dedicated work for the SSCr.

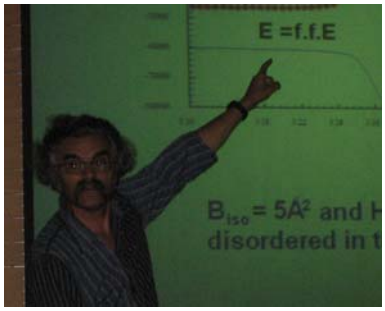
R. Černý presents the candidates for SSCr Committee members for the period 2006-2008 (cf. SGK/SSCr Newsletter 66): W. Steurer (ETHZ) as president, J. Schefer (ETHZ&PSI) as secretary, M. Hennig (Hoffmann-LaRoche), M. Schiltz (EPFL) and K.Yvon (Uni Genève) as Committee Members. Two weeks before the annual meeting Hans Scheel reported that the person whom he had proposed was not willing to succeed him as Vice-President and Section Head. R. Černý therefore proposes to prolong the mandate of H. Scheel by another year to allow for the search of a suitable successor. No other candidates are proposed by the assembly and the candidates are elected unanimously.

12) **Election of the delegate to the Senate of SCNAT** (R. Černý)
He proposes to elect, as usual, the past president, R. Černý, as delegate to the Senate of SCNAT for 2006-2008 and the acting president, W. Steurer, as his proxy. They are elected at unanimity. W. Steurer will represent the SSCr also in Section I of SCNAT.

13) **Election of the auditors** (R. Černý)
The present auditors, Ch. Bärlocher (ETHZ) and K. Schenk (EPFL) are willing to continue in the period 2006-2008 and are elected at unanimity.

14) **Varia**
There are no communications.

Villigen, October 19, 2005
Hans Grimmer, Secretary of the SSCr, 2005



Lecturers:
E. Weckert (DESY), F. Pfeifer (PSI), J.-L. Hodeau (CNRS), A. Sütő (Budapest)

Report from the ECA Council Meeting

Place: Florence on the 25th and 28th August 2005
Present: The SGK/SSCr delegate Prof. Helen Stoeckli-Evans and Prof. Hans Grimmer, delegate for individual members.
Chair: Prof. Hartmut Fuess, the ECA president

Points treated:

1) **Application for membership.**
Tunisia was admitted as a new member and Prof. Mongi Debbabi took a seat as member of the Council.
The president had invited an observer from Armenia and Dr. Bezirganyan reported briefly on the situation of crystallography in his country.

2) **ECANEWS**
The new web master, Prof. Massimo Nespolo, encouraged everyone to send him as much news as possible about events in each country and highlights from national meetings were welcome.

3) **President's report**
New members: A number of countries were being approached and they hope to encourage further contacts to bridge the gap between the North and South, especially with Africa, Middle and Eastern Europe and the Baltic States.
IUCr Newsletter – ECA: Reports on ECM-22, and the relationship with the former Soviet Union countries, has appeared and one is in preparation concerning ECM-21. National members are kindly invited to submit contributions on local meetings and schools.
SIG's: Most are working well. Their representation in the program Committee of the ECM's has to be reconsidered.
EPDIC - ECA relations: A representative of EPDIC has been appointed to take part in the council meetings of ECA and *visa-versa*.
ECA registration: Still registered at the local Chamber of Commerce in Nijmegen and the statutes are in Dutch. Ways will be sought to change this but the European Community does not seem able to cope with the legal aspects of European associations.

4) **Finances**: The financial situation is good especially if the organizers of the ECM's continue to transfer any surplus money to the ECA after the congresses. Prof Duarte will be seconded by Dr. Kuzel who will take charge of collecting the Individual Members fees. A five year fee (50 Euros) has been decided to simplify the procedure. The Councilors approved the audited accounts for 2004. Financial help, ca. 5'000 Euros, for congresses and workshops is available from the ECA. 3 meetings were supported in 2004, and 4 in 2005. Guidelines on how to apply etc. will soon be available.

5) **ECM Meetings.**
Final report was given by the organizers of ECM-22 and they were able to give back 3'800 Euros.
The conflict between ECM in Budapest and EPCIC in Prague was regretted.

ECM-23 2006. 4th – 11th August in Leuven (Belgium). Details were given by Prof. Van Meervelt and more information can be found on the web site www.ecm23.be/

ECM-24 2007. 22nd – 27th August in Marrakech (Morocco). Profs. Mokhlisse and Thalal gave a report and more information is available on the web site www.ecm24.org/

ECM 25 & 26: After various discussions and presentations by Germany/Darmstadt, UK/Edinburgh and Turkey/Istanbul it was decided that ECM-25 2009 will take place in Istanbul and that a joint ECA(ECM-26) and EPDIC meeting will take place in Darmstadt in 2010.

6) ECA – IUCr relations:

The IUCr observer Prof. Viterbo proposed a few items of mutual interest to both ECA and IUCr.

