

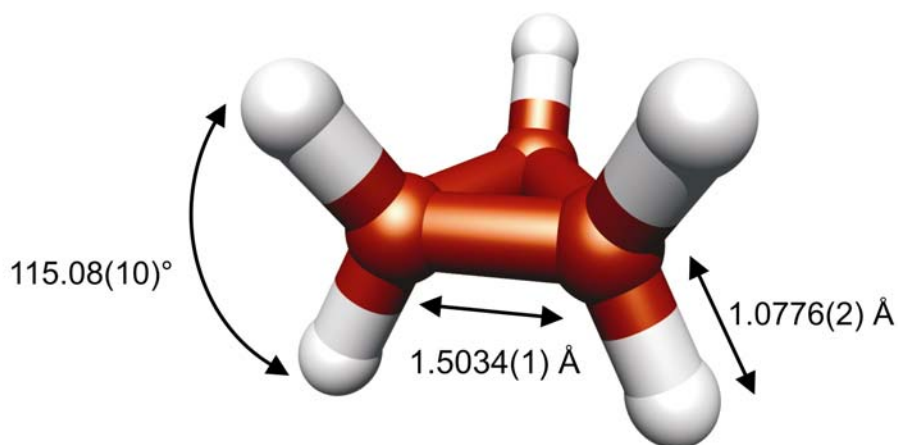
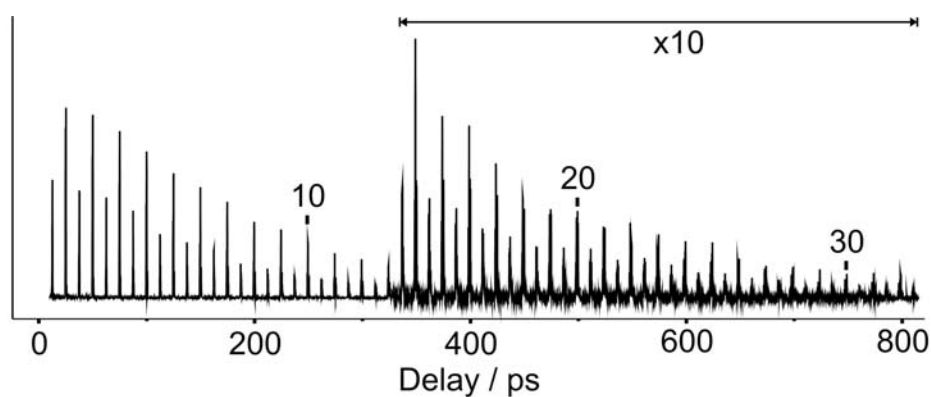


Schweizerische Gesellschaft für Kristallographie
Société Suisse de Cristallographie
Swiss Society for Crystallography

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

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The Structure of Cyclopropane: A Challenge for Crystallographers?

SGK/SSCr NEWSLETTER

with program and abstracts of the **2006 Annual Meeting** in Berne, Oct. 20
and invitation/agenda of the **2006 General Assembly**

No. 69

September 2006

On the Cover:

The rotational constants of cyclopropane, and in general of molecules that exhibit no permanent dipole moment, are not accessible by standard microwave spectroscopy. High resolution femtosecond degenerate four-wave mixing is based on a rotational Raman process and yields molecular constants with microwave accuracy and is applicable to nonpolar molecules. The precise determination of the rotational and centrifugal constants in combination with high level *ab initio* calculations results in highly accurate structures [1] of the molecules under investigation.

Hans M. Frey [hans-martin.frey@iac.unibe.ch] et al., University of Bern.

[1] D. S. Kummli, H. M. Frey, M. Keller and S. Leutwyler,
J. Chem. Phys. **123**, 54308 (2005)

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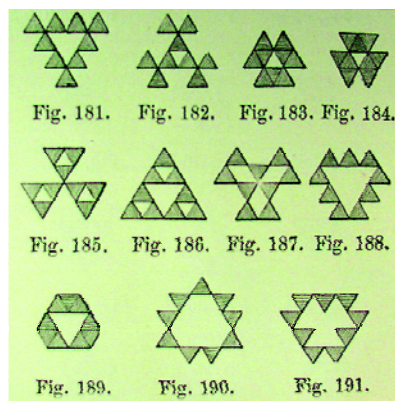
Mobile phone + crystallography = new learning concept?

By Ivan Orlov (ivan.orlov@epfl.ch)

Presented on 23 European Crystallographic Meeting, Belgium

Based on publication in J. Appl. Cryst. (2006). 39, 595-597

The first Kindergarten was created in 1837 by the German crystallographer Friedrich Fröbel. Materials provided to kindergarteners were of course inspired by his passion towards science. The first educational toys, popularly known as Fröbel Gifts, included brightly colored geometric blocks, sticks and paper tiles which could be assembled in various combinations to form two- or three dimensional compositions. The tools were designed to provide intuitive sense of symmetry - including distinction between 2-, 3- and 4-fold rotation axes and even the idea that symmetry might increase as result of object spinning. Thus symmetry exercises and lattice constructions were the primary occupations of millions of children in the first several kindergarten generations in Europe¹. Quoting Fröbel who underlined the 'importance of free play and self-directed activities' in the learning process, one might say that the Gifts were the first platform to learn crystallography while playing a game.



Left: Illustration from 'Practical Guide to Kindergartners', 1910 [2]

Right: Any of the 17 planar groups can be decorated on the phone screen

¹ There is a suggestion that exposure of many girls to crystallography before traditional separated schooling could explain the great proportion of women among the pioneers in X-ray crystallography in the beginning of 20th century [1].



Since a few years, the interactive computer applets caused another breakthrough in crystallography learning by turning self-study to more visual, personal and enjoyable task. Many crystallographers appreciate the online teaching aids created by Chapuis & Hardaker [3] and Weber [4]. The efficiency of Web-crystallography has been largely confirmed during the recent years.

What will be the next learning platform?

According to the Federation of American Scientists, more than 60% of college students are regular mobile game players. This activity is generally considered as a distraction in student's lives, moving their attention away from education to activities commonly seen as inappropriate for their personal development.

We believe that this trend brings quite opposite - an excellent opportunity to improve scientific education by delivering learning content through mobile devices and games. Gaming provide a number of interactions

which develop important skills in the player and also inspires motivation and interest which are indispensable for acquiring new knowledge. Nowadays, when science has an 'image problem' and number of students in natural sciences drops, we shall take the opportunity to use mobile digital media to illustrate the concepts, which are a priori perceived as difficult. This concerns especially physics and chemistry, which handle theory and numerical information, which might be easily formalized.

To launch the initiative, the first mobile phone application for crystallography training - Escher Mobile - is now available at <http://escher.epfl.ch/mobile/>. Designed to illustrate one of the basic concepts - planar symmetry - it enables to decorate the plane with one of the 17 two-dimensional planar groups by various symmetric and asymmetric objects.

The design starts from the selection of a specific group. For each group there is an additional information available - group properties, multiplicity and symmetry elements. Once selected, the unit cell is outlined on the screen along with its asymmetric unit. After picking up a drawing tool the student can design a pattern by drawing or displacing objects on the screen. Any move changes the pattern instantly, providing the ground to observe site symmetries, multiplicity and special positions

associated with a specific group. The resulting pattern can be automatically uploaded to the Escher Web Gallery exhibition or shared by e-mail.²

Currently the crystallographic community is addressing the problem of how to teach students on a worldwide scale, providing the state-of-the art training available to everybody in any part of the globe. We believe that one way of doing that - and interesting adolescents in science - would be a set of learning games devoted to crystallography. The challenge however will not be the development of such software but to use the mobile technologies to transform education into an integral part of daily life to the point where it is no longer recognized as education at all.

After all, as Fröbel declared, 'Play is the engine that drives true learning'.

- [1] B. Kahr, *Cryst. Growth Des.* **2004**, 4, 3-9.
- [2] Wiebé, E. Golden Jubilee Edition. *Paradise of Childhood: A Practical Guide to Kindergartners*; Milton Bradley: Springfield, MA, 1910.
- [3] Chapuis, G. & Hardaker, W. (1999). *J. Appl. Cryst.* **32**, 1164-1168.
- [4] Weber, S. (1999). *J. Appl. Cryst.* 32, 375.

² Escher Mobile is compatible with most of the Java (MIDP 2.0)-enabled mobile phones. Running the program requires no special phone settings except for submitting or emailing images which require WAP service available.

Neuer Schub für die Europäische Forschung

By Stefan Müller (stefan.mueller@euresearch.ch)

National Contact Person NanoMatPro/Energy/Financial & Legal
www.euresearch.ch

Neuer Schub für die Europäische Forschung

Einleitung

Forscher/innen aus Unternehmen, den ETHs, den Eidgenössischen Forschungsinstituten, den Universitäten und Fachhochschulen beteiligen sich bereits seit 1992 aktiv und sehr erfolgreich an den europäischen Forschungsrahmenprogrammen (Framework Programmes, FP). Seit 2004 nimmt die Schweiz als assoziiertes Land am Rahmenprogramm teil und will auch im 7. FP, das voraussichtlich Ende 2006 startet, als gleichberechtigte Partnerin ihre exzellenten Forschungsressourcen für die Europäische Zusammenarbeit einbringen. FP7 wird bis 2013 das Hauptinstrument der Forschungsförderung der Europäischen Union sein und mit einer deutlichen Budgetsteigerung (Budget ca. 53 Milliarden € inkl. Euratom) der europäischen Forschung mehr Schub verleihen.

FP7 Struktur

FP7 zeichnet sich zum einen durch ein hohes Mass an Kontinuität gegenüber FP6 aus. Es enthält aber auch neue Impulse für Grundlagenforschung und Innovation.

FP7 wird sich nach dem Kommissionsvorschlag in die **vier spezifischen Programme** "Cooperation", "Ideas", "People" und "Capacities" gliedern:

- **Cooperation** – Forschungsprojekte im Europäischen Verbund
Dieses Programm beinhaltet folgende neun Themenbereiche, für die die Europäische Kommission spezifische Ausschreibungen lancieren wird:
 - Health
 - Food, agriculture and biotechnology
 - Information and communication technologies
 - Nanosciences, Nanotechnologies, Materials and new Production Technologies
 - Energy
 - Environment and Climate Change
 - Transport and Aeronautics
 - Socio-economic sciences and the humanities
 - Space and Security Research
 - Euratom

Gefördert wird die gesamte Palette der schon in FP6 eingeführten Projektarten: von Forschungs- und Entwicklungsprojekten, über Netzwerke bis hin zur Koordinierung von nationalen Forschungsprogrammen.

- **Ideas** – Grundlagenforschung einzelner Teams
Ein eigenständiger Forschungsrat, ein „Europäischer Nationalfonds“ sozusagen, wird eingerichtet, um die von den Forschenden angeregte „Forschung an den Grenzen des Wissens“ zu unterstützen. Es werden alle wissenschaftlichen und technologischen Fachbereiche, einschließlich der Ingenieurwissenschaften, der Wirtschaft- und Sozialwissenschaften und der Geisteswissenschaften gefördert. Projekte können von einzelnen Forschenden eingegeben werden. Einziges Selektionskriterium ist wissenschaftliche Exzellenz.

