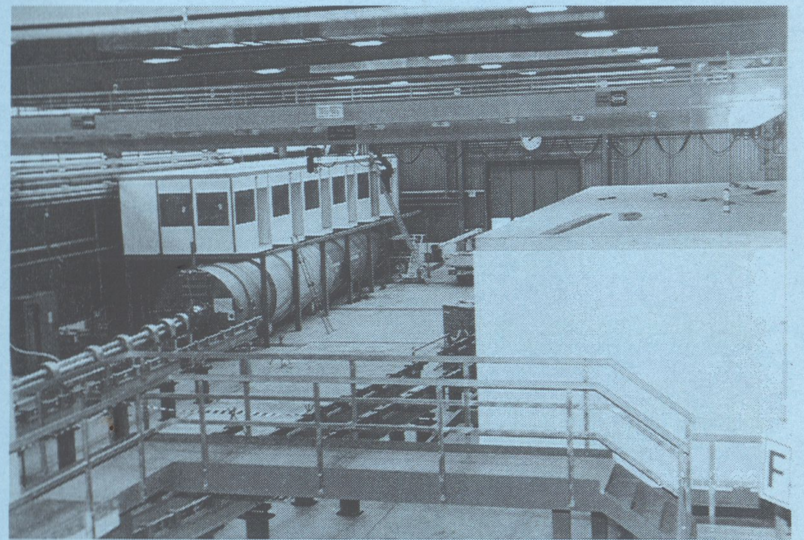
Number 8
Dezember 1995

SWISS NEUTRON NEWS



Schweizerische Gesellschaft für Neutronenstreuung
Société Suisse pour la Diffusion des Neutrons
SGN / SSDN

Umschlagbild

Die SINQ-Leiterhalle im Herbst 1995: Die Kleinwinkelstreuanlage, die Messkabinen und das mit Superspiegel beschichtete Leitersystem sind bereits installiert. Zur Zeit werden die Granit-Tanzböden verlegt und die weiteren Spektrometer aufgebaut.

Impressum:

Herausgeber:	Schweizerische Gesellschaft für Neutronenstreuung	
Vorstand:	Präsident:	Prof. Dr. A. Furrer, ETH Zürich
	Vizepräsident:	Prof. Dr. K. Yvon, Univ. de Genève
	Beisitzer:	Prof. Dr. H.U. Güdel, Univ. Bern
	Sekretär:	Dr. P. Böni, PSI Villigen
Ehrenmitglieder:	Prof. Dr. W. Hälg, ETH Zürich Prof. Dr. K.A. Müller, IBM Rüschlikon und Univ. Zürich	
Rechnungsrevisoren:	Dr. P. Fischer, ETH Zürich Dr. P. Schobinger, ETH Zürich	
Korrespondenzadresse:	Schweiz. Ges. für Neutronenstreuung Laboratorium für Neutronenstreuung ETHZ & PSI CH-5232 Villigen PSI Tel.: 056 / 99 25 18	
Postcheck-Konto:	50-70723-6	
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Inhaltsverzeichnis

Editorial

Herr Prof. Dr. R. R. Ernst (Chemie-Nobelpreis 1991) hat an der Jahrestagung 1995 der Schweiz. Akademie der Naturwissenschaften (SANW) ein viel beachtetes Referat über den "Stellenwert naturwissenschaftlicher Forschung als Stütze von Wirtschaft und Prosperität" gehalten. Er kam dabei auch auf die Rolle der Forscher zu sprechen, die er aufforderte - Zitat - *kommunikativ aktiver zu werden. Kommunikation ist entscheidend für die Zukunft der Forschung und noch wichtiger für die Zukunft der Gesellschaft. In dieser Hinsicht wäre es von grosser Bedeutung, wenn die Forschergemeinschaft ein repräsentatives und politisch starkes Forum hätte, das als einflussreicher Gesprächspartner in wissenschafts-politischen Fragen auftreten könnte. Meines Erachtens erfüllen die heutigen Schweizerischen Akademien diese Aufgabe nur ungenügend. Sie haben weder den notwendigen Rückhalt in der Forscherbasis noch die erforderliche politische Schlagkraft. Ich bin der Ansicht, dass eine einzige Schweizerische Akademie der Wissenschaften, wie sie in zahlreichen andern Ländern besteht, wesentlich wirkungsvoller im Dialog mit der Öffentlichkeit wäre.*

Ein wesentlicher Grund für das zunehmende Ungenügen der Schweizerischen Akademien beruht auf deren starr nach Disziplinen geordneten Strukturen. *Eine der grossen und faszinierenden Herausforderungen der heutigen Zeit liegt im multidisziplinären Ansatz der erkenntnis- und problemorientierten Forschung und Entwicklung* (Prof. Dr. J. Nüesch, Präsident der ETH Zürich, in "Bulletin ETHZ" Nr. 256, Februar 1995). Leider hat sich das erfolgsbestimmende Konzept des interdisziplinären Ansatzes in den Schweizerischen Akademien (noch) nicht durchgesetzt.

Die Schweizerische Gesellschaft für Neutronenstreuung (SGN) bildet ein disziplinenübergreifendes Forum und trägt damit zu einem Abbau der traditionellen, künstlichen und nicht mehr zeitgemässen Fachgrenzen bei. Die Multidisziplinarität der SGN reflektiert sich eindrücklich in der Herkunft der stetig wachsenden Zahl von heute 150 Mitgliedern: 40% Physiker, 20% Chemiker, je etwa 10% Kristallographen, Materialforscher, Ingenieure und Biologen. Gerade wegen ihrer interdisziplinären Ausrichtung hat aber die SGN offensichtlich keinen Platz in der SANW: unser Antrag auf Mitgliedschaft wurde vom Zentralvorstand der SANW zurückgewiesen! Damit beweist die SANW, dass sie eine Öffnung in interdisziplinärer Richtung nicht vollziehen will. Sie sollte sich bewusst sein, dass dann, wenn verkrustete Strukturen nicht mehr verändert werden können, die Institutionen ihren Zweck verlieren.

Albert Furrer
Präsident der SGN

PS: Kürzlich wurde die Gesellschaft der Schweizer Ornithologen (3000 Mitglieder) in die SANW aufgenommen. Quantität ist offenbar wichtiger als wissenschaftliche Qualität. Immerhin - die SANW ist jetzt nicht mehr vogelfrei!

PSI PAUL SCHERRER INSTITUT

4th Summer School on Neutron Scattering

NEW INSTRUMENTS AND SCIENCE AROUND SINQ

18-24 August 1996, Lyceum Alpinum, Zuoz, Switzerland

The main purpose of the Summer School is to give participants an introduction to the basic principles of neutron scattering and its application to the study of condensed matter. The lectures will cover both theoretical and experimental aspects, with particular emphasis on the utilisation of the first-generation neutron instruments installed at the spallation neutron source SINQ at PSI. (SINQ will produce the first neutrons in October 1996). No previous knowledge of the subject is required, but an honours degree in natural sciences (equivalent to the diploma) is essential. A poster session will be organized for participants who wish to present their own results obtained by neutron scattering. ***The list of topics and invited lecturers*** *(* not yet confirmed) includes:*

Introduction to neutron scattering	*W.E. Fischer, Villigen*
Four-circle diffractometer SC3	*J. Schefer, Villigen*
Quasicrystals	*W. Steurer, Zürich*
Optical storage systems	*Th. Woike*, Köln*
Residual stress	*G.A. Webster*, London*
Powder diffractometers HRPT and DMC	*P. Fischer, Villigen*
Supramolecular magnets	*S. Decurtins*, Zürich*
Metal-insulator transitions	*M. Medarde, PSI*
Triple-axis spectrometer DrüchaL	*W. Bührer, Villigen*
Incommensurate phase transitions	*R. Currat*, Grenoble*
Martensitic phase transitions	*W. Petry*, München*
Polarized triple-axis spectrometer TASP	*P. Böni, Villigen*
Identification of magnetic modes by polarization analysis	*B. Dorner, Grenoble*
Invar (small q)	*P.J. Brown*, Grenoble*
Time-of-flight spectrometer FOCUS	*S. Janssen, Villigen*
Dynamics of polymers	*D. Richter, Jülich*
Magnetic excitations studied with time-of-flight spectroscopy	*B.D. Rainford, Southampton*
Small-angle diffractometer SANS	*W. Wagner, Villigen*
Porous materials	*S.K. Sinha*, Argonne*
Polymers and colloids	*P. Schurtenberger, Zürich*
Reflectometer	*D. Clemens, Villigen*
Layered magnets	*H. Zabel, Bochum*
Layered polymers	*M. Stamm*, Mainz*
Non-diffractive methods	*E. Lehmann, Villigen*
Neutron radiography	*J.P. Barton*, La Jolla*
Prompt gamma analysis	*J. Kern*, Fribourg*
Neutron activation analysis	*L. Tobler, Villigen*
Sample environment	
Dynamic nuclear polarization	*H. Stuhrmann, Geesthacht*
Extreme conditions (p,T,H)	*J. Mesot, Villigen*
Data acquisition software and hardware	*D. Maden, Villigen*
Summary	*S.W. Lovesey, Villigen*