1) World Directory of Crystallographers: support and advice on how to improve the situation. Changing from the paper version to the electronic version resulted in the list of names going from 10'000 to only 6'000!

2) IUCr Newsletter: more input from national meetings and schools welcomed.

3) Basic schools on crystallography are required as many people are "doing" crystallography without any expertise!

4) Crystallographic nomenclature: A dictionary of crystallographic terms is being compiled, and help and advice in translation is needed.

Lausanne 13th October 2005 Prof. Helen Stoeckli-Evans (Neuchâtel)

SGK/SSCr Financial Report 2005

UBS Account

Status 1.1.2005	**12'876.91**
Credits:	
Membership dues (120 members)	4'838.00
ECA dues (5 members)	75.00
SANW reimbursement for Annual Meeting 2005	1'532.45
SANW reimbursement for ECA delegate 2005	1'000.00
SANW funds for young scientists travel grants	1'000.00
Refund of withholding taxes	309.54
Interest	69.95
Total Income	**8'824.94**
Debits:	
Sekt. Kristallwachstum (2005)	600.00
Div. Costs (gifts)	319.80
Membership dues to SANW (166 members)	1'162.00
Annual meeting 2005 (Neuchâtel)	2'594.35
Travel Grants to Young Scientists	1'300.00
Travel Grant for ECA delegate (2005)	1'050.00
ECA dues (6 members)	204.85
Cash withdrawal	840.00
Postal charges	54.05
Bank charges	102.30
Withholding Tax	24.50
Total Expenses	**8'251.85**
Income – Expenses	**573.09**
Starting Balance + Income – Expenses	**13,450.00**
UBS Balance 1.1.2006	**13,450.00**

Cash on Hand - 2005
(as of 1.1.2006)

Status 1.1.2005	**524.80**
Credits:	
Drawing from UBS account	840.00
Membership fee R. Pöttgen 2004+2005	120.00
Membership fee H. Huppertz 2005	30.00
Total Income	**990.00**
Debits:	
Travel Expenses, Executive Committee 14.1.2005 and 3.6.2005, Bern	286.00
Fee for internet page of SGK	35.00
Annual meeting 2004, Reimbursement	840.00
Total Expenses	**1161.00**
Income – Expenses	**-171.00**
Starting Balance + Income – Expenses	**353.80**
Cash on Hand 1.1.2006	**353.80**

Status of other Accounts
(as of 1.1.06)

CS (savings account)

Status 1.1.05	**16'525.65**
Transfer from Post account	371.77
Interest (0.875%)	155.35
Withholding Tax (35%)	-54.37
Balance 31.12.05	**16'998.40**

Post Account

Status 1.1.05	369.62
Interest (1.0%)	3.30
Withholding Tax (35%)	-1.15
Transfer to CS 21.11.05	-371.77
Balance 21.11.05	**0.00**

2006 SGK/SSCr Membership Fee

I would like to take the opportunity to thank all the members for promptly paying their membership fees. These will remain unchanged for 2006:

full member	30	CHF / year
student member	10	CHF / year
institutional member	130	CHF / year

- Please pay the fee for 2006 by the end of March **by bank transfer** to the UBS account: IBAN CH39 0027 9279 C029 1110 0
  (old system: BLZ 279, account No. C0291110.0)
  Please add CHF 1.20 if paid at a PTT counter (PC 80-2-2, UBS Zürich, Account No. 230-C0291110.0)
- Several of the fees for 2005 and even a few for 2004 are still missing. A letter indicating the total amount due has been included with this newsletter to the members concerned.
- **Institutional members will be mailed a special invoice.**
- Members of the ECA can also use this opportunity to pay their annual ECA dues (EUR 10.- = CHF 15.-). This way we can make a single foreign bank transfer to the ECA and avoid having each member make an individual one (typically CHF 15.- each). Please note on your payment whether you are also including your ECA membership fees.

Thank you for your cooperation.

Your treasurer,
Michael Hennig

Travel Grants for Young SGK/SSCr Members

The committee will award the grants according to the following rules:

- Preference is given to PhD students
- Proof has to be given that there are no grants available covering the expenses
- A supporting letter by the supervisor of the applicant is necessary

If you whish to apply for a travel grant, please send the above mentioned documents to the President of the SGK/SSCr before October 1, 2006.