Der Scientific Council (ScC) des Europäischen Forschungsrates (ERC) hat weitere Details zur Struktur der Peer Review-Gruppen für die Nachwuchsförderlinie bekannt gegeben. Mit einem Budget von 300-350 Millionen Euro sollen jährlich bis zu 200 „Starting Independent Researcher Grants“ (SIRG) für jeweils maximal fünf Jahre vergeben werden. Die erste Ausschreibung soll spätestens Anfang 2007, eventuell sogar Ende 2006, erfolgen, so dass Ende 2007 die ersten Grants vergeben werden können. SIRG ist offen für Nachwuchswissenschaftler, deren Promotion nicht länger als 10 Jahre zurückliegt. Unabhängig von der Herkunft kann sich jedermann bewerben, solange die Gruppe beabsichtigt das Projekt innerhalb der EU bzw. einem assoziierten Staat durchzuführen. Das elektronische Zwei-Stufen-Antragsverfahren (kurzer Vorantrag, bei erfolgreicher Gesamtauswahl Gesamtantrag) kann in zeitlichen Abständen "subdeadlines", z.B. nach Nachnamen geordnet, erfolgen, um die Masse der Anträge besser zu bewältigen.

Weitere Informationen hierzu erhalten Sie unter den Internetadresse.
http://ec.europa.eu/erc/index_en.cfm
http://ec.europa.eu/erc/pdf/erc-scientific-council_strategy_note_peerreview_panels_en.pdf

- **People** – Laufbahnförderung von Forschenden
Die als „Marie-Curie-Fellowships“ bekannten Massnahmen werden weiter ausgebaut. Mit einer Palette von Aktionen wird einer langfristigen Forschungslaufbahn Rechnung getragen. Besonders gefördert werden die Doktorandenausbildung, die Postdoc-Weiterbildung, Stipendien für hervorragende Wissenschaftlerinnen und Wissenschaftler und die Rückkehr von Forschenden nach Europa im Anschluss an Auslandsaufenthalte. Ein weiterer Schwerpunkt ist der Wissenstransfer zwischen den Hochschulen und der Industrie, welcher durch den Austausch von Personen realisiert wird. Die Forschungs- und Ausbildungsthemen werden von den Antragstellern frei gewählt.
- **Capacities** – Infrastrukturen und Innovation
Unterstützt werden zentrale Aspekte europäischer Forschungs- und Innovationskapazitäten: Forschungsinfrastrukturen; Forschung zugunsten von KMU; regionale forschungsorientierte Cluster; Freisetzung des gesamten Forschungspotenzials in den Regionen der EU; Massnahmen der internationalen Zusammenarbeit. Gesellschaftsrelevante Fragestellungen im Zusammenhang mit Forschung und Technologie (Ethik, Technologie-

Risikoabschätzungen, Gender-Aspekte, etc.) werden im Programm „Wissenschaft und Gesellschaft“ behandelt.

Wie sehen die Teilnahmebedingungen aus?

Die Europäische Kommission hat vor kurzem ihren Vorschlag für das letzte der drei Schlüsseldokumente zum 7. FP, nämlich die Teilnahme- und Verbreitungsregeln verabschiedet. Dieses Dokument ist die Basis für alle Verfahren und Regelungen in Bezug auf die Projektfinanzierung und die Rechte des geistigen Eigentums. Obwohl dieses Dokument noch nicht in der Endfassung aufliegt, ist es sinnvoll in diesem Artikel bereits einige wichtige Änderungen gegenüber FP6 aufzuführen. Es betrifft vor allem die Modifikationen der Teilnahmebedingungen und der Finanzierungsregeln.

Teilnahme und Einreichung:

- Während für Verbundprojekte die Formierung von Konsortien nach wie vor eine wichtige Voraussetzung bleibt, können Einzelteams ihre Finanzhilfen nun beim Europäischen Forschungsrat (ERC) beantragen.
- Im 7. FP wird die elektronische Einreichung die Regel sein.
- Die Einführung eines einheitlichen Registrierungssystems mit einer gemeinsamen Datenbank für alle Kommissionsdienste sollte den Papieraufwand reduzieren helfen.

Finanzielles

- Die folgenden Formen von Finanzhilfen sind vorgesehen: Erstattung zulässiger Kosten (siehe unten), Finanzierung nach Pauschalsätzen (beispielsweise Pauschalbeträge), eine Kombination der beiden sowie Preise und Stipendien.
- In Bezug auf die Erstattung zulässiger Kosten sind einige Änderungen geplant, die es den Teilnehmenden erlauben sollten, mehr Fördermittel als im 6. FP zu erhalten. Die Kostenmodelle des 6. FP werden aufgehoben. Alle Teilnehmende erhalten also die volle Rückerstattung der zulässigen Kosten eines Projekts. Die Kosten für festangestellte Personen können dem Projekt belastet werden (allerdings wird dazu eine Zeiterfassung erforderlich sein). Für Teilnehmende, die ihre indirekten Kosten (beispielsweise für Gebäude, Strom) nicht beziffern können, wird ein Pauschalsatz (flat rate), der noch nicht bestimmt ist, zur Anwendung kommen.
- Die Teilnehmenden werden für die verrechenbaren Kosten ihrer Forschungsaktivitäten wie folgt entschädigt:
 - KMU: 75% (als Anreiz für die Beteiligung von KMU)
 - Öffentliche Einrichtungen und Universitäten: 75%
 - Industrie: 50%
 - ERC-Projekte: bis zu 100%
 - Managementaktivitäten werden wie im 6. FP zu 100% vergütet.
- Rechnungsprüfungszertifikate (Audit-Zertifikate) werden verlangt, aber ihre Zahl pro Projekt und Teilnehmende wird reduziert.
- Exzellenznetzwerken wird eine Pauschalfinanzierung gewährt, die sich nach der Anzahl der im Projekt engagierten Forschenden und der Dauer der Aktion misst. Der Kostenansatz soll 23'500 Euro pro Jahr und Forschenden betragen. Die Zahlungen erfolgen periodisch je nach Fortschritt des Projekts.

- Um die Teilnahme für KMU zu vereinfachen und die Anzahl der durch sie zu liefernden (Bank-)Garantien zu reduzieren, möchte die Kommission einen «Garantiefonds » einführen, der über einen kleinen Teil (wahrscheinlich weniger als ein Prozent) der Beiträge, die Industrie und KMU für Projekte erhalten, finanziert würde.

Wie soll man beginnen?

Wenn Sie die Absicht haben, sich am 7. Rahmenprogramm zu beteiligen, lohnt sich eine gute Vorbereitung. Nachfolgend finden Sie einige Ratschläge.

Verfolgen Sie in diesem Jahr die Anlässe, die Euresearch für Sie organisiert (<http://www.euresearch.ch/eventsfp7>). Im Herbst bieten die Informationsanlässe bereits Details zu den einzelnen Themenbereichen der zukünftigen Ausschreibungen. Die "Infoweeek", die im Januar 2007 von Euresearch gemeinsam mit dem Staatssekretariat für Bildung und Forschung (SBF) durchgeführt wird, eröffnet das 7. Rahmenprogramm und bietet Gelegenheit, Vertreter der Europäischen Kommission zu treffen (16.-19. Januar 2007).

Es empfiehlt sich möglichst jetzt schon mit Kollegen im europäischen Ausland Kontakt aufzunehmen und mögliche zukünftige Projekte zu diskutieren. Umgekehrt können Sie auch versuchen Ihre Stärken in Partnerschaften einzubringen, die sich in Vorbereitung befinden. Die laufenden Projekte unter dem bisherigen Rahmenprogramm sowie kurze Projektbeschreibungen und die Namen der involvierten Partner sind in einer Datenbank unter <http://cordis.europa.eu.int/fp6/projects.htm> ersichtlich. Suchen Sie diese Quelle auf, um zu sehen, welche Teams auf einem ähnlichen oder ergänzenden Gebiet wie Sie arbeiten.

Im letzten Quartal 2006 nehmen die Vorbereitungen für die Projekte konkretere Formen an. Nachdem Sie gezielt Ihren Interessen entsprechenden Veranstaltungen besucht haben, richten Sie Ihren Projektvorschlag so aus, dass er genau auf die Ausschreibung passt. Wir von Euresearch führen gerne ein Pre-Screening für Ihren Antrag durch und unterstützen und begleiten Sie während der Vorbereitungsphase.

Weiterführende Information zum FP7 finden Sie unter www.euresearch.ch/FP7. Wir freuen uns auf Ihre Teilnahme und wünschen Ihnen bereits jetzt viel Erfolg.

News for and from Members

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

Natalia Dalla Favera (Department of Inorganic Chemistry, University of Geneva, 30, Quai Ernest Ansermet, 1211 Genève 4)

Aude Escande (Department of Inorganic Chemistry, University of Geneva, 30, Quai Ernest Ansermet, 1211 Genève 4)

Anke Christine Zürn (Laboratorium für anorganische Chemie, ETH Zürich, HCI H 127, Wolfgang-Pauli-Strasse 10, 8093 Zürich)

Jürgen Ketterer (Ilford Imaging Switzerland GmbH, Research & Development, Route de l'Ancienne-Pepeterie, 1723 Marly)

Travel Grants for Young SGK/SSCr Members

If you wish to apply for a travel grant, please send the above mentioned documents to the president of the SGK/SSCr anytime.

The rules have been modified by the board as following:

1. Only members of the SGK/SSCr can be financially supported.
2. Student members can get up to CHF 500 for a poster presentation and CHF 750 for an oral presentation.
3. Postdocs can be supported only for oral presentations with a maximum of CHF 500.
4. Per institute and year, only two persons can be supported.
5. A 1-2 page scientific contribution to the SGK/SSCr newsletter is expected

New Awards

The Executive Committee of the European Crystallographic Association (ECA) has decided to establish a prize for young scientists (Erwin Felix Lewy-Bertaut-Prize) which will be distributed together with the European Neutron Scattering Association (ENSA).

ECA – European Crystallographic Association: Apply for Individual Membership

The objectives of the Association are: a. to contribute to the advancement of crystallography in all its aspects, including related topics concerning the non-crystalline states; b. to promote European cooperation in crystallography. For these purposes the Association shall have the power: a. to adhere to the International Union of Crystallography as a "Regional Associate", b. to organize meetings and conferences on subjects falling within the purview of the Association, c. to set up committees or other bodies for special purposes, d. to initiate, promote and coordinate crystallographic research requiring European cooperation, e. to organize special projects which shall be financed independently of the regular operations of the Association, f. to participate in joint committees with other associations or other scientific bodies in matters of interest to the Association, g. to do all such things as are appropriate for fulfilling its objectives.

May I recommend you to become an **individual member of ECA** for an additional yearly fee of 10 Euro only. Benefits are e.g. a reduced conference fee at ECA meetings, the next to be held in Marrakech (the reduction is presently 20 Euro), as well as the possibility to suggest new SIG's – scientific interest groups – for example to organize micro symposia at such meetings.

Please contact the homepage of ECA (<http://www.ecanews.org>) for further details.

Missing Addresses of SGK/SSCr Members

We have problems to contact the following members (last known affiliation in brackets):

Dr. S. Rodriguez Belluga (UNIL, Lausanne)

If the new address is known to you, please send an E-mail or FAX to the editor.

News from the Laboratories and Institutes

Starting with the next issue (No. 70 in December 2006), we would like to give to all the laboratories involved in crystallography and related areas the opportunity to present their recent highlights as well as new developments. Up to now, this was already used by the Swiss-Norwegian beam line, but we also invite other facilities and laboratories. Please send short contributions (1-2 pages) to the editor. This will extend the existing possibility to submit individual scientific contributions (which will be open also in the future).

In Memoriam Edgar Ascher

By Hans Grimmer (Hans.Grimmer@psi.ch)



Edgar Ascher, a founding member of the Swiss Society for Crystallography and its second president died in Geneva on July 28, 2006 at the age of 85.