Organization: R. Bercher (Secretary), W.E. Fischer (Chairman), A. Furrer (Programme Chairman)

Residential accommodation will be available at the Lyceum Alpinum in Zuoz (costs: approximately 580 Swiss Francs, including full board, excursion, banquet, and Proceedings). The number of participants will be limited to 100. The language of the School is English. Closing date for applying is ***30 June 1996****. For further information and application forms, contact Renate Bercher, Paul Scherrer Institut, CH-5232 Villigen PSI, Tel.: +41-56-310 34 02, Fax: +41-56-310 32 94.*

Generalversammlung 12. Okt. 1995

Auditorium LG/E26 PSI West, Paul Scherrer Institut, 13.15 Uhr

TRAKTANDEN

1. **Begrüssung:**

   Der Präsident begrüsst die 28 Anwesenden. Entschuldigt: **H. U. Güdel, D.** Maden, K. A. Müller und D. Schwarzenbach.

2. **Protokoll der GV vom 21.10.1994:**

   Das Protokoll der GV vom 21.10.1994 (Swiss Neutron News Nr. 6) wird genehmigt und verdankt.

3. **Jahresbericht des Präsidenten:**

   Im Jahresbericht orientiert der Präsident über die verschiedenen Aktivitäten, die unter Mitwirkung der SGN 1994/95 stattgefunden haben:

   - **Veranstaltungen:**
     - 2. PSI-Sommerschule über Neutronenstreuung, 14.-20. August 1994, Lyceum Alpinum, Zuoz, mit 80 Teilnehmern. Das Thema war "Neutron Scattering from Hydrogen in Materials".
     - GV '94 & Festkolloquium "10 Jahre LNS", 21. Oktober 1994, PSI, Villigen.
       "Resonanzmethoden in der Festkörperphysik"
       * Prof. Dr. F. Mezei, HMI Berlin (Spin-Echo)
       * Prof. Dr. R. R. Ernst, ETH Zürich (NMR)
     - 3. PSI-Sommerschule über Neutronenstreuung, 20.-26. August 1995, Lyceum Alpinum, Zuoz, mit 120 Teilnehmern. Das Thema war "Magnetic Neutron Scattering". Es haben sehr viele junge Wissenschaftler teilgenommen.
   - **Swiss Neutron News:**
     - liefert neueste und aktuellste Informationen
     - Nr. 5 (Juni 1994)
     - Nr. 6 (Dezember 1994)
     - Nr. 7 (Juni 1995)
     - Beiträge sind erwünscht!
     - die hervorragende Redaktionsarbeit von P. Böni wird verdankt

   - **European Neutron Scattering Association (ENSA):**
     - Members (11):
       Austria, Denmark, France, Germany, Hungary, Italy, Netherlands, Spain, Sweden, Switzerland, U.K.
     - Observers:
       * Norway, Russia
       * Delegates from Major European Neutron Sources
       * Delegates from Major European Neutron Source Projects
       * Delegate from European Science Foundation (ESF)
       * Delegate from EC (large facility program)
     - Executive Board:
       * Chairman: D. Richter, Germany
       * Vice-Chairman: A. Furrer, Switzerland
       * Secretary: B. Cywinsky, U.K.
     - Statutes approved by all members
     - Analysis of Questionnaire on Neutron Scattering
     - Expert Workshop "Scientific Prospects of Neutron Scattering with Today's and Future Neutron Sources", January 1996, Autrans, F (participation by invitation)
     - Collaboration among Neutron Providers (monochromators, TOF devices, detectors, software, database)
   - Gesuch der SGN um Aufnahme als Mitglied in die Schweizerische Akademie der Naturwissenschaften (SANW)
   - Ausblick 1996:
     - 4. PSI-Sommerschule über Neutronenstreuung, 11.-17. August 1996, Lyceum Alpinum, Zuoz. Das Thema: "Neutron Scattering Experiments at SINQ on day 1".
     - 1st European Conference on Neutron Scattering (ECNS'96) 8.-11. Oktober 1996 in Interlaken (6.-7. Oktober 1996: Einführungskurs).
     - GV der SGN im Rahmen von ECNS'96
     - Inbetriebnahme der SINQ: **Erste Neutronenstreuexperimente!**

4. Jahresrechnung des Kassiers:

Vermögen 1.1.1994 1101.45

	Einnahmen SFr	Ausgaben SFr
Mitgliederbeiträge	1056.-	
Beitrag Sommerschule Zuoz		770.00
Taxen für Postcheck		25.30
Zins	23.70	
Verrechnungssteuer		8.30
Total	1079.70	803.60
Einnahmen 1994		276.10

Bilanz 31.12.1994

	Aktiven SFr	Passiven SFr
Postcheckkonto	1002.80	
Kasse	374.75	
Vermögen am 1.1.1995		1377.55

Mitgliederbeiträge von ausländischen Mitgliedern:

- Zahlungsmoral sehr gut
- Einzahlungen per Post, Bank
- Einzahlungen bar an Konferenzen, Besuchen am PSI, bei Experimenten

5. Bericht der Revisoren:

Die Rechnungsrevisoren haben die Belege, die Abrechnung und die Bilanz für das Jahr 1994 überprüft und für in Ordnung befunden.

Die Jahresrechnung 1994 wird anschliessend von den Anwesenden genehmigt.

6. Budget für das Jahr 1996:

	Einnahmen SFr	Ausgaben SFr
Mitgliederbeiträge	1050.-	
Sommerschule Zuoz		720.-
Taxen für Postcheck		30.-
Zins	30.-	
Verrechnungssteuer		10.-
Briefmarken		10.-
Total	1080.-	770.-
Einnahmen 1996		310.-

7. Nomination von CH-Vertretern ans ILL:

Der Vorstand schlägt die folgenden neuen Vertreter (ab 2. Halbjahr 1996) für die wissenschaftlichen Komitees am ILL zuhanden des BBW vor:

- K. Yvon für den Scientific Council
- J. Mesot für College 4: Excitations
- Ch. Bärlocher für College 5A: Crystallography

Die Vorschläge werden in stiller Wahl akzeptiert.

8. Varia:

- G. Kostorz berichtet aus dem Scientific Council des ILL:
  - neue Geschäftsordnung verabschiedet
  - wissenschaftlicher Rat wird unabhängiger → verursacht Mehrarbeit für die Mitglieder (z.B. Einführung von Rapporteurs, die Spektrometer begutachten)
  - Die bisherigen 5-Jahresverträge für Postdoktoranden (als Instrument Scientists) sind nach französischem Recht illegal
- Prof. Y.Y. Stavissky vom Institute for Nuclear Research RAS, Moscow, richtet eine Grussbotschaft von der russischen Neutronenstreugemeinde an die SGN

Um 14.00 Uhr wird die Behandlung der Traktanden abgeschlossen.

Der Sekretär der SGN, Dr. P. Böni

Zuoz School on Neutron Scattering - 1995

G.H. Lander (written for NEUTRON NEWS)

As Günter Bauer put it in describing the 2nd summer school in the small town of Zuoz (some 20 km from St. Moritz in the Engadine valley) - "A tradition is in the making". Indeed, it is. This year from 20-26 August, almost 90 "students" and some 30 lecturers assembled in this lovely Swiss village to discuss "Magnetism and Neutron Scattering". The numbers themselves are impressive - 48 from Switzerland, 20 from Germany, 14 from France, ending with 2 from Japan, 1 each from India and Korea. Two further breakdowns of the attendance show that the attendance was split 50/50 between young and "old" (i.e. more than a student or postdoc), and approximately equally between those working at neutron centers and elsewhere.