News of Members

We welcome the following new members of the SGK/SSCr:

M. Jean-Noël Chotard (Laboratoire de Cristallographie, Université de Genève, 24, Quai Ernest-Ansermet, CH-1211 Genève 4)

Dr. Miroslav Kobas
(Detector Group, Swiss Light Source, OFLB-006, CH-5232 Villigen PSI)

Dr. Jean-Philippe Rapin (Laboratoire de Cristallographie, Université de Genève, 24, Quai Ernest-Ansermet, CH-1211 Genève 4)

Dr. Marisa Medarde (Labor für Entwicklung und Methoden, Festkörperforschung mit Neutronen und Myonen, WHGA-242, CH-5232 Villigen PSI)

Dr. Vladimir Pomjakushin (Laboratorium für Neutronenstreuung, ETH Zürich und Paul Scherrer Institut, WHGA-133, CH-5232 Villigen PSI)

Dr. Olga Smirnova (Laboratoire de Cristallographie, Université de Genève, 24, Quai Ernest-Ansermet, CH-1211 Genève 4)

Awards Received by SGK/SSCr-Members

Prof. Dr. A. Furrer: 2005 Walter Hälg Prize
(http://sgn.web.psi.ch/sgn/prwh_2005.pdf)

Professor Albert Furrer, former head of the Laboratory for Neutron Scattering ETHZ&PSI, was honoured by this prize in recognition of the important role he played in developing new and interesting magnetic materials using neutron scattering methods. He received the prize together with his long-time collaborator, Prof. H.-U. Güdel, from the University of Berne. The prize was awarded by ENSA at the ICNS2005 meeting in Sidney/Australia.

Awards Open for Application

Prix A.F. Schläfli	**Link/Deadline**
Der **Prix A.F. Schläfli** zeichnet eine **wissenschaftliche Arbeit von hoher Qualität** aus, die **von nicht habilitierten Schweizer Nachwuchsforschenden** realisiert wurde.	http://www.scnat.ch/d/Preise/Prix_Schlaefli/ 31.3.2006

In Memoriam

Prof. Hans H. Günthard has died on February 2, 2006 in the age of 90. He founded the Laboratory for Physical Chemistry of ETH. Professor Günthard was a member of our society since its foundation in 1968.

Summary of the Workshop on Crystal Growth Technology, IWCGT-03

Beatenberg, Switzerland, September 10-18, 2005

The 3rd International Workshop on Crystal Growth Technology (IWCTG-03) was held in Beatenberg, Switzerland. 38 Speakers lectured on research and numerical simulation of crystal growth processes, crystals growth processes, crystal growth industry, crystal machining and crystal characterizations. The successful workshop ended with a panel discussion on the future of crystal growth and an award to the three best lecturers of the conference. As a result of the well organized conference, Hans J. Scheel was put into charge to organize the next workshop, **IWCGT-04**, to be held at the same place in **Beatenberg** from **May 18-25, 2008**. Congratulation to the organizers! (A full report is printed in the IUCr newsletter **13**,3 (2005), page 26-28 has been included in the last mailing).

Annual Meeting 2006

The annual meeting 2006 will be held in Bern on the occasion of the retirement of Prof. H.-B. Bürgi, Laboratory for Chemical and Mineralogical Crystallography. An announcement will follow. It will start **October 20, 2006 at 9^{45}** at the *Departement für Chemie und Biochemie*, **Freiestrasse 3, 3012 Bern**.
Present Title of the Symposia :
Expanding the boundaries of crystallography with topics on

crystallography
- in the gas phase
- on surfaces
- in picoseconds
- with electrons

A poster session will take place during the lunch break. The authors of the best four posters submitted before the meeting will be invited to give five-minute 'appetizer-presentations' immediately before the lunch break.
More information will be available closer to the date of the meeting from http://www.krist.unibe.ch/events.html.

Godfathers for Maturity Work

Maturity work is an ideal starting point to motivate young people for a career in science, as they are getting a first insight view. However, support from our side is essential.

Are you interested to be a godfather of such a work? Please have a look on the web site **www.maturitywork.ch** or contact Annabelle Cuttelod (031 310 4026, cuttelod@scnat.ch) for further information.

News from SNBL

The Swiss-Norwegian Beamlines at the ESRF have recently celebrated 10 years of user operation (1995 – 2005). During this period, almost 500 refereed publications have appeared in the scientific literature using data from SNBL, and new papers are now appearing at a rate of about 70 per annum. Although the beamline profits from the existence of a very active community of well-established users, we are also keen to encourage new user groups from Switzerland and Norway to come to the beamline and to explore the many possibilities offered by the various techniques which are available at SNBL. These techniques include high resolution powder diffraction, EXAFS, single crystal diffraction and protein crystallography. The emphasis has shifted over the years more and more towards materials science and related projects, but bio-crystallography continues to contribute about 10% of the scientific output of SNBL.

We have now begun a very active program of upgrading and extending the technical facilities which we provide as part of the SNBL equipment pool. Recent acquisitions include two new Helium flow cryostats used either for combined powder/EXAFS experiments or for single crystal diffraction. These devices will allow us to cover a temperature range from 4K to 400K. In combination with our existing heaters and furnaces, we can extend the high temperature range accessible at SNBL up to about 1300K. The new cryostats are designed to allow simultaneous access for the synchrotron beam, and an external light source for investigating photo-excited states. In addition, the x-ray transmission and fluorescence signal can be monitored and a Raman spectrum measured. A series of combined test experiments (diffraction-Raman and/or EXAFS) at non-ambient conditions (5-1000K) have recently been performed in order to demonstrate the versatility of this new equipment in fields ranging from zeolite and metal-organic framework chemistry to electronic properties of oxides and mixed valence polycyanides.