He was born on January 6, 1921 in Győr (Hungary), started secondary school in Vienna, but being of Jewish origin, looming Nazism incited his family emigrating to Zagreb, where he had to learn Croatian, the language in which he passed his maturity exam in 1939. During World War II he fled to Italy, where he became one of the 73 children and adolescents having

found refuge in the now famous "Villa Emma" in Nonantola [1]. From there he finally succeeded to enter Switzerland in 1943. He studied at the Universities of Basle and then of Lausanne, where he received his "licence ès sciences" in 1949 and became an assistant to Prof. A. Perrier. In 1954 he received his doctoral degree with a thesis on the Hall effect in ferromagnetic Fe-Ni-alloys.

In 1955 Edgar joined Battelle Institute in Geneva, where he started with experimental and then changed to theoretical work. His main interests were in symmetry and its applications to solid state physics. Particularly fruitful were the collaborations with his colleagues Aloysio Janner and Hans Schmid, who later became professors in Nijmegen and Geneva, respectively.

Together with Aloysio Janner he applied modern algebraic methods to the study of the structure of crystallographic space groups [2,3] and later to relativistic symmetry groups of systems with periodicity in space and time.

With Hans Schmid he worked on boracites and their electric, magnetic and magnetoelectric properties, culminating in the demonstration of the coexistence of spontaneous magnetization and polarization in boracites containing 3d-transition metals [4].

Edgar determined the tensors of those Heesch-Shubnikov point groups permitting the bilinear magnetoelectric effects. He derived upper and lower bounds on the magnetoelectric susceptibility tensor and upper bounds for various other electric and magnetic properties.

Forty years ago, he investigated properties of spontaneous currents, determined the corresponding 31 magnetic point groups for crystals permitting a time-odd polar vector and predicted related new phenomena [5]. Later he extended these results to the description of kinetolectric and kinetomagnetic effects in crystals [6]. Astonishingly, even today that time-odd polar vector is still ignored in most solid state physics textbooks. In recent times these 31 groups have received great practical importance since they describe those magnetoelectric crystals that permit a spontaneous toroidal moment.

The most fruitful years of his crystallographic and solid state physics research were from 1964 to 1969, when eleven of his thirteen most frequently quoted papers appeared, the remaining two were published in 1977 and concerned symmetry aspects of phase transitions [7,8].

I got to know Edgar in 1968, when I joined the Battelle Advanced Studies Center as a member of his group. I met a friendly, modest man who liked to play on words, and I was impressed by his wide interests and his knowledge of languages: Hungarian, Croatian, Italian, German, French, English, Russian, ...

Edgar was invited to many places to give lectures on a wide range of topics. As examples, I shall just mention the lectures he gave at EPFL in 1972 and 1973: Within the scope of "Enseignement du 3e cycle de la physique en Suisse romande" he gave an excellent series of lectures on "Extensions et cohomologie de groupes" with applications to crystallographic space groups, and he lectured on "Limites à la croissance: considérations méthodologiques au sujet du 'modèle du monde' proposé par Forrester". Another lecture series was entitled "Mathematical Models and Contemporary Problems". At that time he was offered a professorship at EPFL, which he declined.

In 1974 he started collaborating with the International Center for Genetic Epistemology of Jean Piaget. In the last thirty years his research encompassed philosophy, psychology, linguistics, history, and, in particular, sociology. A considerable number of publications in the "Revue européenne des sciences sociales" testifies to the immensely wide range of his interests.

Although he wrote his last crystallographic paper in 1982, Edgar Ascher remained a member of the SSCr until his death. Our thoughts are with his wife Corinna, his son Stéphane, and his sister Alice.

I am grateful to Corinna Ascher for the picture of Edgar and to Hans Schmid for much information on his life and work.

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- [7] E. Ascher, J. Kobayashi, Symmetry and phase transitions: the inverse Landau problem, *J. Phys. C: Solid State Phys.* **10** (1977) 1349-1363
- [8] E. Ascher, Permutation representations, epikernels and phase transitions, *J. Phys. C: Solid State Phys.* **10** (1977) 1365-1377

Used Diffraction Equipment

We are offering here old equipment which may be of interest for our community. If you have X-ray or neutron diffraction related equipment in a reasonable condition which is preferably in operating condition or at least may be used as spare parts, please send a note with all the relevant information to the editor.

Equipment	Offered by	Contact
Presently, no equipment is advertised here.	--	--

Invitation for the General Assembly October 20, 2006 in Bern

Freiestrasse 3, 3003 Bern, 16⁴⁵ – 17⁴⁵

1. Approval of the Agenda
2. Minutes of the Annual General Assembly in Lausanne, October 13, 2005
(published in SGK/SSCr Newsletter 67)
3. Reports from the SGK/SSCr of the
 - a) president (W. Steurer)
 - b) treasurer (M. Hennig)
 - c) Auditors (C. Bärlocher, K. Schenk)
4. Presentation of the Budget 2007 and membership fees 2007 (M. Hennig)
5. Reports from the SKT/SCT
 - a) treasurer (K. Fromm)
 - b) Auditors
6. Presentation of the SKT/SCT Budget 2007 (K. Fromm)
7. Report of the delegate to the ECA Council Meeting Leuven 2006
8. Award of travel grants (W. Steurer)
9. Election of the section head of SKT/SCT (W. Steurer)
10. Election of the auditors (W. Steurer)
11. Amendments to the by-laws of the SGK/SSCr (W. Steurer)
 - a) establishing the possibility to make a new Sektion Biologische Kristallographie (SBK)/Section Biological Crystallography (SBC)
Discussion of the possible adds/changes to be made to the by-laws
 - b) further small modifications.
12. Next annual meeting of the SGK/SSCr (W. Steurer)
13. Varia

Appendix to point 11 of the agenda (changes of the statuten/by-laws):

Art. 17 bis (alt)

Der Vorstand wählt aus seiner Mitte den Sekretär für die IUCr, zwei Delegierte an jede General Assembly der IUCr (verbunden mit Internationalem Kristallographenkongress) sowie Delegierte an eventuelle weitere Körperschaften (diese letzteren brauchen nicht dem Vorstand anzugehören). Die Amtsdauer des Sekretärs für die IUCr beträgt sechs Jahre; er besorgt den Verkehr mit der IUCr und ist der eine Delegierte. Er wird jeweils für zwei aufeinanderfolgende General Assemblies, der zweite Delegierte nach Uebereinkunft gewählt. Der Präsident der SGK ist gleichzeitig Vorsitzender des Schweizerischen Komitees für die IUCr. Der Sektionsleiter der SKT ist gleichzeitig der Vorsitzende des Schweizerischen Komitees und Delegierter im IOCG; der zweite Delegierte ist sein Sekretär.

Art. 17 bis (neu)

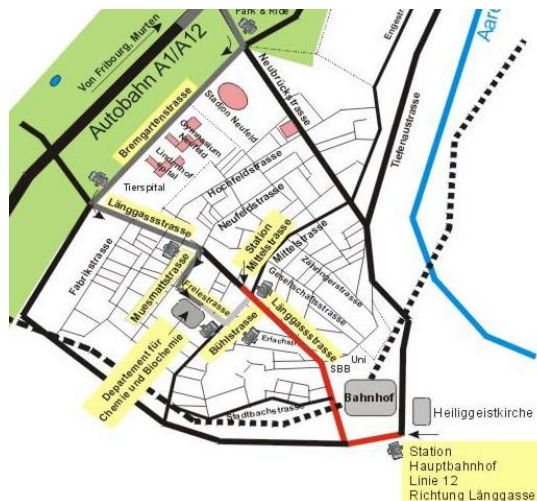
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Further modifications:

To be discussed at the meeting (point 11a).

Annual Meeting of the SGK/SSCr in Berne, October 20

Expanding the boundaries Crystallography in the gas phase, on surfaces, in picoseconds



- 09h45 – 09h50 Welcome by the President **Walter Steurer**
- 09h50 – 10h35 **Michael Wulff**, ESRF, Grenoble (F), “*Molecular dynamics studied by single-pulse X-ray diffraction*”
- 10h35 – 10h45 Discussion
- 10h45 – 11h00 Coffee break / Poster session
- 11h00 – 11h45 **Samuel Leutwyler**, University of Bern, “*Hydrogen Bonding and p-Stacking, a Gas Phase Perspective*”
- 11h45 – 11h55 Discussion
- 11h55 – 12h15 ‘**Appetizer Presentations**’ to the Poster Session: (oral, 5 Min. each)
- 12h15 – 13h30 Lunch at the Posters, Sandwiches and Soft Drinks provided
- 13h30 – 14h15 **Roman Fasel**, EMPA, Dübendorf, “*Expressions of chirality upon two-dimensional crystallization*”
- 14h15 – 14h25 Discussion
- 14h25 – 14h55 **Vladimir Dmitriev**, Swiss Norwegian Beam Lines: “*Scientific highlights from SNBL and other important developments*”, Information by the Swiss Steering Committee of the SNBL
- 14h55 – 15h25 **Bruce Patterson**, SLS, **Jürg Schefer**, SINQ, “*Scientific highlights from SLS and SINQ*”
- 15h25 – 15h45 Coffee break / Poster session
- 15h45 – 16h30 **Nenad Ban**, ETH, Zürich, “*Crystallographic studies of fatty acid synthases: supersize enzymes*”
- 16h30 – 16h40 Discussion
- 16h45 – 17h45 General Assembly of the SGK/SSCr
- 18h00 **Apero** followed by **Dinner**. Hans Grimmer, former president of the SGK/SSCr and his wife, will be our invited guests on the occasion of his retirement.

Lecture Abstracts (Berne, 2006)

Molecular Dynamics Studied by Single-Pulse X-Ray Diffraction

Michael Wulff

European Synchrotron Radiation Facility, FR-38043 Grenoble, France

Beamline ID09B is dedicated to fast pump and probe experiments from crystals and liquids. In the experiments ultrashort laser pulses excite a subset of molecules in the sample and the scattering from delayed hard X-ray pulses probe the structure at a given delay τ . By Fourier transforming the measured scattering $S(Q, \tau)$, we can produce a movie of the electron density, at atomic resolution, as a function of time. The time resolution is 100 picoseconds limited by the X-ray pulse from a synchrotron. The quality of the experimental data is strongly dependent on the wavelength and the intensity of the X-ray and laser beam. On ID09B at the ESRF we produce a very intense, quasi-monochromatic X-ray beam with a monoharmonic undulator, the U17, where the emission is concentrated in the first harmonic in the energy spectrum. The energy of the first harmonic can be varied between 15-20 keV and the bandwidth $\Delta E/E$, is 3%. This harmonic contains up to 1×10^{10} photons per pulse, a factor of 500-1000 more than a conventional monochromatic beam from a silicon monochromator. This beam is focused by a toroidal mirror into a $0.10 \times 0.06 \text{ mm}^2$ spot. The X-ray time structure on the sample is slowed down by the use of a high-speed chopper that ensures that the X-ray and laser pulses arrive in pairs of pulses at 1000 Hz. We will show how time resolved X-ray diffraction is improving our understanding on show on how photosensitive proteins work [1] and how smaller molecules change structure and exchange energy with the surrounding during chemical reactions in solution [2,4].