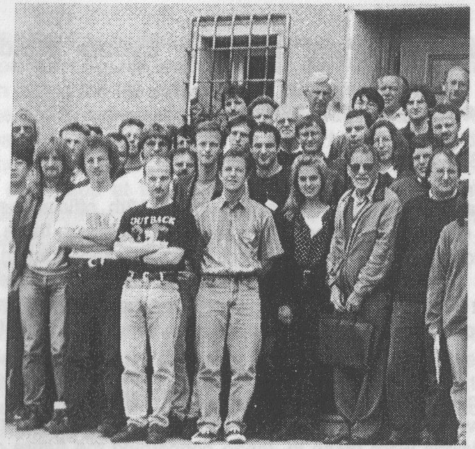
The Zuoz "schools" are at a high level - indeed they may be more accurately compared to a series of seminars, except for the first day, which is truly elementary in nature. In some sense they approximate a Gordon Conference. Despite this high level, or perhaps, because of it, the Zuoz schools attract a very diverse audience, all of whom certainly enjoy themselves and have the pleasure of listening to some of the world's experts. [Gabe Aeppli (AT&T) and Chuck Majkrzak (NIST) flew from the US to give a talk, and 2 days later flew home!].

This years school, as for the previous ones, insisted on (and got) written texts from the speakers ahead of time, and have been published by World Scientific. Some of the subjects discussed after the "Principles and Methods" of the first day, were static magnetic properties, critical and dynamical effects, strongly correlated electron systems, magnetic clusters, the use of polarized neutrons, reflectometry in the study of magnetism, and non-neutron methods such as muons and synchrotron x-rays. The latter a noble gesture on the part of the organizers in view of the feelings sometimes expressed between the two camps - how many neutron scatterers are invited to talk at synchrotron schools?

One leaves these schools with a high sense of optimism - Switzerland surely has more neutron scatterers per head than any other country, and they are busy constructing one of the few "new" sources being turned on anywhere in the world - the SINQ, which is due to start operation at the end of 1996.

Predictably, in Switzerland, the organization is flawless. Much of that is due to the combination of the principal characters in the tradition of the Zuoz Schools: Renate Bercher (secretary), Walter Fischer (School chairman) and Albert Furrer (programme chairman)

Next years' school - same place from 11-17 August 1996, will be organized on "New Instruments and Science around SINQ". My advice is to reserve your tickets now - visiting Zuoz is worth every minute, both from a professional and personal sense!



Prominent participants at the Zuoz School 1995: Alex Müller (front row), Gerry Lander and Günter Bauer (back row).

ICANS-XIII and ESS-PM4, Two Important Neutron Events Held in Switzerland
- separate locations, common topics and joint proceedings

G.S. Bauer, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

The International Collaboration on Advanced Neutron Sources held its 13th official meeting (ICANS-XIII) at the Paul Scherrer Institut (PSI) from October 11 to 14, 1995. Although there were only 8 formal members in the collaboration, 132 participants attended the meeting, coming from 40 different laboratories and institutions. It was particularly encouraging to see that, besides the old friends we have shared our interest in new neutron sources with for many years, several young people have entered the scene and were able to make important contributions to the field.

The topic of new sources could be seen to be as acute as ever. Several important events since ICANS-XII made this meeting a particularly exciting one: The AUSTRON-study has been completed and both, ANL and LANL have produced impressive documents on upgrade options for their respective facilities. Crucial decisions were taken in Japan concerning the future of the KEK-accelerating complex which lead to a complete rethinking of the KENS-II-project. Also the European Spallation Source Study had finally received funding from the EU which gave the project work a significant boost. To acknowledge this and to make information exchange as intense as possible without requiring excessive duplication of presentations, ICANS-XIII and the 4th General Meeting of the ESS-project group were moved close together (in time and location).

The new interest in the long pulse option which has developed steadily since ICANS-XII reflected itself in a significant number of contributions to this topic.

The probably most decisive event, the negative decision on the ANS project in the US, which deprived the world neutron scattering community of its hope to have a next generation reactor neutron source soon, had an immediate effect also on the ICANS-group of laboratories:
Oak Ridge National Laboratory as the preferred alternative site for the US spallation neutron source project study has applied and was warmly welcomed as a new member of the collaboration. We all wish them success in the duty they have taken on and will be happy to share our knowledge and experience in every possible way.

There is a lot to share, indeed. Understanding of instruments has greatly progressed and the new capability, developed mainly in Los Alamos, to simulate whole instruments by Monte Carlo methods will certainly help to improve our abilities in doing things right from the onset. Operational experience from existing sources, in particular ISIS, is growing steadily and we are beginning to realise that some of the goodies, like uranium targets and methane cold moderators will not be able to carry on in the same way as the source power rises into the Megawatt range.

Oak Ridge itself was able to make a first contribution which may in fact have some potential for the future but will also require substantial development work: in a joint paper with PSI the proposal was made to move solid methane pellets in a liquid hydrogen bath through the moderator vessel by mechanical means and thus prevent higher polymers that are formed under the irradiation from clogging the pipework and the moderator vessel.

Even more futuristic ideas came from our Russian colleagues who proposed to use a subcritical arrangement of uranium-nitride cooled with gallium to produce a short pulse high intensity source with only a modest accelerator system.

There were numerous topics to be discussed among the participants and these discussions also carried on when some 50 attendants took advantage of the Sunday between ICANS-XIII and ESS-PM4 to participate in an excursion-transfer from PSI to Weinfelden, where the European Spallation Source team held their 4th Plenary Meeting. Although the nice weather that had been on during the full week of the ICANS-meeting slowly started to change, the visit to the summit of the Säntis mountain turned out as spectacular as ever. In view of the awe-inspiring sheer rock of the Säntis massive all of the brave hikers who had previously decided they would walk up or down rather than using the cable car finally changed their minds and did as everybody else. After a short stop at the Canton's capital the participants got their final taste of Appenzell at the Demonstration Dairy at Stein where everyone was introduced to the intricacies of Swiss Cheese making and had an opportunity to taste the different flavours of the three special varieties of this Appenzell product.

The Hotel Thurgauer Hof in the friendly little town of Weinfelden (nomen est omen!) was an ideal location for the ESS-PM4-meeting from October 16 to 19. Traditionally these gatherings are meant as a forum for accelerator experts, target developers and future users of ESS to exchange information and coordinate their efforts. Among the 106 participants a accelerator language was much more dominant than at ICANS-XIII because most of the accelerator related talks had been scheduled there.

The ESS-accelerator system has now been defined to feature a 1.334-GeV 50 Hz H^--linac with 3.75 mA time average current at 6% duty cycle and two pulse compressor rings to produce double pulses of less than 1 μs duration on the target. Significant progress was made in tracing individual particles to determine losses, a problem that needs careful attention at the power level in question (5 MW extracted beam).

However, there was also good news on the target side: after more than half a year of exploring different options, the ESS-Target Group had agreed to settle for a mercury liquid metal target and to make this their first priority option. The task to make this work is certainly not an easy one, but solutions seem to be visible for all of the most crucial problems such as pressure waves resulting from the short 100 kJ power pulses and the need to maintain a certain minimum temperature at all times to avoid the brittle regime of irradiated steel etc.

While it is certainly true that the meeting fully accomplished its scientific and technical goals, so did the Wednesday night boat ride on the Lake of Constance with a visit to the island of Mainau on the social side. Many a participant will certainly keep long term memories of it!

A final note:
Papers presented at ICANS-XIII and ESS-PM4 will be published in joint proceedings (2 volumes of over 900 pages altogether) which are already in press and will be available as of mid January 1996.

Information on ICANS is accessible on the World Wide Web under the URL

http://www.pns.anl.gov/icans/icansdescript.html.

An ESS-page is to come up soon.

Groups of ICANS-XIII participants visiting the SINQ-site on a guided tour were impressed by the craftsmanship and precision that was particularly visible at the present state of construction. With the neutron guide system largely completed and work on the "Tanzboden" in progress the guide hall will soon be ready for installation of instruments. The small angle scattering facility is already in place (back, left) and the analyser part of the single crystal diffractometer (back, right) is waiting to be moved to the target hall.