In addition to the ancillary equipment mentioned above, we are investing a substantial amount of resources in a major refurbishment of the X-ray optics for powder and EXAFS experiments. The existing channel-cut monochromator will be replaced by a double-crystal monochromator with feed-back control allowing either Si(111) or Si(311) crystal orientations to be selected. We have also received delivery of new x-ray mirrors for harmonic rejection, consisting of silicon substrates with different strips of metal coating. These mirrors are longer, and have a better surface quality than our previous optical components. In addition, we have purchased jointly with the EPFL a new detector which is a convenient and compact device for fluorescence EXAFS measurements in either experimental hutch. Finally, we are pleased to announce that we will shortly have achieved a staff level of three full-time scientists on each of the two Swiss-Norwegian beamlines, in addition to our existing technical and secretarial support. We are very grateful to the various organizations in Norway and Switzerland that have contributed generously to allow us to reach this staff level. We now believe that we can provide both a good service to our users and have sufficient manpower to be able to sustain a high quality in-house research program.

The management of our governing body (the SNX Foundation) has signed in 2005 a collaboration agreement with the steering committee of the Dutch-Belgian beamline consortium (DUBBLE). This agreement allows SNBL to share resources, manpower, equipment and infrastructure facilities with the DUBBLE beamline at the ESRF. In addition, we now have a mechanism to exchange beamtime between our two Collaborating Research Groups (CRGs). This is the first formal collaboration agreement to be signed between CRGs, and has been warmly welcomed by the directors of the ESRF and by our funding agencies. We recently took advantage of this agreement in order to borrow a MarResearch CCD detector from DUBBLE to replace our standard Mar345 image plate for a series of single crystal experiments where rapid data collection was an advantage. Although the CCD is only half the size of the image plate, the readout of the CCD is more than an order of magnitude faster than the image plate. This allowed, for example, our protein crystallography groups from Oslo and Tromso to double their data throughput during their last beamtime. In return, some Belgian PX users will have access to SNBL. The agreement also includes the provision of beamtime for R&D projects of mutual interest, and we will therefore be taking advantage of some in-house beamtime on the SAXS/WAXS set-up at DUBBLE for a project to characterize protein crystallization mechanisms using small angle scattering.

We will conclude this report with some examples of current scientific activities carried out by our users. We very much encourage also new groups to come to SNBL and to evaluate for themselves the technical possibilities offered by SNBL for their projects. Please visit our web site (http://www.esrf.fr/exp_facilities/BM1A/index.htm) and feel free to contact us for further information.

Vladimir Dmitriev
Phil Pattison

Examples of Scientific Activities at SNBL

The crystal structure of tyrolite mineral

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To be published in American Mineralogist (2006)

Copper arsenates are common minerals in oxidation zones of the sulfide ore deposits. There are more than 70 different copper arsenate mineral species reported so far. The limited stability of these natural phases is largely responsible for the release of As into the biosphere. Structural investigations of secondary As-bearing phases may therefore help to elucidate mechanisms of transportation and accumulation of As under natural conditions. Tyrolite, a complex copper arsenate carbonate hydrate, was first described by Haidinger in 1845 from Schwaz-Brixlegg, Tyrol, Austria (Figure 1). Since that time, tyrolite has been found in more than 128 localities all over the world. The chemical composition $CaCu_5(AsO_4)_2(CO_3)(OH)_4.6H_2O$ and orthorhombic space group (Pmma) have been assigned to tyrolite in 1956. In 1990 a monoclinic polymorph of tyrolite, called clynotyrolite, has been discovered in

China. Crystal structures of both tyrolite and 'clinotyrolite' have been unknown till now, primarily due to the poor quality of the crystals.

We have now solved the crystal structure of these minerals using the combination of modern area detector technologies and high-intensity synchrotron radiation available at the Swiss-Norwegian Beamline (BM1A), together with a tiny, carefully selected single crystal fragment about 50 microns in size. The crystal structure (Figure 2) is based upon complex slabs consisting of Cu, As, and Ca coordination polyhedra. The slabs are about 26 Å = 2.6 nm thick and thus can be considered as nanolayers. In tyrolites, a two-dimensional nanosized substructure of transition metal ions (Cu^{2+}) is sandwiched between the layers of dielectric Ca^{2+} cations and H_2O molecules. This feature of the structure of tyrolite is very unusual and has not been previously observed in oxysalt minerals. The nanometer scale of the layer structures containing magnetic Cu^{2+} cations, combined with the weak hydrogen bonds which link the layers together, makes tyrolite attractive for material science investigations.