- [1] "Watching a Protein as it Functions: 150 ps Time-resolved Structures of a Myoglobin Mutant at 1.7 Å Resolution"
F. Schotte, M. Lim, T. A. Jackson, A. Smirnov, J. Soman, J. S. Olson, G. N. Phillips, M. Wulff, and P. A. Anfinrud.
Science, **300**, 1944-1947, 2003.
- [2] "Visualising Chemical Reactions in Solution by Picosecond X-ray Diffraction",
Plech, M. Wulff, S. Bratos, F. Mirloup, R. Vuilleumier, F. Schotte and P.A. Anfinrud.
Physical Review Letters, vol 92, no 12, p 125505-1, 2004.
Stuart Rice, *Nature*, Vol **429**, p 255, 2004
- [3] "Ultrafast X-ray Diffraction of Transient Structures in Solution", H. Ihee, M. Lorenc, T. K. Kim, Q. Y. Kong, M. Cammarata, J. H. Lee, S. Bratos, M. Wulff,
Science, **309**, 1223-1227, 2005.
- [4] "Spatio-temporal reaction kinetics of an ultrafast photoreaction pathway visualized by time resolved liquid x-ray diffraction",
T. K. Kim, M. Lorenc, J. H. Lee, M. Lo Russo, J. Kim, M. Cammarata, Q. Kong, S. Noel, A. Plech, M. Wulff, and H. Ihee. *PNAS*, vol. **103**, no. 25, 9410–9415, 2006

Expressions of chirality upon two dimensional crystallization

Roman Fasel

Swiss Federal Laboratories for Materials Testing and Research (Empa)
nanotech@surfaces Laboratory, Dübendorf / Thun, Switzerland

In his famous experiment in 1848, Pasteur manually separated left- and right-handed ammonium sodium tartrate crystals under the microscope and observed opposite optical activity of their aqueous solutions. There are two intriguing aspects in this groundbreaking experiment: i) Handedness is transferred from molecular structure into the macroscopic shape of the crystal, and ii) the two mirror-like forms of the molecules crystallized into homochiral conglomerates allowing manual separation. The mechanisms of both processes are still poorly understood - we are not able to predict the shape of a crystal based on the molecular structure, nor do we understand why mixtures of left- and right-handed molecules (racemate) only sometimes crystallize into homochiral conglomerates.

A promising approach is studying two-dimensional (2D) crystallization phenomena via scanning tunnelling microscopy (STM). During the last years, we have investigated the 2D crystallisation of the polycyclic aromatic hydrocarbon heptahelicene. I will show that, under repulsive conditions, heptahelicene shows a transfer of chirality from the individual molecules into homochiral assemblies. For a small enantiomeric excess, a strongly non-linear amplification of chirality is observed.

In a second part, I will focus on the geodesic fullerene fragment ("buckybowl") hemifullerene, which represents half of the C_{60} carbon framework. No successful separation of the hemifullerene enantiomers has been reported up to date. Upon deposition on a Cu(110) surface, however, homochiral one- and two-dimensional organometallic nanostructures are formed. Both structures can be understood by local enantioseparation driven by enantioselective interaction with chiral kink sites.

While STM is the method of choice for studying molecular pattern formation, it does in general not allow to draw quantitative conclusions regarding the molecular conformation. In a last part, I will therefore present a complementary method that yields direct quantitative structural information for molecular adsorbates: Synchrotron-radiation angle-scanned X-ray photoelectron diffraction (XPD) allows to determine the handedness of adsorbed chiral molecules, and to distinguish and identify the enantiomers, in a straightforward way.

Scientific Highlights and New Developments at SNBL

Vladimir Dmitriev

Swiss-Norwegian Beam Lines at ESRF, Grenoble, France

Events and improvements on the Swiss-Norwegian beam-lines (SNBL) will be presented in the talk. The ESRF has recently revealed its long term strategy. The essence of these changes and the implication for SNBL will be summarised. Equally, significant progress in instrumentation development has been made over the last months. This includes a considerable extension of the available energy range (5-70

keV on SNB), the acquisition and integration of a He-Cryostats (down to 5 K) combined with the simultaneous use of different techniques (Diffraction, EXAFS and Raman spectroscopy). These improvements will be demonstrated on a selection of some experiments carried out by our users.

Crystallography Highlights from the Swiss Light Source

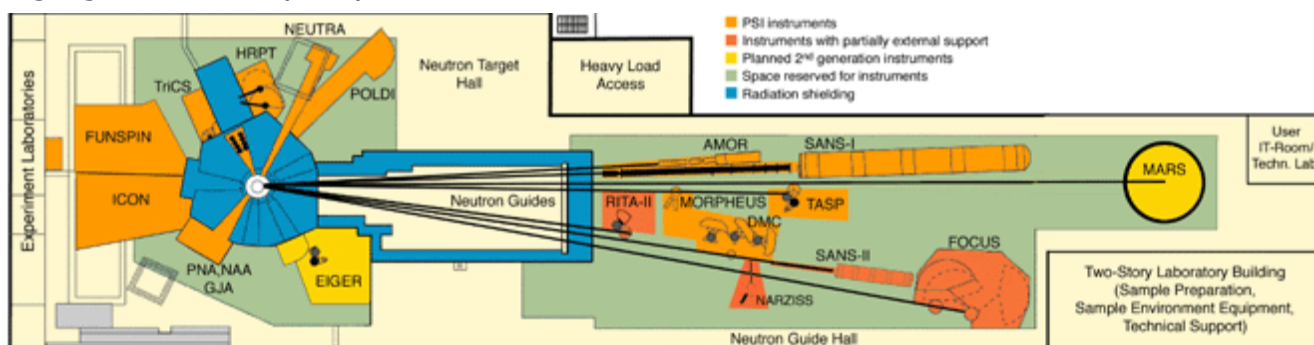
Bruce D. Patterson, Swiss Light Source, Paul Scherrer Institut, 5232 Villigen
Bruce.Patterson@PSI.CH

The Swiss Light Source is a 2.4 GeV electron storage ring with 10 X-ray beam lines presently in operation and another 6 under construction. Among the recent crystallography highlights from our facility are results from glancing-incidence diffraction on oxide surfaces, high-resolution and time-resolved powder diffraction on organic and inorganic systems, resonant soft X-ray diffraction studies of orbital order in perovskites and large-molecule protein crystallography. Important progress in several of these fields has been triggered by the in-house detector development.

Highlights and Developments at the Swiss Neutron Spallation Source SINQ

J. Schefer Laboratory for Neutron Scattering, ETHZ & PSI, 5232 Villigen
Jurg.Schefer@PSI.CH

The continuous Swiss Neutron Spallation Source SINQ has started operation in 1996. In 2005, 351 experiments have been performed by 352 scientists. In 2006, a new liquid target (MEGAPIE) has been successfully installed, increasing the neutron flux up to 60%, depending on wavelength and beam position. This test-target opens the possibility to increase the proton flux far above its current level of 1.8 to mA (whereof 1.3mA on SINQ as a result of losses when passing the muon target). We present the status of the instrumentation operated by the Laboratory for Neutron Scattering, ETHZ&PSI - focusing on diffraction instruments – as well as scientific highlights from the past years.



Nenad Ban, ETH, Zürich

Fungal $\alpha_6\beta_6$ heterododecameric fatty acid synthase (FAS) harbors all catalytic domains required for *de novo* fatty acid synthesis. Recently, a 5Å resolution x-ray crystallographic electron density map of *Thermomyces lanuginosus* fatty acid synthase allowed fitting of homologous enzymes that catalyze the individual reaction steps [1]. The catalytic domains are embedded into well-defined structural features, which serve as a matrix and define the architecture of the huge assembly. The synthesis is compartmentalized in two large reaction chambers, each containing three sets of active sites and three flexible acyl carrier proteins that transfer substrates between the catalytic domains. This architectural solution differs considerably from the mammalian multienzyme [2], which catalyzes the same conserved reaction pathway but evolved as a homodimer.

Very recently, we were able to collect a dataset from a FAS crystal diffracting to 3.1Å, which allows us to build and refine an atomic model of the FAS particle. Thus, we now have the possibility to analyze the catalytic centres of the enzymatic domains in detail and to understand the structural role of interdomain linkers and insertions, which define the overall architecture of the FAS complex.

- [1] Jenni S, Leibundgut M, Maier T, Ban N. (2006) *Science* **311**,1263-1267. Architecture of a Fungal Fatty Acid Synthase at 5 Å Resolution.
- [2] Maier T, Jenni S, Ban N. (2006) *Science* **311**, 1258-1262. Architecture of Mammalian Fatty Acid Synthase at 4.5 Å Resolution.

Poster Abstracts (Berne, 2006)

Centrosymmetric and Pseudo-Centrosymmetric Structures Refined as Non-Centrosymmetric

H. D. Flack,^{a*} G. Bernardinelli,^a D. A. Clemente,^b A. Linden^c and A. L. Spek^d

^aLaboratoire de Cristallographie, University of Geneva

^bDipartimento dei Materiali e delle Risorse Naturali, Università di Trieste sede di Pordenone, Italy,

^cInstitute of Organic Chemistry, University of Zurich and

^dDepartment of Crystal and Structural Chemistry, Bijvoet Center for Biomolecular Research, Utrecht University, The Netherlands.

The behavior of the Flack parameter for centrosymmetric and pseudo-centrosymmetric crystal structures based on crystal structures published as being non-centrosymmetric is presented. It is confirmed for centrosymmetric structures that the value obtained for the Flack parameter is critically dependent on the Friedel

coverage of the intensity data approaching 0.5 for a coverage of 100% and sticking near the starting value for a coverage of 0%. For pseudo-centrosymmetric structures, even those very close to being centrosymmetric, it is found that it is often possible to obtain significant values of the Flack parameter. A theoretical basis for this surprising result is established. It has also been possible to establish an *a-priori* estimate of the standard uncertainty of the Flack parameter based only on the chemical composition of the compound and the wavelength of the radiation. The poster concludes with preliminary presentations of bias in the Flack parameter and other novel results. Results are published in [1].

[1] Flack, Bernardinelli, Clemente, Linden & Spek, *Acta Cryst.* **B62** (2006)

An Alternative Approach for the Description of Modulated Structures Using Differential Geometry

Philippe Kocian and Gervais Chapuis

Laboratoire de Cristallographie, École Polytechnique Fédérale de Lausanne
E-mail: philippe.kocian@epfl.ch

Differential geometry is a theory that has been existing for one and a half century and is much solicited in many physical topics, but not a lot in crystallography. In fact, Hans Wondratschek [1] hints at this mathematical topic, when introducing two spaces for the description of the symmetry operations : the *point space* and the associated *vector space*. In our work, we think of \mathbf{R}^n as a differential manifold in which we consider n -dimensional lattices, be they smoothly modulated or not. The focus of our viewpoint is to say that each node of the lattice is linked to an origin point not by a vector, but by a curve belonging to a family $\{c_\lambda \mid \lambda \in M\}$, where M is a \mathbf{Z} -module. If we parameterize each of these curves between 0 and 1, we can see that the extremities of the corresponding velocity vectors at 0 generate a periodic lattice of translations in the tangent space. Using this approach, it seems that the symmetry of modulated structures can be described without erring in a higher dimensional space (super space) and the diffraction pattern of such structures could be better understood considering the Fourier transform in the tangent space.

[1] H. Wondratschek, *Introduction to space group symmetry : Basic concepts*, taken from : *International Tables for Crystallography*, Vol. A, pp 720 – 721, Kluwer Academic Publishers, Dordrecht, 2002.

L. Massüger¹, L.B. McCusker¹, Ch. Bärlocher¹, F. Gozzo² & B.Schmitt²

¹Laboratory of Crystallography, ETH Zurich, 8093 Zurich

²Swiss Light Source, PSI, 5232 Villigen

lars.massuger@mat.ethz.ch

In 1999, Wessels *et al.* [1] demonstrated the practical viability of the 'texture method' for resolving reflections that overlap in a powder diffraction pattern. More information about the relative intensities of overlapping reflections could be obtained, by collecting synchrotron data on a textured, polycrystalline sample as a function of sample orientation. In contrast to other related approaches, a full texture analysis was used to establish how the crystallites were oriented in the sample. This information was then used to extract a single set of single-crystal-like reflection intensities via a joint refinement procedure using all diffraction patterns (between 5 and 1296) simultaneously.