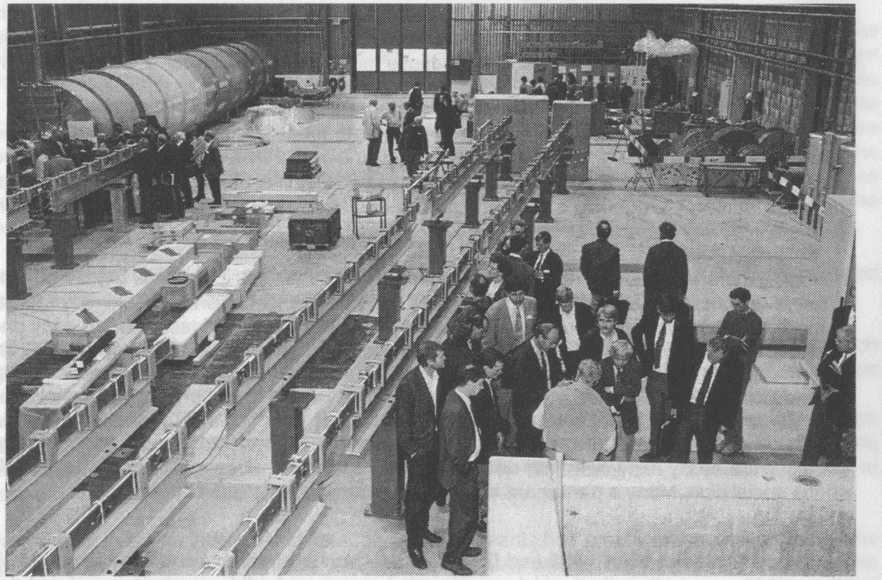


Photo: A. Müller, PSI

THIRD EUROPEAN SUMMER SCHOOL ON "SCATTERING METHODS APPLIED TO SOFT CONDENSED MATTER"

2 - 8 June 1996
BOMBANNES, Gironde - France

This school proposes advanced training for young researchers at post-graduate and post-doctoral level (typically aged 25 to 35 years). The organizers will especially encourage the participation of women researchers, students whose place of work is in a less favoured region and researchers who work in industry. It will be devoted to a practical approach to neutron, X-ray, and light scattering experiments involving theoretical principles, mathematical transformation back to real space and structural model calculation of the scattering. It is aimed to young colloid and polymer scientists (using scattering methods in their home laboratory or at large-scale facilities) who have already some background in this domain and want to learn complementary techniques and to exchange their experience. Primary objective is to explain current methodology of static and dynamic scattering techniques (avoiding both under and over-exploitation of data) rather than a general course on colloids and polymers. Basic information on data interpretation, on the complementarity of the different types of radiation, as well as information on recent applications and developments will be presented.

The school will be held at the vacation centre "Les Bruyères" in Bombannes with accommodation (full board) and lecture room located at the same site. The possibility of a common leisure activity (sailing, which is available nearby at the U.C.P.A. sailing centre) will ensure close contact between students and lecturers.

INTRODUCTORY LECTURES prepared by:
P. Pusey University of Edinburgh; **J. Teixeira** LLB CEN Saclay; **O. Glatter** University of Graz; **J.S. Pedersen** Risø National Laboratory; **Th. Zemb** CEN Saclay; **C. Williams** LURE Orsay; **R. Klein** University of Konstanz; **B. Farago** Institut Laue-Langevin Grenoble; **J.A. Nielsen** Risø National Laboratory; **R. May** Institut Laue-Langevin Grenoble; **P. Schurtenberger** ETH Zürich; **G. Porte** Université Montpellier; **D. Richter** IFF-Forschungszentrum Jülich; **P. Lindner** Institut Laue-Langevin Grenoble; **F. Boué** LLB-CEN Saclay;

SHORT CONTRIBUTIONS: the evening sessions will be devoted to **OBLIGATORY** short contributions (15 min each) given by the participants where the specific project and associated problems should be presented and discussed.

PROGRAMME:
23 HOURS GENERAL LECTURES (morning and late afternoon sessions)
10 HOURS LEISURE ACTIVITIES (afternoon sailing course)
16 HOURS PARTICIPANTS CONTRIBUTIONS (evening sessions)

SPONSORING INSTITUTIONS: The school is sponsored by **IFF Jülich, ILL Grenoble, PSI Villigen, Risø National Laboratory, CEA Saclay.**

PARTICIPATION FEES: **620 ECU (≈ 4000 FF)**
INCLUDING: accommodation (full board, single bedrooms), leisure activity with course (sailing, windsurfing), transport from and to BORDEAUX station or airport, lecture material.

Depending on subsidy decisions by further sponsors, the organisers could probably contribute to travel expenses for participants in exceptional cases.

THE SCHOOL WILL BE STRICTLY LIMITED TO 35 PARTICIPANTS FROM EUROPEAN COUNTRIES !

PREREGISTRATION to be returned to the address given below

Surname: Firstname:

Date of Birth: Place of Birth: Nationality:

Adress of University/ Institute/ Company:

Phone: Fax: e-mail:

Please send preregistration to **Dr. P. LINDNER, Institut Laue-Langevin, BP 156, F-38042 GRENOBLE cedex 9, FRANCE FAX: (33) 76 20 71 20; e-mail: lindner@ill.fr**

THE EUROPEAN NEUTRON SCATTERING
ASSOCIATION (ENSA) AND
THE PAUL SCHERRER INSTITUTE (PSI)

First Announcement

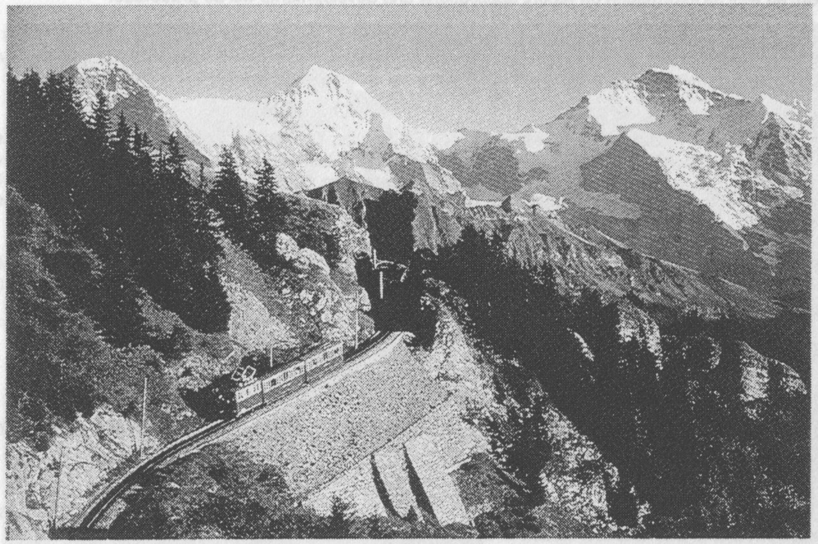


Photo: Tourismus Organisation Interlaken

ECNS'96

1*st* European Conference on Neutron Scattering

(Introductory Course: October 6-7, 1996)

8 - 11 October 1996 Interlaken Switzerland

The European Neutron Scattering Association (ENSA)

decided to hold the 1*st* European Conference on Neutron Scattering (ECNS'96) at Interlaken, Switzerland, October 8-11, 1996. At present European neutron scattering is seeing a renaissance (resumption of operation of existing neutron sources, new neutron sources, new neutron source projects) which will soon result in a large body of novel neutron scattering results. The scientific program will be set up by the ENSA Program Committee. Particular efforts will be made to encourage participation of young scientists, i.e., a large number of grants will be available for qualified Ph.D. and postdoctoral students. Also, the program will start with a **two-days' introductory course (October 6-7, 1996) on neutron scattering and instruments**, particularly for participants with little or no knowledge of the field.

The Paul Scherrer Institute (PSI), Villigen,

assisted by the Swiss Society for Neutron Scattering, is responsible for the organization of ECNS'96. A one-day visit to the spallation neutron source SINQ at PSI will be part of the conference program.

Important Dates and Deadlines

December 31, 1995	Deadline for submission of preregistration forms
June 1, 1996	Deadline for submission of abstracts
July 15, 1996	Notification of authors about acceptance
August 15, 1996	Deadline for early registration
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Conference Secretary / Further Information

Dr. J. Mesot
Laboratorium für Neutronenstreuung
ETH Zürich & Paul Scherrer Institut
CH-5232 Villigen PSI, Switzerland
Tel.: +41 - 56 - 310 40 29
Fax: +41 - 56 - 310 29 39
E-mail: ECNS@psi.ch

SINQ - Where we stand (November 1995)

G.S. Bauer, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

The target date for the first beam on SINQ is October 1996 and we are all eager to be constantly reassured that things are converging toward this date. The following short status update may help everyone's own judgement.