Figure 1: Tyrolite mineral

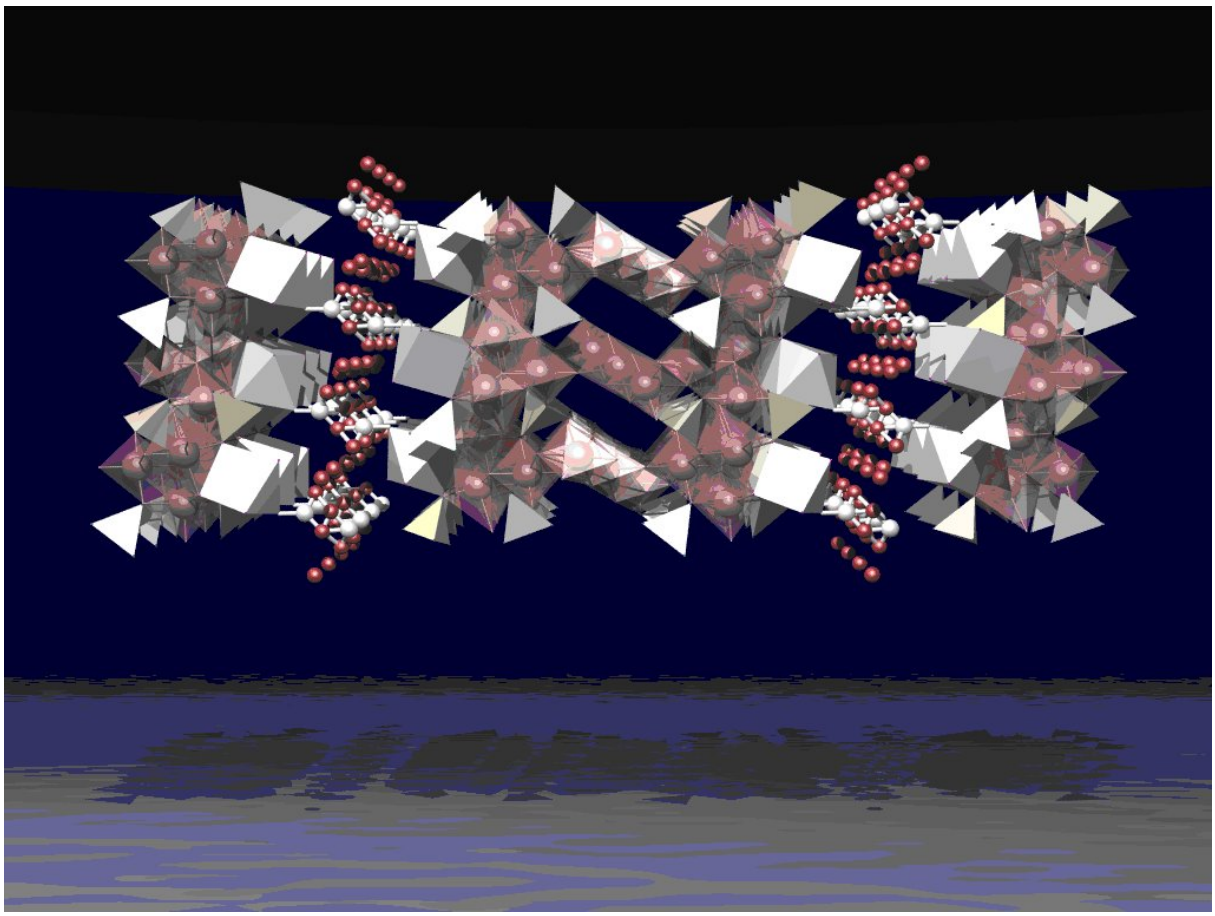

Figure 2: Tyrolite crystal structure

Synthesis and structure of Mu-33, a new layered aluminophosphate.

Marichal,C., Chezeau, J.M., Roux, M., Patarin, J., Jorda, J.L., McCusker, L.B., Baerlocher, C. and Pattison, P.
Microporous and Mesoporous Materials, **90** (2006) 5-15

Although the use of high resolution powder diffraction techniques for the structure solution of zeolites and related microporous materials has enjoyed considerable success, sometimes the complexity of the crystal structure can present serious challenges to even the best quality powder data. However, if the powder sample consists of a collection of very small single crystals, then the analysis of one of these tiny crystallites may provide the route to a successful structure solution. In the case of Mu-33, a new layered aluminophosphate, the crystals in the sample appeared to be quite large in two dimensions but unfortunately very thin indeed (ca. 5μm) in the other dimension (as seen in Fig 3).