The data collection strategies for both, reflection and transmission geometries have been described [2]. Both have their drawbacks. The reflection mode experiment requires 3 days of synchrotron beam time per sample, extreme corrections to the data for higher tilt angles, and a large homogeneously textured specimen. The transmission mode experiment (using an area detector) allows the beam time to be reduced to *ca* 6h per sample, involves no tilt correction, and requires only a very small sample, but these advantages are gained at the expense of data resolution. In an attempt to improve the resolution of the transmission geometry setup, the experiment has been adapted to accommodate the one-dimensional Si microstrip detector on the powder diffractometer on the Materials Science Beamline at the SLS [3]. This setup has allowed the resolution of the data to be improved both in 2θ (from 0-35 deg to 0-60 deg) and in peak width (from *ca* 0.06 deg 2θ to *ca* 0.03 deg 2θ) with an acceptable increase in the amount of beam time required (*ca* 12h per sample).

The data analysis software has been modified to accommodate the data from the Si-microstrip detector, and now possibilities for the further optimization of the experiment are being investigated. New techniques for preparing textured samples are being developed, the data analysis software is being improved, and the data collection itself is being optimized. For the latter, it was reasoned that once the orientation distribution function (ODF) has been determined for a specific sample, the sample orientations that will yield the best resolution of the overlapping reflections can be identified using a cluster analysis approach. Data collection can then be concentrated on these specific orientations (*ca* 10% of all possible orientations) to yield fewer patterns (without loss of information) with better counting statistics. This, in turn, facilitates the final intensity extraction step, which uses all of these patterns simultaneously.

[1] Wessels T., Bärlocher Ch., McCusker L.B., *Science*, 1999, **284**, 477

[2] Bärlocher Ch., McCusker L.B., Prokic S., Wessels T.,
Z. Kristallogr., 2004, **219**, 803

[3] Schmitt B. *et al.*, *Nucl. Instr. And Meth.*, 2004, A **518**, 436

Powder Diffraction and Electron Microscopy Combined to Solve a Complex Zeolite Structure

Fabian Gramm, Christian Bärlocher, Lynne B. McCusker
Laboratory of Crystallography, ETH Zurich, 8093 Zurich

Many industrially important materials, ranging from ceramics to catalysts to pharmaceuticals, are polycrystalline and cannot be grown as single crystals. This means that non-conventional methods of structure analysis must be applied to obtain the structural information that is fundamental to the understanding of the properties of these materials. Transmission Electron microscopy (TEM) might appear to be a natural approach, but only relatively simple structures have been solved by TEM. Powder diffraction is another obvious option, but there the overlap of reflections with similar diffraction angles causes an ambiguity in the relative intensities of those reflections. Various ways of overcoming/circumventing this problem have been developed, and for complex zeolite structures, the FOCUS algorithm [1,2] has proven to be an effective one for structures with up to 12 Si-atoms in the asymmetric unit

To access even more complex zeolite structures, an attempt was made to combine phase information from high-resolution transmission electron microscopy (HRTEM) images with diffraction intensities extracted from a high-resolution powder diffraction pattern. Because FOCUS operates in both real and reciprocal space, phase information can be incorporated directly into the algorithm in a simple way. The results from a series of tests on ITQ-22 [3], the most complex zeolite structure known to date, showed clearly that the phase information facilitated structure solution. For ITQ-22, with 16 (Si,Ge)-atoms in the asymmetric unit, the computing time required to solve the structure could be reduced from *ca.* 31 days for a single correct solution (no phase information used) to 44 h for 2 correct solutions (31 phases input). When 124 phases were used, the correct solution was found 2248 times in just 12 h.

With this new combination of powder diffraction and HRTEM data, it was possible to solve the previously unknown structure of the zeolite TNU-9 ($[H_{9.3}[Al_{9.3}Si_{182.7}O_{384}]]$) [4] with 24 topologically distinct (Si,Al)- and 52 O-atoms in the asymmetric unit.

- [1] Grosse-Kunstleve, R.W., McCusker, L.B. & Bärlocher, *J. Appl. Crystallogr.* **30**, 985-995 (1997)
- [2] Grosse-Kunstleve, R.W., McCusker, L.B. & Bärlocher, Ch., *J. Appl. Crystallogr.* **32**, 536-542 (1999)
- [3] Hong, S.B., Lear, E.G., Wright, P.A., Zhou, W., Cox, P.A., Shin, C.-H., Park, J.-H. & Nam, I.-S., *J. Am. Chem. Soc.* **126**, 5817-5826 (2004)
- [4] Corma, A., Rey, F., Valencia, S., Jorda, J.L. & Rius, J., *Nature Materials* **2**, 493-497 (2003)

Ch. Bärlocher,^{a*} L.B. McCusker^a and L. Palatinus^b,
^aLaboratory of Crystallography, ETH Zurich, 8093 Zurich and ^bLaboratory of
Crystallography, EPF Lausanne, 1015 Lausanne
E-mail: Bärlocher@mat.ethz.ch

The charge flipping (CF) algorithm is an alternative method for structure solution that uses an iterative procedure to reconstruct approximate electron densities from diffraction data [1,2]. It has proven to be highly successful for medium-sized structures, and seems to work best when large areas of "empty space" are present. This criterion of "emptiness" is well fulfilled in the structures of zeolites. Therefore an investigation of the potential of the CF algorithm for solving complex zeolite structures from powder diffraction data was undertaken.

Real powder data suffer from both limited resolution in reciprocal space and the overlap of reflections with similar d -spacings. In a series of tests with different zeolite structures, the tolerance of the CF procedures to these limitations was evaluated. In one test, simulated and real data for the zeolite ZSM-5 ($Pnma$; $a=20.1\text{\AA}$, $b=19.7\text{\AA}$, $c=13.1\text{\AA}$; 38 atoms per asymmetric unit) were used with the following results:

- (a) simulated single crystal data with different resolutions in reciprocal space \Rightarrow perfect solution for $d(\text{min}) \leq 1.1\text{\AA}$.
- (b) as (a) but with 506 groups of equipartitioned intensities (i.e. 1428 of 2188 reflections considered to be strongly overlapping) \Rightarrow good solution
- (c) as (b) but with 1755 reflections considered to be overlapping (462 groups) \Rightarrow **no** solution
- (d) real powder data ($d(\text{min}) = 0.98\text{\AA}$; FWHM 0.05 to $0.09^\circ 2\theta$; 2630 of 3052 reflections overlapping), intensities extracted using the Le Bail procedure \Rightarrow partial solution (Fig 1):

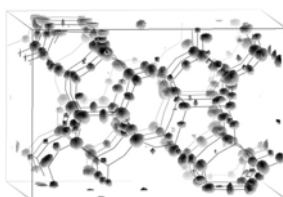


Fig.1: extracted (LeBail) data

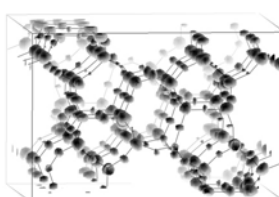


Fig.2: repartitioned (HM) data

Next, a histogram matching procedure that allowed the intensities of the overlapping reflections to be repartitioned during the CF solution process was implemented in the program Superflip [3]. Using this procedure and the data from (d) above (471 overlap groups; criterion for overlap: $0.2 * \text{FWHM}$) an almost perfect solution was obtained (Fig. 2):

The CF method works in space group $P1$, which is a particular advantage for powder data, where the correct symmetry often cannot be determined from the pattern. This aspect proved to be critical in the solution of an unknown layer silicate structure (orthorhombic, $a=11.5\text{\AA}$, $b= 8.5\text{\AA}$, $c= 27.9\text{\AA}$, $d(\text{min}) = 1.02\text{\AA}$, 410 of 733 reflections overlapping). It was solved in space group $I1$, and the solution showed the non-centrosymmetric space group $Ima2$ to be the most likely one. The solution with best

R-value allowed 22 of the 24 atoms (Si, O, C, N and water molecules) to be located directly in the CF map.

These results show that the CF algorithm works well with good powder data, even for limited resolution, that the repartitioning of overlapping peaks significantly increases the success rate for structures with strong peak overlap, and that the algorithm is robust towards symmetry ambiguity.

[1] Oszlányi, G. and Sütö, A. (2004). *Acta Cryst.* **A60**, 134-141

[2] Oszlányi, G. and Sütö, A. (2005). *Acta Cryst.* **A61**, 1347-15

[3] Palatinus, L. and Chapuis. G. <http://superspace.epfl.ch/superflip/>

The Effect of Crystal Symmetry on the Spectral Decomposition of the Linear Elastic Tensor

Hans Grimmer

Laboratory for Development and Methods, Condensed Matter Research with Neutrons and Muons, Paul Scherrer Institut, CH-5232 Villigen PSI

E-mail: hans.grimmer@psi.ch

In a series of papers Theocaris & Sokolis [1-3] described the spectral decomposition of the elastic compliance and stiffness fourth-rank tensors for crystals with different point group symmetries. They found that the number of different eigenvalues plus the number of different "eigenangles" is equal to the number of independent tensor components for monoclinic, orthorhombic, tetragonal, hexagonal and cubic crystals as well as in the isotropic case [1,2]. For trigonal crystals they found a result that did not fit into the general picture sketched above [3]. We, therefore, reconsidered the trigonal case, obtaining a different result, which is consistent with the general picture.

The compliance and stiffness tensors being invariant under inversion, $\bar{1}$, the restrictions on their form imposed by point group symmetry will depend only on the Laue class. Because there are 11 Laue classes of crystallographic point groups, the number of different restrictions cannot be larger than 12 if also the isotropic case is included. It is shown that the inclusion of non-crystallographic point groups (e.g. of quasi-crystals) does not lead to additional types of restrictions. As is well known

(see e.g. [4]), the restrictions are the same for the two hexagonal Laue classes and also for the two cubic Laue classes. Forte & Vianello [5] distinguish only 8 symmetry classes of elastic tensors, not 10. It is shown that this is due to the fact that the tensors of the two trigonal Laue classes belong to the same symmetry class; similarly the tensors of the two tetragonal Laue classes (See Grimmer [6]).

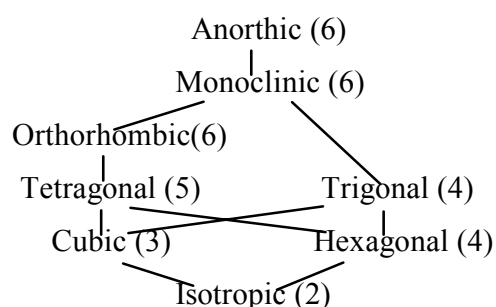


Fig.1: Hierarchy of the 10 symmetry classes of linear elastic tensors. The numbers of different eigenvalues are given in parentheses.

- [1] P.S. Theocaris, D.P. Sokolis, Acta Cryst. **A55**, 635-647 (1999).
- [2] P.S. Theocaris, D.P. Sokolis, Acta Cryst. **A56**, 319-331 (2000).
- [3] P.S. Theocaris, D.P. Sokolis, Z. Kristallogr. **215**, 1-9 (2000).
- [4] J.F. Nye, Physical Properties of Crystals: their Representation by Tensors and Matrices. 2nd edition, Clarendon Press, Oxford 1985.
- [5] S. Forte, M. Vianello, J. Elasticity **43**, 81-108 (1996).
- [6] H. Grimmer, Acta Cryst. **A62**, 168-173 (2006).

Order and Disorder in a Mn based Prussian Blue Analogue: Synchrotron Diffraction and Magnetic Susceptibility Study.