Much of the difficulties the project team had to fight in the past had to do with the complicated double-walled moderator tank, next to the target the core part of the neutron source. The most difficult parts of this tank have now been successfully manufactured and assembled (Fig. 1) - a great relief for the people in charge. Both, the thermal neutron scatterer which is to provide neutrons to the High Resolution Powder Diffractometer (HRPT) and the Single Crystal Diffractometer (SC3) in the target hall and the cold source setup are complete. The cold source is presently undergoing out-of-pile, cryogenic tests. The neutron guide system which it is to feed is almost complete and the tanzboden is presently being layed down. The part so far installed turned out to be completely to specifications and we are looking forward to seeing it completed soon (see Figure in the report on ICANS-XIII and ESS-PM4 in this issue). Instrument control cabins have also been delivered and have been put in place. With the difficulties that had arisen with the supplier of our water circuit valves now resolved, installation of the plant services is expected to proceed speedily. Good progress is also being made with the control system and the computerized visualisation system.

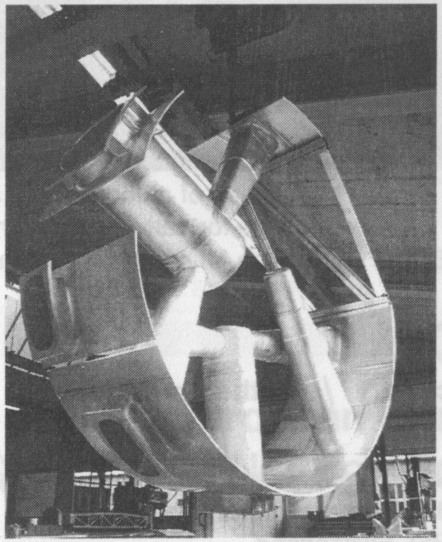


Figure 1: The delicate central part of the moderator tank with the beamhole thimbles and special moderator housings is taking shape at the manufacturers workshops (Photo Alusuisse Road & Rail AG).

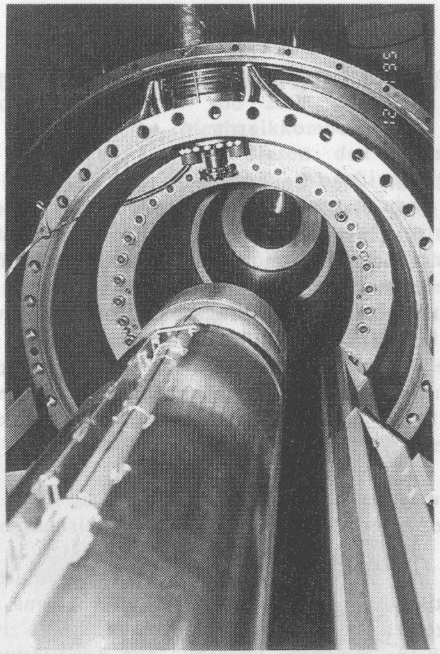


Figure 2: The cold moderator plug with the D_2-vessel at its front end being inserted in the vacuum housing for cryogenic tests.

Prototypes of the day-one target and its safety hull have been manufactured and the target exchange flask is nearing completion in the manufacturers workshops.

Good news also come from the accelerator operations. The current level of 1.3 mA, which was the goal for the period before the present shutdown has been achieved and operations became amazingly stable after a few initial problems in the power supply system had been cured. During the 1991 to 1995 operations periods the current averaged over the full period developed from 132 μA (1991) via 194 μA (1992), 458 μA (1993) and 562 μA (1994) to the respectable figure of 811 μA in 1995 and there is every reason to believe that, in 1997, 1.5 mA will be achieved, delivering 1 mA to SINQ as planned.

In summary, while things look good at present, a huge amount of work remains yet to be done and everybody's cooperation is required to ensure efficient use of funds and human ressources in order to be able to fulfil the tight schedule. This also applies to instrument designers and builders who compete for help from the same people also needed to complete the source proper.

SINQ-Instrumentierung: Mechanik

(P.Keller)

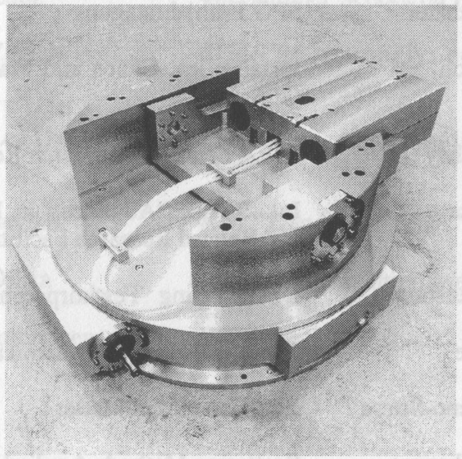
Die Mechanik für die Spektrometer an der SINQ ist in ihren Ausführungen sehr vielfältig. So benötigt man einerseits feinmechanische Geräte für Justierungen und andererseits riesige Gussteile für Abschirmungen. Auch bei den angewendeten Werkstoffen sind oft nicht alltägliche Anforderungen gestellt, wie: Unmagnetisch, strahlungsbeständig und strahlungsabschirmend, sowie Einsatz im Vakuum. Die bis jetzt ausgeführten Konstruktionen von Instrumenten umfassen eine Zeichnungsdokumentation von total etwa tausend Detail- und Zusammenstellungszeichnungen. Im Folgenden sollen nun der derzeitige Stand einzelner Instrumente, sowie deren Besonderheiten erläutert werden.

Die beiden Dreiachsenspektrometer Drüchal und Tasp befinden sich in der Leiterhalle. Deren Monochromatorabschirmungen sind in ihrer Funktionsweise aussergewöhnlich: Im Gegensatz zu anderen Neutronenstreuzentren, die für die Abschirmung viele radiale Segmente mit je einem Pneumatikzylinder verwenden, läuft bei uns eine kreisförmige Kette von einzelnen Abschirmsegmenten auf einer zirkularen horizontal angeordneten Schiene mit zwei Ebenen. Auf der tieferen Ebene fahren die Segmente unter dem Neutronenleiter durch und werden anschliessend durch ein Hubsystem automatisch und ohne Unterbruch der Rotationsbewegung auf die höhere Schiene probenseitig des Leiters angehoben. Die Analysatorabschirmungen beruhen auf dem Prinzip von radialen Abschirmsegmenten, welche pneumatisch gehoben werden. Anstelle von vielen Zylindern arbeitet dieses System jedoch mit nur einem Zylinder. Ein mechanisches System entscheidet, welche Segmente gehoben werden müssen. Bei beiden Monochromatorabschirmungen sind die Einzelteile fertig hergestellt. Bei jener des Drüchals hat die Montage soeben begonnen. Auch die Probentische werden demnächst in Montage gehen. Die Analysatorabschirmungen befinden sich in der Fertigung. Bei den Detektorabschirmungen ist die Konstruktion demnächst abgeschlossen.

Die beiden Spektrometer TOPSI und DMCG, in der Leiterhalle platziert, verwenden ebenfalls denselben Monochromatorabschirmungstyp. Die Unterbauten dazu sind nahezu endgefertigt. Die Fertigung der Oberbauten folgt demnächst. Da diese beiden Instrumente zuvor im Saphir bei unterschiedlicher Strahlhöhe verwendet wurden, müssen die Probentische und die Detektoreinheiten noch angepasst werden.

Das Spektrometer SC3 und HRPT besitzen eine gemeinsame Monochromatorabschirmung. Da diese direkt am Strahlkanal in der

Targethalle angeordnet ist, erreicht diese aus abschirmtechnischen Gründen das kolossale Gewicht von 280t. Im Strahlkanal der Targetabschirmung sitzen diverse Mechanikkomponenten, wie Antriebe, Drehgeber und Sensoren. Um zu diesen den Zugang einfach zu gewährleisten, kann die gesamte Abschirmung auf einem Luftkissengleitmodul verschoben werden. Dieses Modul ist bereits fertig hergestellt und wartet auf seine Montage. Die Abschirmungen bestehen aus schweren Gussblöcken, Kunststoffplatten und Stahlplatten, welche demnächst in Fertigung gehen werden. Bei den Instrumenten selbst sind beim SC3 die meisten Komponenten schon hergestellt. So ist die Detektormechanik bereits fertig montiert. Beim HRPT ist der Probentisch und die Detektorabschirmung in Konstruktion.



Rotationsmodul mit Ankopplungsmechanismus für den Probentisch.

Viele Instrumente haben Komponenten, welche auf Luftkissenfüssen gleiten. Wir benötigten deshalb "Tanzböden". Die üblichen Marmorböden sind im Neuzustand sehr gut, da der Stein jedoch eher weich ist, treten schnell Abnützungen durch "Winderosion" auf. Wir suchten deshalb eine Lösung mit einem härteren Boden. Längere Entwicklungen führten zur Realisierung eines Granitbodens mit geläppten Platten.