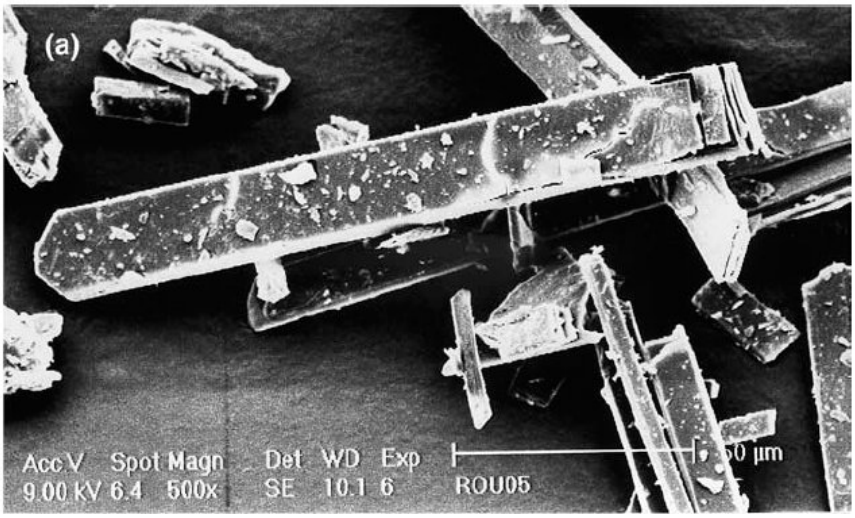

Figure 3: Crystals of the lamellar aluminophosphate Mu-33.

Although too thin for single crystal data collection in the home laboratory, diffraction data from a microcrystal of dimensions 200 x 25 x 5 μm^3 were measured on station BM1A of the Swiss-Norwegian Beamlines. These data were of sufficient quality to allow the structure to be solved, but structure refinement proved to be difficult. Therefore high resolution powder diffraction data were collected using the powder diffractometer on station BM1B of SNBL.

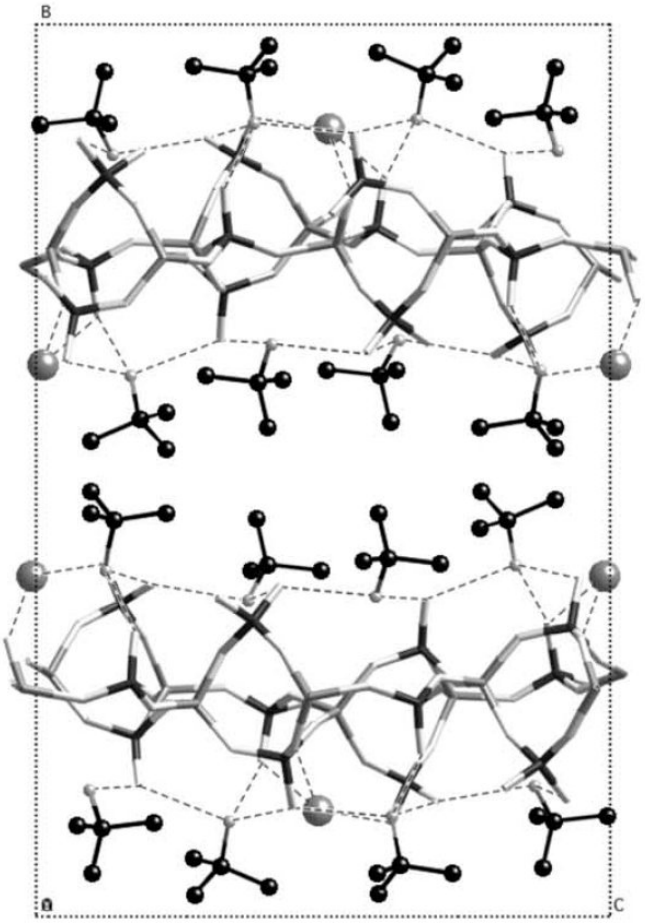

Figure 4: The crystal structure of Mu-33

The complete structure, consisting of aluminophosphate layers, 4 independent tert-butylamine species and one water molecule is shown in Fig. 4. Although the structure of this new layered material could be solved from single-crystal synchrotron data collected on a microcrystal, it is interesting that high resolution synchrotron powder data were required for a satisfactory refinement of the structure. This result illustrates nicely the complementary nature of the two techniques, and shows how it can be helpful to have both of these techniques available at SNBL.

Application of the Charge-Flipping Algorithm to the Solution of Modulated Crystal Structures

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Introduction

The algorithm named *charge flipping* [1] is an iterative algorithm for *ab initio* reconstructions of the electron density from x-ray diffraction data. It was originally thought to be a mere toy, interesting for its simplicity, but not likely to be a widely applied structure solution method. However, the algorithm was soon used to solve a first real structure [2] and it was also very early recognized as a powerful tool for structure solution of aperiodic crystal structures using the superspace approach [3]. The applicability of the algorithm to modulated structures represents an important breakthrough in this field. This is because the standard procedure of solving modulated structures included two steps: first the average, periodic structure must be solved, and only then the modulation can be reconstructed. Especially the first step is highly non-trivial for structures with strong modulation. Contrary to the standard procedure, charge flipping reconstructs the electron density directly in superspace without the need to determine first the average structure.