Chernyshov Dmitry,^a Bürgi Hans-Beat^{b*} Ambrus Christina,^b Hauser Jürg^b and Decurtins Silvio^b

^aSwiss-Norwegian Beam Lines at the ESRF, France, ^bUniversity of Berne, Switzerland, E-mail: hans-beat.buergi@krist.unibe.ch

The metal-substituted analogues of Prussian Blue have attracted renewed interest due to their unique combination of magnetic and optical properties. Current research in this field is aimed at designing transparent and optically tunable magnetic materials. A fundamental problem for such design is the presence of intrinsic structural disorder - $M(CN)_6$ vacancies filled by $(H_2O)_6$ clusters - which strongly affects magnetic and optical properties. We characterize the $Mn^{2+}[Mn^{3+}(CN)_6]_{2/3} \cdot (6H_2O)_{1/3}$ analogue with synchrotron diffraction, neutron magnetic scattering and magnetization measurements. Synchrotron diffraction from a single crystal revealed a pronounced diffuse signal linked to a correlated distribution of $[Mn^{3+}(CN)_6]$ vacancies filled by $(H_2O)_6$ water clusters. A complex frequency dependence of the real and imaginary parts of the magnetic susceptibility near T_c , somewhat similar to that of a cluster-glass, indicates a correlated disorder of magnetic centers.

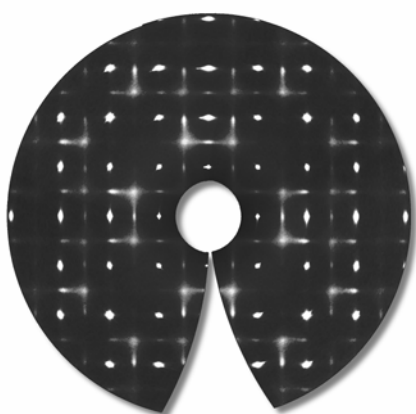


Fig. 1: Structural Disorder in $Mn^{2+}[Mn^{3+}(CN)_6]_{2/3} \cdot (6H_2O)_{1/3}$ As seen from diffuse scattering.

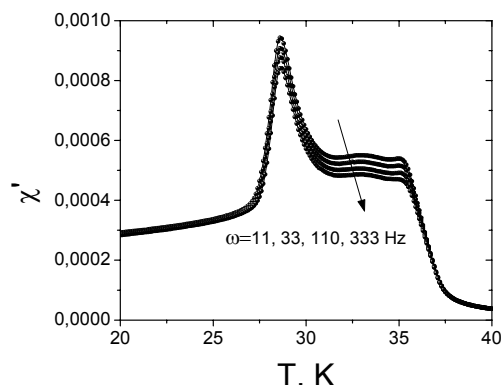


Fig. 2: Frequency dependence of the real part of the ac- susceptibility.

Monte Carlo Simulation of the Incommensurate Structure of p Azoxyphenetol

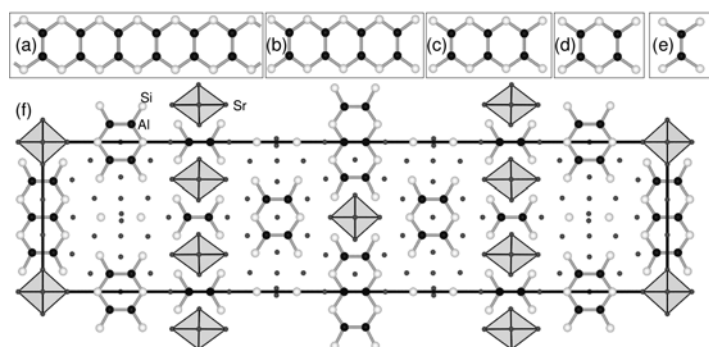
E. Germaine¹, C. B. Pinheiro², K. Schenk¹ and G. Chapuis¹,
¹Laboratory of Crystallography, Ecole Polytechnique Federale de Lausanne (EPFL),
Lausanne,
²Laboratório de Difração de Raios X, Universidade Federal Fluminense (UFF),
BoaViagem, Brasil.

The aim of this work is to describe the behavior of an incommensurate molecular crystal using molecular dynamics simulations (MD). Incommensurate crystals are part of the more general class of aperiodic material. In addition to diffraction methods, molecular dynamical methods can be applied in order to give some information on the mechanisms leading to the aperiodicity of crystalline structures. Incommensurate crystals exhibit sometimes characteristics of disorder which should also be included in the modeling. The calculations are performed with the parallel code *ddgmq* [1]. The compound is p-Azoxyphenetol (PAP) [2]. This compound exhibits two distinct crystalline phases from melting down to 100K. Phase II, stable above 356 K is described by a triclinic space group. Phase I is incommensurately modulated. The disorder is due to the distribution of the oxygen of the azoxy group on two possible sites. Currently a model has been investigated in order to determine the correct sequence of the oxygen position with the development of a code based on the metropolis algorithm. Our aim is to find the configuration with the lowest energy. This structure will be used to initiate the molecular dynamic simulations.

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New Sr Intermetallics with Planar Al/Ge and Al/Si Anions

Michael Rhode, Marco Wendorff and Caroline Röhr
Institut für Anorganische und Analytische Chemie, Universität Freiburg, Germany
caroline@ruby.chemie.uni-freiburg.de



Planar anions with considerable p_{π} - p_{π} interactions between heavier main group 13 and 14 elements are observed in several alkaline earth trielides and tetrelides. The most prominent compounds are those of the AlB_2 structure type, for instance the digallides of Sr and Ba [1-3], or mixed triel/tetrelides like SrAlGe

[4], both with graphite analogous planar nets.

Starting from the planar chains $[Al_{2/2}Ge_2Al_{2/2}]$ of condensed six-membered rings (a) in $Sr_3Al_2Ge_2$ [5] (Ta_3B_4 structure type), a series of aluminide-silicides and -germanides with chain pieces consisting of three (b), two (c) and one (d) six-membered ring and finally only of the oxalate analogous segment $[Ge_4Al_2]$ (e) of the chain have been prepared and characterized on the basis of single crystal data. The formal disruption of the chains is achieved by the incorporation of $[OSr_6]$ octahedra, chains of which (connected *via* common corners) exactly fit the distance between the planar anions (as do the $[OBa_6]$ octahedra in $Ba_{11}[In_6][O]_3$ [6], which contains the same type of anion). The most curious compound presented in this series of new Sr intermetallics is $Sr_{54}Al_{18}Si_{32}O_3$ (f) (space group *Immm*, $Z=2$) where one lattice constant is only 482.5 pm in size (which corresponds to the distance between the planar anions in all compounds, in (f) perpendicular to the plane of paper) whereas one of the other lattice parameters is 7395.6 pm in length. This compound (= $Sr_{54}[Al_2Si_4]_2[Al_4Si_6]_2[Al_6Si_8][Si]_4[O]_3$) contains the planar anions $[Al_2Si_4]$ (e), $[Al_4Si_6]$ (d) and $[Al_6Si_8]$ (c) together with isolated Si^{4-} and O^{2-} . The puzzling bonding situation in these type of polar intermetallics at the *Zintl* border is calculated (using the DFT FP-LAPW approach) and discussed for the structures with manageably small unit cells.

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- [5] A. Widera, H. Schäfer, Z. Naturforsch. **32b**, 1349 (1977)
- [6] M. Wendorff, C. Röhr, Z. Anorg. Allg. Chem. **632**, 1792 (2006)

Standardless Neutron Powder Diffraction 2D-detector Calibration

Antonio Cervellino^a, Uwe Filges^b and Lukas Keller^a

^a Laboratory for Neutron Scattering, ETH Zurich & PSI Villigen, 5232 Villigen

^b Laboratory for Development and Methods, ETH Zurich & PSI Villigen, 5232 Villigen

Calibration of 1D powder diffraction detectors means normally the precise quantification of wavelength, diffraction angle zero bias and instrumental resolution function. The calibration of cylindrical 2D detectors entails the correction of additional more complex aberrations due to a) the exact position of the sample center-of-mass in the z direction (orthogonal to the scattering plane), b) the sample position and beam direction in the scattering plane. Following the work of Ref. [1], we have developed an algorithm [2] that is able to evaluate the latter corrections directly on the collected data without using a standard. This reduces the need for frequent standard calibrations and increases the instrument availability for experiment, while increasing the quality of the data set. As Ref. [1] was concerned with frontal flat detectors instead of lateral cylindrical detectors, there are several differences due to the different geometry; therefore the algorithm has been evolved

accordingly. In particular, the vertical (z direction) sample centering is performed first, while in a second stage the smaller effects of sample off-centering and beam inclination (in the scattering plane) are corrected for. The first stage – as in Ref. [1] – finds the z centering by maximizing the sharpness of the signal integrated along the cone-cylinder intersection curves, which are the isolines for the scattering angle 2θ (and the transferred momentum q) on the detector face. This stage should be incorporated in the data reduction algorithm and be repeated for each dataset, as the sample height is bound to depend on the sample and however can be performed in < 1 s CPU time. The second stage – to be performed at calibration time and optionally at data reduction time for each dataset - uses the multiple correlations of signal profiles extracted at different constant-z lines on the detector face to determine the in-plane geometric corrections. Maximizing again the sharpness has given acceptable results in the first simulations [3]. More sophisticated methods are being evaluated, including point wise correlation. The latter exploits general signal analysis methods (damped oscillation [1] or wavelet [4] decomposition) to have the signal in a generic analytic form. The first instead uses only the deformation of the abscissa (2θ or q) as a function of the geometry.

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J. Appl. Cryst. (2005) 38, 685-687.

Phase Transformations in Cyanometalate Complexes

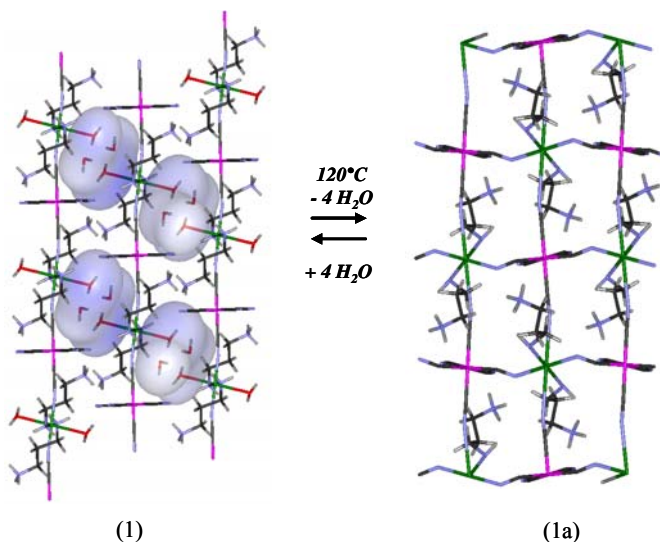
O. Sereda¹, A. Neels¹, H. Stoeckli-Evans¹, F. Stoeckli¹, D. Semenyshyn², O. Borova²
and Y. Yatchyshyn²

¹ Institut de Microtechnique, Université de Neuchâtel, CH-2009 Neuchâtel

² Institute of Chemistry, Lviv Polytechnic National University, Lviv, Ukraine

E-Mail: olha.sereda@unine.ch

There is growing interest in coordination polymers having high-dimensional structures because of the unique physicochemical properties arising in the bulk. In particular, much effort has been made to the design highly ordered structures with paramagnetic metal centers [1-4]. It is known that hexacyanometalate ions, $[M(CN)_6]^{n-}$, are good building blocks to form bimetallic assemblies, such as



Prussian blue, $\text{Fe}^{\text{III}}_4[\text{Fe}^{\text{II}}(\text{CN})_6]_3 \cdot n \text{H}_2\text{O}$. We have used $[\text{M}'(\text{L})_2]^{2+}$ (L=diamine ligands) complex cations, instead of simple metal ions as in Prussian blue analogues, to prepare bimetallic assemblies. We will present some new cyanide-bridged metal-organic frameworks $[\text{M}'(\text{L})_2]_m[\text{M}(\text{CN})_n]_2$ (where $\text{M}'=\text{Cu}$, $\text{M}=\text{Ru}$, Ni), and discuss their structural features and phase transformations, a number of which are reversible.