Die uns noch verbleibende Zeit bis zur Inbetriebnahme der SINQ, wird vor allem durch Montagen und durch die Fertigung diverser kleinerer Komponenten und Zubehörteile, beansprucht.

Konferenzen 1996/97

Datum	Ort	Thema
1996		
25.2.-2.3	Planneralm, A	11*th* Workshop "Correlated Systems & Superconductivity"
25.2.-4.4	Grenoble	HERCULES
4.-15.3.	Jülich	Ferienkurs "Streumethoden zur Untersuchung kond. Mat."
7.-8.3.	Neuchâtel	SPG Frühjahrstagung
11.-12.3.	Zurich	Instabilities, Chaos and Fractals in Crystal Growth
11.-15.3.	Bombay	IAEA Seminar "Research Reactors"
19.-21.3.	Osaka	Int. Symp. "Advances in Neutron Optics and Related Research Facilities"
25.-29.3.	Regensburg	DPG-Tagung "Festkörperphysik"
9.-21.4.	Erice	X-ray and neutron dynamical diffraction
22.-25.4.	Baveno-Stresa	EPS Condensed Matter
2.-8.6.	Bombannes (Gironde)	Scattering Methods Applied to Soft Condensed Matter
9.-15.6.	Crete (Greece)	5*th* Int. Conf. "Applications for Nuclear Techniques"
7.-11.7.	Budapest	5*th* World Congress on Superconductivity
13.-20.7.	Eger, Hungary	2*nd* Int. Summer School on High-T_c Superconductivity
7.-12.7.	Minnesota	Rare Earth Research Conf.
21.-25.7.	Campinas, Brazil	10*th* Int. Conf. on Small-Angle Scattering

Datum	Ort	Thema
2.-6.8.	Karlsruhe	MOS'96 HTSC
4.-9.8.	Denver	SPIE's Annual Meeting "Optical Science, Engineering, and Instrumentation"
5.-7.8.	Gaithersburg	Neutron Scattering Satellite Meeting to XVII IUCr
8.-17.8.	Seattle, USA	17*th* Int. Congress on Crystallography
8.-14.8.	Prague	Conf. on Low Temperature Physics
18.-24.8.	Zuoz	4*th* Summer School on Neutron Scattering
19.-22.8.	Zürich	SCES'96 (strongly correlated electron systems)
25.-30.8.	Les Diablerets	Properties and Applications of M-H Systems
9.-13.9.	Sevilla	EPS "Trends in Physics"
24.-27.9.	Osaka	Physics of Transition Metals
8.-11.10.	Interlaken	ECNS'96
1997		
28.2.-4.3.	Bejing	M^2S-HTSC-V
17.-21.8.	Toronto	ICNS'97

Neue Mitglieder

P. Böni

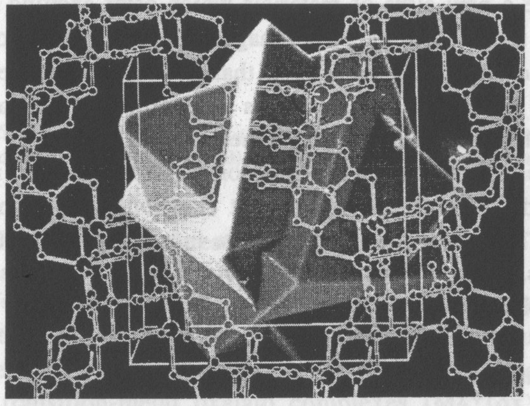
Seit dem 30. Juni 1995 sind acht Mitglieder der SGN beigetreten und damit hat sich der Mitgliederbestand der Schweizerischen Gesellschaft für Neutronenstreuung auf 150 erhöht:

- P. Keller, Laboratorium für Neutronenstreuung ETHZ & PSI
- S. Schorr, Hahn-Meitner-Institut
- H.P. Andres, Universität Bern
- R. Cerny, Universität Genf
- G. Vogl, Universität Wien
- R. Feyerherm, ETHZ
- F. Carsughi, Forschungszentrum Jülich
- U. Gasser, Laboratorium für Neutronenstreuung ETHZ & PSI

Magnetism and Supramolecular Chemistry

S. Decurtins[‡], R. Pellaux[‡], R. Huber[‡], H.W. Schmalle[‡], P. Fischer[†]
[‡]Anorganisch-Chemisches Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland
[†]Laboratorium für Neutronenstreuung, ETH & PSI, CH-5232 Villigen, Switzerland

MOLECULAR MAGNETISM HAS MANY APPEALING OBJECTIVES TO REACH



From magnetochemistry to solid state supramolecular magnetochemistry. Single crystal of a chiral 3D network compound with transition-metal ions as spin carriers.

1. Molecular Tectons and Supramolecular Chemistry

Chemical synthesis has the power to produce new molecules, which in the present context may be called **"molecular tectons"**. The word *Tecton*, — from the Greek, tekton, builder — is well known as a term referring to geological structures. The term may be applied equally well to structure on a microscopic scale. The name has been proposed for any molecule whose interactions are dominated by particular associative forces that induce the self-assembly of an organized network with specific architectural or functional features.

Cleverly designed tectons provide chemists with the tools of a powerful molecular-scale construction set. They enable them to engineer materials having a predictable order and useful solid-state properties.

Analogously, **supramolecular chemistry**, characterized as chemistry beyond the molecule, aims to design systems exhibiting molecular self-organization. Evidently, both terms express the strategy of the synthetic chemist creating novel materials which combine a selected set of properties, for instance from the areas of photophysics, photochemistry, magnetism and electronics.

Accordingly, it is the aim of our studies as outlined in this concise report, to explore a new class of materials which offer exciting new opportunities, mainly in the fields of molecular magnetism [1,2] and photophysics [3]. It is of interest, to engineer a compound that is not only magnetic but which also possesses additional characteristics not normally associated with magnetic solids such as transparency or nonlinear optical properties.

A possible approach is to exploit host/guest solids, i.e. supramolecular compounds, where each component contributes its own physical characteristics. The two entities could behave independently, resulting in composite properties, or they might interact synergetically, potentially leading to new physical phenomena.

2. Crystal Engineering

As chemistry is moving from the molecular to the supramolecular systems in the sense that, having learned how to synthesize molecules, it has been realized that if we want them to perform sophisticated physico-chemical functions it is necessary to assemble them correctly in space.

In particular, molecular magnetism, by essence of supramolecular nature, results from the collective features of components bearing free spins and on their arrangement in organized assemblies. Materials studied in this field comprise three categories: i) all organic with spins residing on moieties made up only of first row elements and all bridges comprised of first row elements; ii) organic/metallic with spins both on first row moieties and on molecules containing spin in d-orbitals, with the spin contribution of both systems essential for formation of the magnetic state; and iii) organic-bridged metallic with spins only in moieties containing d-orbitals and the interaction between selected spins relying upon spinless bridges containing first row elements.

In that scheme, we are following approach iii), based on the use of preorganized transition-metal complexes as spin carrier centers and mutually complementary molecular partners (see Figure 1). Due to their coordinating properties, they are predisposed to form two- (2D) and three-dimensional (3D) target structures [4-6].

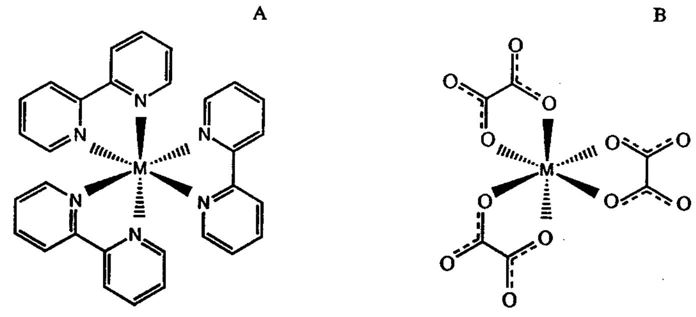


Figure 1: Schematic representations of the two chiral (the Λ-isomer is shown) preorganized cationic (A) and anionic (B) coordination entities. M = transition-metal ion as spin carrier.

2.1. The Chiral 3D Host-Guest System

Specifically, for the design of the chiral 3D supramolecular host-guest system, the mutual interaction of two distinct, complementary molecular subunits or coordination entities will be necessary. In the present case, these are anionic, tris-chelated transition-metal oxalato complexes $[M^{z+}(ox)_3]^{(6-z)-}$, ox = $C_2O_4^{2-}$, and cationic, tris-chelated transition-metal diimino complexes, for instance $[M(bpy)_3]^{2+/3+}$, bpy = 2,2'-bipyridine (see Figure 1).