Operation of the algorithm

The algorithm has been described in detail in [1] and its generalization towards superspace is described in [3]. Its basic operation is schematically illustrated in Fig. 1. The electron density is described on a *d*-dimensional grid, where *d* is 3 for the standard periodic structures and higher (typically 4) for modulated structures. The structure solution by charge flipping proceeds in iterative cycles. The iteration is initialized by assigning random phases to the experimental structure amplitudes. From this trial solution an electron density is calculated by inverse Fourier transform. This electron density is modified in such a way, that all grid points with density below a certain positive threshold δ are multiplied by -1 (flipped). New temporary structure factors are calculated by Fourier transform of this modified density. The phases of these temporary structure factors are combined with the experimental amplitudes and such a set of structure

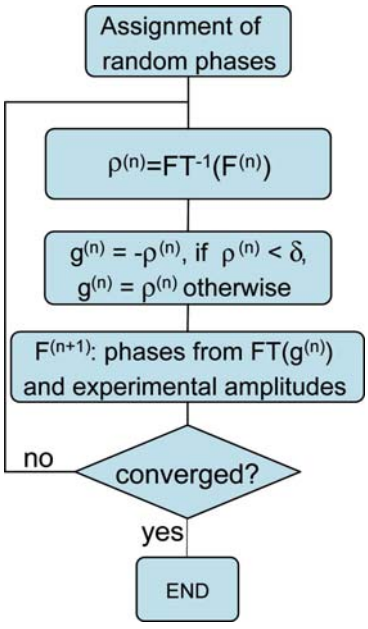

Figure 1: Schematic flowchart of the operation of the charge-flipping algorithm. FT stands for Fourier transform.

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factors enters the next cycle of iteration. δ is the only parameter of the whole algorithm.

A modification of the algorithm has been developed [4] that improves the probability of convergence by a special handling of the weak reflections. If a reflection is considered weak, the calculated amplitude of its temporary structure factor is retained, and its phase is shifted by $\pi/2$. This induces an additional perturbation in the phase space and leads to an improved performance of the algorithm.

Applications

The usability of the algorithm for structure solution of aperiodic structures was established by testing it on several experimental datasets of modulated structures ranging from simple inorganic structures with small modulation to complex organic structures with modulations exceeding 1Å. A selection of the tested structures is given in Table 1.

The structure of quininium (R)-mandelate deserves a special attention. This structure exhibits extreme modulations, which prevented the solution of the average structure by standard methods. The structure was solved with difficulties in an 18-fold superstructure approximation, which contains 1260 atoms in the unit cell [5]. The complexity of the structure is underlined by the fact that the early attempts to solve this structure by charge flipping failed. However, the improved algorithm with the special handling of weak could solve the structure immediately and without problems. Later thorough tests showed that even the original version of the algorithm is capable of solving the structure, albeit with a relatively low success rate.

Apart from solving all test structures, for which the structure solutions have been known, charge flipping has been already successfully used to solve unknown modulated structures of 2-phenylbenzimidazole [6] and chromium(II)-diphosphate [7].

Conclusions

Charge flipping is a powerful tool for structure solution of aperiodic structures. Just recently its ability to solve the quasicrystal structures has been demonstrated [8]. The fact that the modulated structures can be solved directly in superspace without the intermediate step of solving the average structure is the major advantage of charge flipping in comparison to other structure solution methods for aperiodic structures. Moreover, the method is still in its infancy and improvements of its performance can be expected in future.

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Table 1: Overview of some of the structures used for testing the charge-flipping algorithm with experimental data of modulated structures. V_{UC} represents the volume of the unit cell, "atoms" is the number of non-hydrogen atoms in a primitive unit cell.

structure name	**symmetry**	**composition**	**V_{UC}**	**atoms**
tantalum germanium telluride	Pnma(00γ)s00	$TaGe_{0.354}Te_2$	347.3	16
Lanthanum niobium sulphide	F'm2m(α00)00s	$(LaS)_{1.14}NbS_2$	439.9	5.32
4,4'-azoxyphenetole	I2(α0γ)0	$C_{16}H_{18}N_2O_3$	1457.0	42
Quininium (R)-mandelate	P21(α0γ)0	$C_{20}H_{25}N_2O_2^+ \cdot C_8H_7O_3^-$	1214.6	70
tetraphenylphosphonium hexa- bromotellurate-(IV) bis{dibromoselenate(I)}	C2/m(α0γ)0s	$[(C_6H_5)_4P]_2$ $[TeBr_6(Se_2Br_2)_2]$	2913.9	130
hexamethylenetetramine sebacate	P21(α0γ)0	$N_4(CH_2)_6 \cdot (CH_2)_8(COOH)_2$	942.1	48
hexamethylenetetramine resorcinol	I'mcm(0β0)s0s	$N_4(CH_2)_6 \cdot C_6H_4(OH)_2$	1232.4	32
$Ce_{13}Cd_{58}$	Amma(00γ)s00	$Ce_{13}Cd_{58}$	6692.3	77

Call for Proposals

Beside normal proposals, most facilities allow urgent beam time requests. Please check directly with the facility.