Powder X-ray diffraction analysis has been used to characterize the new materials obtained after desorption of water by heating. The *ab initio* [5] structure solution for compound **1a**, for example, enabled us to study the structural changes (from **1** to **1a**) and to explain the desorption process. Reversibility and selectivity of the solvents has also been proven by adsorption and desorption of solvent followed by X-ray powder diffraction.

- [1] O. Kahn, *Adv. Inorg. Chem.* **1995**, *43*, 179.
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Interplay of Spin Conversion and Structural Phase Transformations

Karl W. Törnroos¹, Brita Vangdal¹, Dmitry Chernyshov², Marc Hostettler³, Hans-Beat Bürgi³

¹*Department of Chemistry, University of Bergen, Norway*

²*The Swiss-Norwegian Beam lines at the ESRF, Grenoble, France*

³*Laboratory of Crystallography, University of Bern*

E-mail: karl.tornroos@kj.uib.no

The family of solids of $[\text{Fe}^{\text{II}}(\text{2-picolylamine})_3]\text{Cl}_2 \cdot \text{alcohol solvate}$, consists thus far of nine different alcohols. Of these the 2-propanol solvate is outstanding in terms of the structural complexity it displays upon induction of the temperature-dependent (2 to 300 K) and fully reversible high spin ($t_{2g}^4 e_g^2$) \leftrightarrow low spin ($t_{2g}^6 e_g^0$) crossover process.

The spin crossover progresses very differently in terms of both steepness and $T_{1/2}$ (the temperature with a 1:1 ratio of HS and LS iron centers) in each of the six solvates, despite their structures being otherwise isostructural.

In some cases the spin conversion is even absent.

The 2-propanol solvate displays dramatic structural ordering in addition to its magnetic ordering process. The structural ordering is accompanied by two 1st order phase transitions and two hysteresis loops. Clearly there exists an intricate interplay

between the magnetic and the structural ordering processes. We have attempted to map these processes using various macro- and microscopic techniques, including X-ray diffraction experiments at 21 temperatures.

The Swiss Norwegian Beamline – BM01A

D Chernyshov[§], V Dmitriev[§], Y Filinchuk[§] and P Pattison^{§*}

[§]Swiss-Norwegian Beamline, ESRF, BP220, Grenoble Cedex, FRANCE and *Laboratory of Crystallography, EPFL, CH-1015, Lausanne

The Swiss-Norwegian beamlines at the European Synchrotron Radiation Facility have now been in user operation for over a decade. Over the last few years, the scientific activities on the beamline have become more and more focused on solving problems in materials science and crystal chemistry. We present here an overview of the operational characteristics of the beamline and the equipment available on BM01A. Although originally conceived as a station for single crystal diffraction and macromolecular crystallography, the combination of point detector, CCD area detectors and image plate provides a very versatile tool for many types of X-ray diffraction and scattering experiments. Some examples are given of recent results which demonstrate the capabilities of the beamline.

Spherical Neutron Polarimetry Analysis with FullProf: soon a reality

Marc Janoschek^{1,2}, M. Medarde^{3,1}, J. Rodríguez-Carvajal⁴ and B. Roessli¹

¹Laboratory for Neutron Scattering, ETH Zürich and Paul Scherrer Institute,,
CH-5232 Villigen PSI

²Physik-Department E21, Technische Universität München, James-Franck-Strasse,
DE-85747 Garching, Germany

³Laboratory for Developments and Methods, Paul Scherrer Institute,
CH-5232 Villigen PSI

³Institute Laue Langevin, 6, rue Jules Horowitz, B.P. 156,
FR-38042 Grenoble Cedex 9, France

Contact address: marisa.medarde@psi.ch

Because the scientific community using spherical neutron polarimetry (SPN) is relatively small, the available software able to handle SNP data is also scarce. At present, the only crystallographic analysis package including this possibility is the Fortran 77 Cambridge Crystallographic Subroutines Library written by P.J. Brown, J.C. Matthewman and J.P. Wright [1].

In collaboration with J. Rodríguez-Carvajal (ILL, Grenoble), author of the Rietveld analysis program FullProf and the Crystallographic Fortran 95 Modules Library (CrysFML) [2], we have developed new module to be included in FullProf which will add the possibility of handling SNP data. The reasons for such development are threefold:

1. With 3 CRYOPAD and 3 MUPAD devices in operation, spherical neutron polarimetry is becoming more popular. There is thus an urgent need of user-friendly software.

2. FullProf fits into this category and it is well known among the neutron scattering community. Hence, to learn how to use a new option will only represent a small investment for most neutron scattering users.

3. FullProf and the CrysFML package are written in modern Fortran 95 and in modular form, being relatively simple the implementation of new options.

For a given a magnetic structure (expressed as a Fourier series), the new module calculates the polarization matrix at any Bragg reflection, in the case of a single magnetic domain. Upgrades to include multiple domains, as well as the possibility to refine the Fourier coefficients are also planned.

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Reconsideration of polymorphism in Salicylideneaniline

Frédéric Arod^{a*}, Philip Pattison,^{a,b} Kurt Schenk,^a and Gervais Chapuis,^a

^aLaboratoire de Cristallographie, École Polytechnique Fédérale de Lausanne

^bSNBL-ESRF, Grenoble, France

E-mail: frederic.arod@epfl.ch

Organic compounds exhibiting photo- or thermochromicity are of considerable interest owing to their properties and possible applications. The photochromism of salicylideneaniline (SA) was discovered by Senier *et al.* at the beginning of last century, and in 1964, Cohen *et al.* [1] observed its polymorphism. It is generally accepted that the stable form of SA in the ground state is the enol form, with an intramolecular hydrogen bond between the hydroxyl proton and the nitrogen atom. Upon photoexcitation of this enol form with UV light, it undergoes an ultrafast proton transfer from the hydroxyl group to the nitrogen, due to the electronic redistribution in the excited state. The proton transfer generates a keto tautomer in the excited state. We report on the α 2-polymorph structure of SA in the ground state [2]. We also describe a new polymorph, β , which features a planar SA molecule and is therefore thermochromic. We did also revisit the α 1-polymorph structure of SA described by Destro *et al.* [3], but reconsidering their hypothesis. We suggest a lowering of the symmetry with the aim to improve the structure solution. A phase transition between the β form and the α 1 form is observed. Finally, we discuss the different packing observed in these polymorphs, with the goal of understanding their structure-property relationships [4].

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submitted to *Crystal Growth Design*.

C. Besnard, F. Camus, M. Fleurant, P. Pattison*, M. Schiltz
Laboratoire de Cristallographie, EPFL, Lausanne, Switzerland.

*also :Swiss Norwegian Beamline, ESRF, Grenoble, France

J. P. Wright, I. Margiolaki, A. N. Fitch, M. J. Jenner
European Synchrotron Radiation Facility (ESRF), Grenoble, France.

R. Kahn

Institut de Biologie Structurale, IBS, Grenoble, France

During recent years, there has been a major interest for protein powder diffraction¹. The method has proven to be useful in such domains as the study of polymorphism and the investigation of ligand binding¹. A major limitation of protein powder diffraction in ab-initio structural determination is the problem of peak overlap that occurs at high angles, hampering the determination of individual reflection intensities in this part of the pattern. However, given the high-quality information contained in the low angle part, the determination of a solvent envelope should still be possible. Molecular envelopes on model proteins such as Hen Egg White Lysozyme and Porcine Pancreatic Elastase have been successfully extracted by the application of the Single Isomorphous Replacement method. In order to help deconvoluting the overlapping peaks in the high-angle part of the powder pattern, the anisotropic shifts of the unit-cell parameters induced by changes in pH (lysozyme) or radiation damage (elastase) were exploited in a multiple-pattern Pawley intensity extraction.

¹ B. Von Dreele (2003) *Methods Enzymol.* **368**, 254-267

Extracting structural information from protein powder diffraction data

Camus Fabrice^a, Besnard Céline^a, Fleurant Marc^a, Margiolaki Irene^b, Wright Jonathan P.^b, Pattison Phil^{a,c}, Schiltz Marc^a

^a *Laboratory of Crystallography, Ecole Polytechnique Federale de Lausanne*

^b *ESRF, Grenoble (France)*

^c *SNBL, ESRF, Grenoble (France)*

It is sometimes difficult and/or time-consuming to obtain crystals of suitable size for single crystal X-ray diffraction measurements. However if a microcrystalline material can be obtained, it is still possible to perform powder diffraction experiments. Although the collapse of the three-dimensional reciprocal space into a one-dimensional powder diffraction pattern gives rise to a severe loss of information, the availability of high-resolution powder diffractometers and synchrotron sources enables the recording of high-quality powder patterns from proteins. From these spectra, a set of valid intensities can be extracted and/or Rietveld refinement can be carried out [1-2]. It is thus possible to investigate the binding of ligands or heavy atoms to biological macromolecules [3]. We present here results obtained recently in this field. Emphasis will be put on low-resolution phase determination by the methods of isomorphous replacement and contrast variation.

By using extracted intensities from a series of powder diffraction patterns, the location of heavy-atom is possible and a low resolution structure envelope could even be obtained for some small proteins. We present here data for PPE (porcine pancreatic elastase) in which the radiation-induced anisotropic lattice expansion was used as a way to uncorrelate the intensities of overlapping peaks.

On the other hand, contrast variation by solvent exchange is commonly used in small-angle scattering studies, both with X-rays and neutrons, and allows ab initio phasing and molecular envelope determination [2]. We present here our first results on using the solvent contrast variation method in powder diffraction studies.

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Combined high resolution powder and single crystal diffraction analysis, to determine the structure of $\text{Li}_{1+x}\text{Ce}^{\text{III}}_x\text{Ce}^{\text{IV}}_{6-x}\text{F}_{25}$

G. Renaudin¹, E. Mapemba¹, M. Dubois¹, M. El-Ghozzi¹, D. Avignant¹, R. Černý²

¹*Laboratoire des Matériaux Inorganiques, Université Blaise Pascal de Clermont-Ferrand,*

Campus scientifique des Cézeaux, Aubière, France

²*Laboratoire de cristallographie, Université de Genève, 24 quai Ernest-Ansermet, Genève*

Corresponding e-mail address: guillaume.renaudin@ensccf

$\text{Li}_{1+x}\text{Ce}_6\text{F}_{25}$ is the first mixed valence cerium fluoride compound. This compound presents interesting electronic and ionic conductor properties. Intercalation-deintercalation of lithium ions into the $\text{Li}_{1+x}\text{Ce}^{\text{III}}_x\text{Ce}^{\text{IV}}_{6-x}\text{F}_{25}$ host matrix has been realized by electrochemical control of the $\text{Ce}^{4+}/\text{Ce}^{3+}$ ratio. This fluoride can be considered as a model material for potential application as an electrode or an electrolyte for a battery. Then crystallographic study has been performed in order to investigate the long-range ordering of trivalent and tetravalent cerium atoms (by way of valence calculation based on the refined structural parameters) and the localisation and mobility of alkaline lithium cations.

Moderate temperature solid-state synthesis has been used to prepare single crystals. Single-crystal X-ray diffraction intensity data were collected at room temperature using a Stoe IPDS II image plate diffractometer. A tetragonal lattice ($a = 8.855(2)$ Å and $c = 22.968(5)$ Å) was observed and the structure was solved and refined in the space group $P4_3$ ($R_{\text{int}} = 0.054$, $R_{\text{F}} = 0.080$, $R_{\text{wF}} = 0.151$ and $S = 1.39$ for 165 parameters refined from 4583 unique reflections). In order to check the tetragonal lattice of the compound, high resolution synchrotron powder diffraction has been performed on a powdered sample (from the same synthesis) at the Swiss-Norwegian Beam Line (SNBL) at ESRF Grenoble.