A short characterization of the key structural elements shows that both coordination compounds have in common that they gain enhanced stability from the chelate effect, which in turn is expressed in their specific molecular topology. As a further consequence of this $[M(L^\wedge L)_3]$ type of connectivity, each coordinated metal ion represents a chiral center with D_3 point-group symmetry, showing either Δ- or Λ-helical chirality. Furthermore, the chelation mode of the transition-metal ions determines unambiguously shape and rigidity of these preorganized complexes, inasmuch as the specific configuration leads to the typical three-bladed propeller geometry.

With respect to the aim of attaining a high level of organization, both molecular entities exhibit a complementary functionality. The anionic, tris-chelated oxalato complexes are able to build up an extended polymeric host system, whereas the cationic complexes act as templates to initiate the formation and finally the crystallization of a three-dimensionally, covalently connected open framework. Simple topological rules will determine the connectivity of the 3D network structure which is known to be of a three-connected ten-gon (10,3) type. In short, this structure type is formally composed of $[M^{z+}(ox)_{3/2}]^{(3-z)-}$ subunits, whereby each one represents a three-connected point. Four of these units together (Z = 4) will have the necessary number of six free links to build the 3D net. Identically oriented links repeat at intervals of (Z + 1) points, so that circuits of $2 \cdot (Z + 1)$ points are formed. Thus, the structure represents a uniform net in the sense that the shortest path, starting from any point along any link and returning to that point along any other link, is a circuit of ten points (see Figure 2).

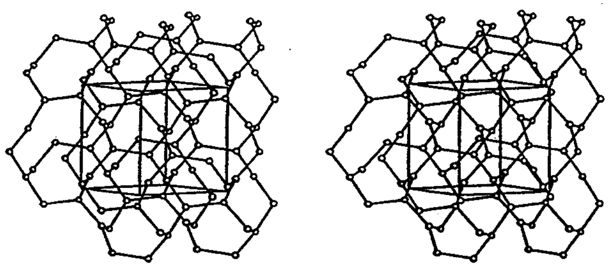


Figure 2: Stereoview of the 3-connected 10-gon (10,3) network topology.

The topological principle implies for the 3D case, that only subunits of the same chirality are assembled (an alternation of the chirality would lead to the 2D structural motif). Consequently, the uniform anionic 3D network-type with stoichiometries like $[M^{II}_2(ox)_3]_n^{2n-}$ or $[M^IM^{III}(ox)_3]_n^{2n-}$ is chiral, as it is composed of 2n centers exhibiting the same kind of chirality. Naturally, this chiral topology is in line with the symmetry elements which are present in the crystalline state of these 3D frameworks, which in sum constitute either one of the enantiomorphic cubic space groups $P4_332$ or $P4_132$ for the former and the cubic space group $P2_13$ for the latter stoichiometry. Thereby, the 2n metal ion centers occupy special sites with a three-fold symmetry axis.

Furthermore, extended helical geometries are encountered through the three-dimensional repetitive assembling of subunits with helical chirality (see Figure 3). Thus, the framework structure may alternatively be seen as composed of either right-handed (Λ-chirality) or left-handed (Δ-chirality) helices with a 4_1 arrangement, running in three perpendicular directions while simultaneously being covalently bound to each other.

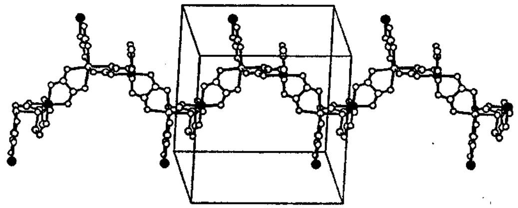


Figure 3: View of a helical strand along a 2_1 axis from a $[M^IM^{III}(ox)_3]_n^{2n-}$ type compound.

In addition, the chiral, cationic tris-chelated guest complexes fit perfectly into the elaborate pattern of vacancies. Within the channel-system they occupy the n available chiral sites with point symmetry 32 ($P4_332/P4_132$) or 3 ($P2_13$). At least for the former case, the molecular D_3 point-group symmetry of the guests is fully retained. In analogy to a "lock and key effect", a Δ–Δ or Λ–Λ pairing in the chirality of the host-framework and the guests is observed.

One of the main attractions in studying these 3D extended network compounds is the fact that the synthetic route allows for a large variation of the metal ions, mainly within the first-row transition-metal series but also extendable to e.g. Ru, Os, Rh ions in case of the templating cationic complexes. Thus, an overall stoichiometry of e.g. $[M^{II}(bpy)_3]^{2+}{}_n\ [M^{II}_2(ox)_3]_n^{2n-}$ results.

2.2. The Honeycomb Layer Compound

The anionic tris-chelated oxalato complexes may also form infinitely extended sheets of hexagonal symmetry. The discrimination between the formation and crystallization either of a 2D or a 3D supramolecular host-guest system with analogous network stoichiometries relies on the choice of the templating counter-ion. Evidently, the template cation determines the crystal chemistry.

In particular, $[XR_4]^+$, (X = N, P; R = phenyl, n-propyl, n-butyl) cations initiate the growth of 2D sheet structures containing $[M^{II}M^{III}(ox)_3]_n^{n-}$, M^{II} = Cr, Mn, Fe, Co, Ni, Cu, Zn; M^{III} = V, Cr, Fe, network stoichiometries [6,7]. Figure 4 shows a sector from a 2D honeycomb layer.

As noted above, in contrast to the chiral 3D network compounds, the 2D framework topology implies an assembly of coordination entities with alternating chirality between nearest neighbouring centers. Although these 2D compounds are not chiral, they express a structural polarity due to the specific arrangement of the templating cations (see Figure 4b). These organic cations which are located between the anionic layers determine the interlayer separation which typically shows values in the range of 8-9 Å, but also the molecular packing arrangement of the solids, hence the resulting space group, for instance R3c for $[P(Ph)4]^{+}$, $[N(Pr)4]^{+}$ and P63 for $[N(Bu)4]^{+}$. Altogether, a careful examination of the structural parameters like spacing between the layers or symmetry and degree of distortion of the coordinating ligand sphere around the magnetic centers are a prerequisite for a thorough understanding of the magnetic properties.

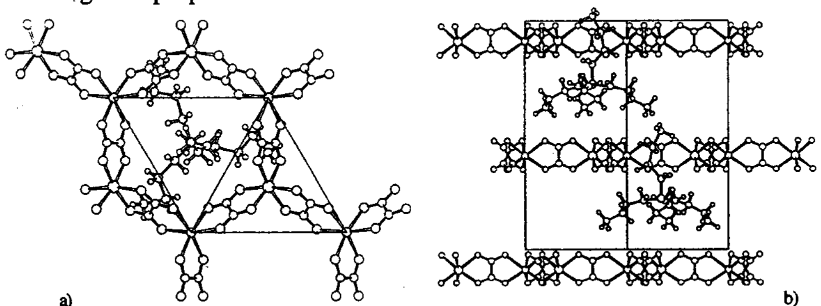

a) b)

Figure 4: Sector from the $\{[N(Bu)_4][Mn^{II}Fe^{III}(ox)_3]\}$ layer compound.
a) [001] projection; b) [110] projection.

3. Molecular Magnetism

Clearly, where major break-throughs must be expected in the field of molecular magnetism is in the association of properties which are not met in traditional magnets, for instance if photophysical properties are associated with magnetic phase transitions.

Generally, any synthetic strategy aimed at designing molecular magnets has to answer the questions i) how to control the interaction between the nearest neighbouring magnetic spins and ii) how to control parallel alignement of the magnetic spin vectors over the 3D lattice. Naturally, if the compounds assume a 2D layer structure, the magnetic properties depend on the nature of both the intra- and inter-layer magnetic interactions.

With respect to the first question, it is well-known, that the oxalate bridge is a good mediator in both antiferromagnetic and ferromagnetic interactions between similar and dissimilar metal ions, therefore it has been widely used to

construct polynuclear compounds in the search for new molecular-based magnets. Naturally, in search for an answer to the second question, effort has to been given to the investigation of the magnetic ordering behaviour of the above described 2D and 3D systems. In the following, a brief account of the current state of the ongoing investigations by means of the neutron scattering technique will be given.