Facility	Deadline(s)	Link
SLS: Swiss Light Source		
All except PX lines	March 15, Nov. 15	user.web.psi.ch
Protein beam lines (PX)	Feb. 15, June 15, Oct. 15	user.web.psi.ch
SINQ: Swiss Spallation Neutron Source		
All instruments except irradiation	May 15, Nov. 15	user.web.psi.ch
SμS: Swiss Muon Source		
All instruments	Dec. 5	user.web.psi.ch
ESRF: European Synchrotron		
All instruments, long term proposals	Jan. 15	www.esrf.fr
All instruments, short term proposals	March 1, Sept. 1	www.esrf.fr
SNBL: Swiss Norwegian Beam Line		
	March 1, Sept. 1	www.esrf.fr/ exp_facilities/BM1A
ILL: Institut Laue Langevin		
All Instruments	Sept. 19, 2006	www.ill.fr

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Calendar of Forthcoming Meetings

Date	Location	Meeting / Link	Abstract Deadline
2006			
March 13-24	Jülich Germany	10th Laboratory Course: Neutron Scattering http://www.fz-juelich.de/iff/wns_lab06	expired
April 3-6	Freiburg Germany	14th Annual Meeting, German Crystallographic Society http://opal.kristall.uni-frankfurt.de/DGK	expired
May 10	Villigen CH	8th SINQ User Meeting http://sinq.web.psi.ch/sinq/usmeet_8/meet8.html	open
June 9-18	Erice Italy	The Structure and Function of Larger Molecular Assemblies, http://www.crystalerice.org/2006.htm	expired
April 27-29	Grenoble France	ILL Millenium Symposium and European Users Meeting, http://vitraill.ill.fr/symposium/welcome.jsp	20. March 2006
June 18-22	St. Charles USA	ACNS 2006 American Soc. Neutron Scattering http://www.acns2006.anl.gov	20. March 2006
July 22-27	Honolulu USA	ACA, American Crystallographic Association http://www.xray.chem.ufl.edu/aca2006	1. March, 2006
Aug. 4-6	Leuven Belgium	Satellite Conference of ECM-23 on "Mathematical and Theoretical Crystallography" http://www.lcm3b.uhp-nancy.fr/mathcryst/leuven2006.htm	
Aug. 6-11	Leuven Belgium	ECM 23 European Crystallographic Meeting http://www.ecm23.be	1. March 2006
Aug. 19-26	Zuoz CH	5th PSI Summer School on Condensed Matter Neutrons, X-rays and Muons for Nanostructures http://num.web.psi.ch/zuoz2006	to be announced
Aug. 27 - Sept. 2	Siena Italy	IUCr School on Basic Crystallography http://www.iucr.org/iucrtop/comm/cteach/siena2006/	30. June 2006
Aug. 28 - Sept. 2	Nancy France	Summer School: Analyse structurale par diffraction des rayon X, cristallographie sous perturbation	
Sept 1-4	Geneva CH	EPDIC 10 : European Powder Diffraction Conference http://www.sgk-sscr.ch/EPDIC10/EPDIC10.html	1. April 2006
Sept. 11-13	Bristol GB	EMPG XI: mineralogy, petrology and geochemistry http://www.empg2006.org	1. June 2006
Sept. 28-29	Villigen CH	7th SLS User Meeting http://sls.web.psi.ch/view.php/users/affairs/umeetings/Umee2006/index.html	to be announced
Oct. 4-6	Hamburg Germany	Synchrotronstrahlung, Neutronen und Ionenstrahlen an Grossgeräten 2006, http://www.sni2006.de	15. May 2006
Oct. 20	Bern CH	SKG/SCCR annual meeting, Freiestr. 3 http://www.sgk-sscr.ch	to be announced
2007			
Aug. 22-27	Marrakech Morocco	ECM-24: European Crystallographic Meeting http://www.ecm24.org.	to be announced
June 7-17	Erice Italy	Engineering of Crystalline Materials Properties http://www.crystalerice.org/2007.htm	to be announced
June 25-29	Lund Sweden	4th European Conference on Neutron Scattering http://www.ecns2007.org	to be announced
2008			
May	Gargnano Italy	Summer School on Mathematical and Theoretical Crystallography, http://www.lcm3b.uhp-nancy.fr/mathcryst/gargnano2008.htm	to be announced
May 18-25	Beatenberg CH	IWCGT-4 Fourth International Workshop on Crystal Growth Technology http://www.beatenberg.ch/IWCGT-4	to be announced

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