The powder pattern clearly showed numerous peak splittings due to a lowering of the lattice symmetry. The pattern was successfully indexed with a monoclinic cell ($a = 8.82391(7) \text{ \AA}$, $b = 22.9188(2) \text{ \AA}$, $c = 8.85384(7) \text{ \AA}$ and $\beta = 90.6093(2) \text{ deg}$), corresponding to a weak distortion of the tetragonal cell previously observed for the single crystal. The definitive structure was solved and refined in the monoclinic space group $P2_1$ by using both single crystal data and the synchrotron powder pattern. 68 independent crystallographic sites were refined (328 parameters refined from 8776 unique reflections with $R_{\text{int}} = 0.053$, $R_F = 0.075$, $R_{\text{wF}} = 0.142$ and $S = 1.11$). The original structure, which is composed of opened and locked slabs, will be presented. Two kinds of lithium sites were observed. One, in the locked slab, is fixed, while the other, in the opened slab, is allowed to move into a bidimensional channel network. The ^7Li MAS-NMR spectrum of the compound confirms the presence of two different lithium environments. Valence calculation performed on the cerium sites clearly indicates long-range ordering of trivalent and tetravalent cerium atoms in the different structural slabs. A comparison between the average tetragonal $P4_3$ structure and the definitive monoclinic $P2_1$ structure will be given. Both models show the same main structural characteristics.

Crystal structures of carbon containing Zirconium and Titanium-Zirconium Deuterides

M. N. Guzik¹, B. Hauback², K. Yvon¹

¹*University of Geneva, Laboratory of Crystallography, Quai Ernest – Ansermet 24, CH – 1211 Geneva 4*

²*Institute for Energy Technology, P.O. Box 40, NO – 2027 Kjeller, Norway*

During last years, carbohydrides compounds have been investigated because of their potential using as a hydrogen storage materials revealing high volumetric efficiency. While the structures of different carbohydrides were reported, an atomic environment of hydrogen in carbon – containing hydrides is not understood completely. Thus, interactions between carbon and hydride (deuterium) atoms should be still improved.

Ti – Zr carbo – deuterides samples of following nominal compositions:

1. $\text{Ti}_{0.66}\text{Zr}_{0.33}\text{C}_{0.57}\text{D}_{0.92}$
2. $\text{Ti}_{0.66}\text{Zr}_{0.33}\text{C}_{0.53}\text{D}_{0.29}$
3. $\text{ZrC}_{0.44}\text{D}_{0.89}$

have been prepared by thermal radiation and cold synthesis and self – propagating high – temperature synthesis and put at our disposal [1]. The compounds crystallize with face – centred cubic (f.c.c.) and hexagonal close – packed (h.c.p.) metal atom arrangements. The samples were studied by X – ray and neutron powder diffraction. The joint Rietveld structure refinements show that carbon atoms occupy only octahedral interstices either nearly ordered (h.c.p.) or disordered (f.c.c.), while deuterium atoms are located on different interstitial sites: tetrahedral in the trigonal phase and octahedral in the cubic. In contrast to previous study [2], in f.c.c. metal atoms arrangement, D atoms do not occupy tetrahedral interstices, even weakly.

- [1] Samples put at our disposal by Prof. S. K. Dolukhanyan (Institute of Solid State Physics of Armenian Academy of Sciences, 375044 Yerevan, Armenia.
- [2] G. Renaudin, K. Yvon, S. K. Dolukhanyan, N. N. Aghajanyan, V. Sh. Shekhtman, J. Alloys Comp. **356 – 357** (2003) 120.

La₂MgNi₂H₈, the first mixed polyanionic transition metal hydride

J-N. Chotard, Y. Filinchuk, K. Yvon

Laboratory of Crystallography, University of Geneva, 1211 Geneva 4

Following our discovery of a hydrogen induced insulating state in the LaMg₂Ni-H system [1] we have investigated the closely related La₂MgNi₂-H system. Hydrogenation of tetragonal La₂MgNi₂ at 10 bar and 100°C leads to a complex metal hydride of composition La₂MgNi₂H₈ having monoclinic symmetry. In contrast to LaMg₂NiH₇ which displays tetrahedral [NiH₄]⁴⁻ complexes that are isolated from each other, La₂MgNi₂H₈ displays two types of polyanionic hydrido complexes having novel geometries. The complexes are ordered and represent the first case of a mixed polyanionic metal hydride system in the literature. The metal and deuterium atoms were located by collecting high resolution synchrotron and neutron powder diffraction data, respectively. The structure (26 independent atoms) was solved by a direct space method and then refined by the Rietveld method. The Ni-H distances vary from 1.43 to 1.91Å. Some hydrogen atoms are coordinated by La and Mg atoms only in octahedral [La₄Mg₂]-type or tetrahedral [La₂Mg₂]-type configurations. The hydride does not desorb hydrogen below 190°C and 1.10⁻¹ mbar pressure and segregates into LaH₃ and other unidentified phases above 300°C.

- [1] K. Yvon, G. Renaudin, C. M. Wei, and M.Y. Chou, Phys. Rev. Lett. **94**, 066403 (2005)

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Please check directly with the facility.

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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	mid September, February	www.ill.fr
FRM-II		
All instruments		user.frm2.tum.de

Calendar of Forthcoming Meetings

Date	Location	Meeting / Link	Abstract Deadline
2006			
Oct. 20	Bern CH	SKG/SSCR annual meeting, Freiestr. 3 http://www.sgk-sscr.ch	Expired
Nov. 27- Dec. 1	Boston USA	MRS Fall Meeting, http://www.mrs.org/s_mrs/sec_mtgdetail.asp?CID=6073&DID=167209	Expired
Dec. 7-8	Berkley USA	MinerMineralogical Society of America Short Course Neutron Scattering in Earth Sciences	

2007

Jan 14-19	Havana Cuba	International School on Mathematical and Theoretical Crystallography www.lcm3b.uhp-nancy.fr/mathcryst/havana2007.htm	
March 5-9	Bremen Germany	Deutsche Gesellschaft für Kristallographie Deutsche Gesellschaft für Kristallwachstum und Kristallzüchtung, Jahrestagung http://www.dgk-dgkk-2007.uni-bremen.de/	Nov. 15, 2006
April 26-29	Dongguang China	ICANS XVIII – Neutron Spallation Sources http://icans-XVIII.ac.cn	Dec. 31, 2006
June 7-17	Erice Italy	Engineering of Crystalline Materials Properties http://www.crystalerice.org/2007.htm	to be announced
June 25-29	Lund Sweden	4 th European Conference on Neutron Scattering http://www.ecns2007.org	to be announced
June 7-17	Erice Italy	Engineering of Crystalline Materials Properties http://www.crystalerice.org/2007.htm	Nov. 30, 2006
July 21-26	Salt Lake City, USA	Annual Meeting of the American Crystallographic Society aca.hwi.buffalo.edu	to be announced
August 5-11	Turin Italy	41 st IUPAC World Chemistry Congress http://www.IUPAC2007.org	to be announced
August 13-17	Manchester UK	9 th Int'l Conference on Biology and Synchrotron Radiation www.srs.ac.uk/bsr2007	March 31, 2007
Aug. 22-27	Marrakech Marocco	ECM-24: European Crystallographic Meeting http://www.ecm24.org	to be announced
Sept. 10-13	Nürnberg Germany	Euromat 2007: Advanced Materials and Processes http://euromat2007.fems.org	Jan. 31, 2007
Oct.7-9	Garmisch Germany	Size-Strain V http://www.mf.mpg.de/ss-v	Feb. 28, 2007

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
May 31 – June 5	Knoxville USA	Annual Meeting of the American Crystallographic Society www.hwi.buffalo.edu/ACA	to be announced
August Sept. 1-11	Japan Warsaw Poland	IUCR EPDIC-11 European Powder Diffraction Conference	to be announced to be announced
Nov. 17-20	Ghent Belgium	14 th International Conference on Thin Films http://www.ICTF14.UGent.be	to be announced

2009

August	Istanbul Turkey	ECM-25: European Crystallographic Meeting http://www.ecm25.org	to be announced
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Become a Member of SGK/SSCr

If you are working in the field of crystallography, you will be interested to become a member of our society. For more information as well as online registration, please have a look on our website (<http://www.sgk-sscr.ch>). Presently, the yearly membership fee is sfr. 30 (sfr. 10 for students). For new members, the membership is free until the end of 2006. Please note: SGK/SSCr members can also apply to be a member of the subsection crystal growth (no additional charge) or for individual membership of the European Crystallographic Association, ECA (additional charge: 10 Euro).

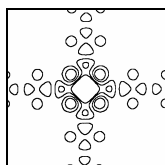
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Interest	
Membership subsection crystal growth	Yes () No ()
Birth date	Day: Month: Year:
Language(s)	
Major research interests	
Highest degree received	
from university	
Present position	

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Schweizerische Gesellschaft für Kristallographie
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Membres du Comité pour la période 2006 – 2008

Président

Prof. Dr. W. Steurer

Laboratorium für Kristallographie
ETH Zürich
HCI G 511, Wolfgang-Pauli-Str. 10
CH-8093 Zürich
Tél.: +41 44 632 66 50 Fax: +41 44 632 11 33
e-mail: WALTER.STEURER@MAT.ETHZ.CH

Vice-Président

Dr. Hans J. Scheel (2006)

Scheel Consulting
Sonnenhof 13
CH-8808 Pfäffikon
Tél.: +41 33 841 25 26 Fax: +41 33 841 25 27
e-mail: HANS.SCHEEL@BLUEWIN.CH

Secrétaire

Dr. Jürg Schefer

Laboratorium für Neutronenstreuung ETHZ & PSI
Paul Scherrer Institut, WHGA-244
CH-5232 Villigen PSI
Tél.: +41 56 310 43 47 Fax: +41 56 310 29 39
e-mail: JURG.SCHEFER@PSI.CH

Trésorier

PD Dr. Michael Hennig

F. Hoffmann - La Roche
Pharma Research 65/319
CH-4070 Basel
Tél.: +41 61 688 60 46 Fax: +41 61 688 74 08
e-mail: MICHAEL.HENNIG@ROCHE.COM

Prof. Dr. Marc Schiltz

Laboratoire de Cristallographie 2
BSP 514
Bâtiment Science Physique UNIL
CH-1015 Lausanne
Tél.: +41 21 693 06 31 Fax: .. 05 04
e-mail: MARC.SCHILTZ@EPFL.CH

Prof. Klaus Yvon

Institut de Cristallographie
Université de Genève
24, Quai Ernest Ansermet
CH-1211 Genève 4
Tél.: +41 22 379 62 15/31 FAX .. 68 64
e-mail: KLAUS.YVON@UNIGE.CH

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

Animateur

Dr. Hans J. Scheel

Trésorière

Prof. Dr. Katharina Fromm

Departement Chemie
Universität Basel
Spitalstrasse 51
CH-4056 Basel
Tél.: +41 61 267 10 04
Fax: +41 61 267 10 21
e-mail: KATHARINA.FROMM@UNIBAS.CH

SGK/SSCr Newsletter

Editor : Dr. Jürg Schefer
Laboratory for Neutron Scattering
ETH Zürich and Paul Scherrer Institute
Building WHGA-244
CH-5232 Villigen PSI, Switzerland

e-mail: Jurg.Schefer@psi.ch

<http://www.sgk-sscr.ch>

Bank Account: UBS Genève IBAN CH39 0027 9279 C029 1110 0

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