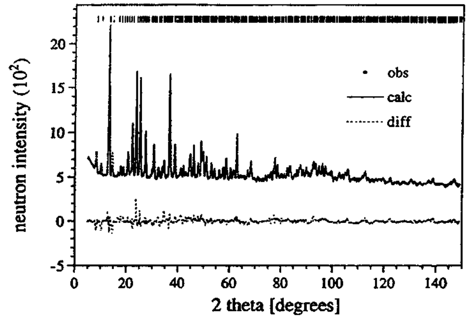


Figure 5: Observed, calculated and difference neutron diffraction patterns of a polycrystalline sample of **1** at T = 30 K (paramagnetic phase). Diffractometer D2B at the high-flux reactor of the Institute Laue-Langevin (ILL) in Grenoble; high intensity mode with neutron wavelength λ = 1,593 Å.

Thereby, we report on neutron diffraction experiments, performed on a 3D polycrystalline sample with stoichiometry $[Fe^{II}(d_8\text{-}bpy)_3]^{2+}{}_n[Mn^{II}{}_2(ox)_3]_n{}^{2n-}$ (**1**), with the goal to determine the magnetic structure of this helical supramolecule in the antiferromagnetically ordered phase, thus below T_N = 13 K [8]. The existence of this magnetically ordered phase has formerly been suggested from magnetic dc-susceptibility measurements which revealed a rounded maximum at about 20 K in the χ_M versus T curve (thus T_N < 20 K) as well as a Weiss constant Θ of -33 K in the $1/\chi_M$ versus T plot [5]. Accordingly, a magnetic ac-susceptibility experiment revealed an ordering temperature around 15 K. This long-range magnetic ordering originates basically from the exchange interaction between neighbouring Mn^{2+} ions, mediated by the bridging oxalate ligands.

In oder to confirm the room-temperature crystal structure to be valid down to helium-temperatures, the polycrystalline compound **1** has been investigated by neutron diffraction at several temperatures. Between 300 K and 1.8 K, all the measured neutron diffraction patterns are consistent with a crystal structure which is described in either one of the enantiomorphic pair of the cubic space groups $P4_332$ / $P4_132$. In Figure 5, the good agreement of observed and calculated neutron intensities is illustrated with the data of the paramagnetic phase at T = 30 K. Consequently, no crystallographic phase transition could be detected, only the lattice parameter shows the expected thermal contraction: a = 15.427(2) Å (300 K); 15.374(2) Å (150 K); 15.359(1) Å (100 K); 15.353(1) Å (60 K); 15.349(1) Å (30 K); 15.348(1) Å (1.8 K).

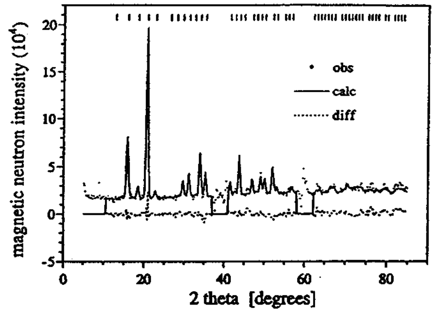
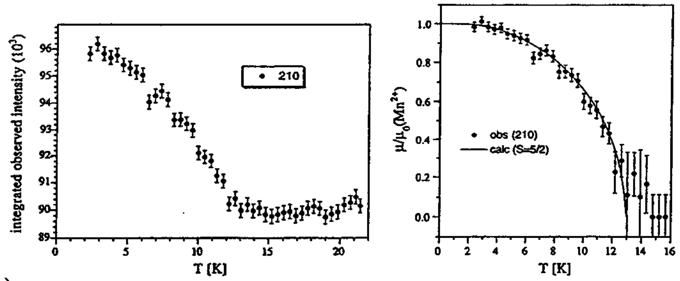


Figure 6: Observed [difference I(1.8 K) - I (30 K)], calculated and difference magnetic neutron diffraction patterns of 1 with long-range AF order due to the magnetic Mn^{2+} moments. Diffractometer D1B at the high-flux reactor of the Institute Laue-Langevin (ILL) in Grenoble; neutron wavelength λ = 2.5154 Å.

Furthermore, as anticipated, an increase of the intensities due to long-range antiferromagnetic ordering of the Mn^{2+} ions could be detected with the neutron diffraction measurements performed in the temperature range from 30 K to 1.8 K. Figure 6 illustrates the observed [difference I(1.8 K) - I(30 K)], calculated and difference magnetic neutron diffraction patterns. Thereby, it has to be noted that the increase of the intensities corresponds to a propagation vector **K** = 0, i.e. a magnetic unit cell being equal to the chemical cell. The temperature dependence of the dominant magnetic intensity (210) at 2Θ = 21.1°, as shown in Figure 7a, indicates an ordering temperature T_N = 13(0.5) K, in good agreement with the magnetic susceptibility experiments. As a further aspect, the observed sublattice magnetization is compared with the theoretical derivation from a mean-field approximation for a S = 5/2 spin value which originates from the high-spin d^5-electron configuration of the Mn^{2+} ions. Figure 7b illustrates good agreement between the experimental data and the theoretical values.

Finally, it remains to discuss the determined magnetic moment configuration of this three-dimensionally linked Mn^{2+} network. With respect to space group $P4_132$, the Mn^{2+} ions occupy sites 8 c; x,x,x with x = 0.64907. The best agreement between observed and calculated magnetic neutron



a) b)

Figure 7: a) Temperature dependence for increasing temperature of the integrated magnetic neutron intensity of the (210) peak. b) Sublattice magnetization within the 3D Mn^{2+} network of compound 1 as a function of temperature and its relation to the theoretical line derived from the mean-field approximation.

intensities was achieved with a collinear, antiferromagnetic arrangement of Mn^{2+} moments according to the three-dimensional irreducible representation τ_4, which is derived from the enantiomorphic pair of the chiral, cubic crystallographic space groups $P4_332$ / $P4_132$ [9]. Thereby, the ordered magnetic moment at 1.8 K amounts to μ_{Mn} = 4.6(1) μ_B, where μ_B is the electron Bohr magneton. The saturation magnetization, M_S, is related to the equation $M_S = g \cdot \mu_B \cdot N \cdot S$, where S is the spin quantum number, N the Avogadro number and g the electron g-factor. Thus, a g·S value corresponding to the number of unpaired electrons of 4.6 is obtained, which is compatible with the expected 5 unpaired electrons (g = 2) from the Mn^{2+} ions. Naturally, in the present experiment, no information about a preferred direction of the magnetic moments with respect to the crystallographic axes can be gained from the polycrystalline sample with cubic symmetry.

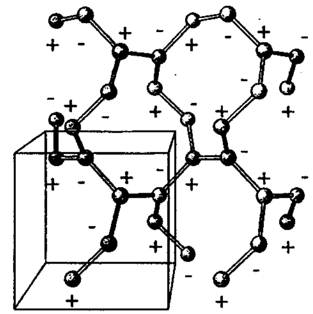


Figure 8: A scheme of the AF, collinear configuration of the magnetic moments originating from the Mn^{2+} ions, which constitute the chiral 3D network compound 1.

Figure 8 depicts the pattern of the magnetic structure within the 3D manganese(II) network. Despite the three-dimensional helical character of the framework structure incorporating the magnetic ions, a two-sublattice antiferromagnetic spin arrangement has now proved to occur, hence no helimagnetic structure has shown up. After all, a behaviour which is in accordance with the typical isotropic character of the Heisenberg ion Mn^{2+}.

4. Concluding Remarks

In conclusion, the outlined neutron diffraction experiments have successfully proven to trace for the first time the spin configuration defining the 3D antiferromagnetic phase of a representative compound of novel, helical 3D supramolecular materials. In the mean time, positive results have also been obtained in case of a ferromagnetically ordered phase for a 2D honeycomb layered material.

Not mentioned in this report is the whole aspect of the photophysical properties of these supramolecular materials. Some exciting phenomena have already proved to occur and ongoing studies will focus to look for any combined properties resulting from these molecular based materials.

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Schweizerische Gesellschaft für Neutronenstreuung (SGN)
Société Suisse pour la Diffusion des Neutrons (SSDN)

Anmeldeformular

Name:..

Vorname:..

Akad. Titel:..

Geschäftsadresse:..

....

....

Telefon:..

Telefax:..

Telex:..

E-Mail:..

Privatadresse:..

....

....

Telefon:..

Zustelladresse: Geschäft/Privat ? (Nichtzutreffendes streichen)

Datum: .... Unterschrift: ....

Bitte senden an:

Sekretariat SGN, c/o Laboratorium für Neutronenstreuung, 5232 Villigen PSI

(Jahresbeitrag: Fr. 10.--)