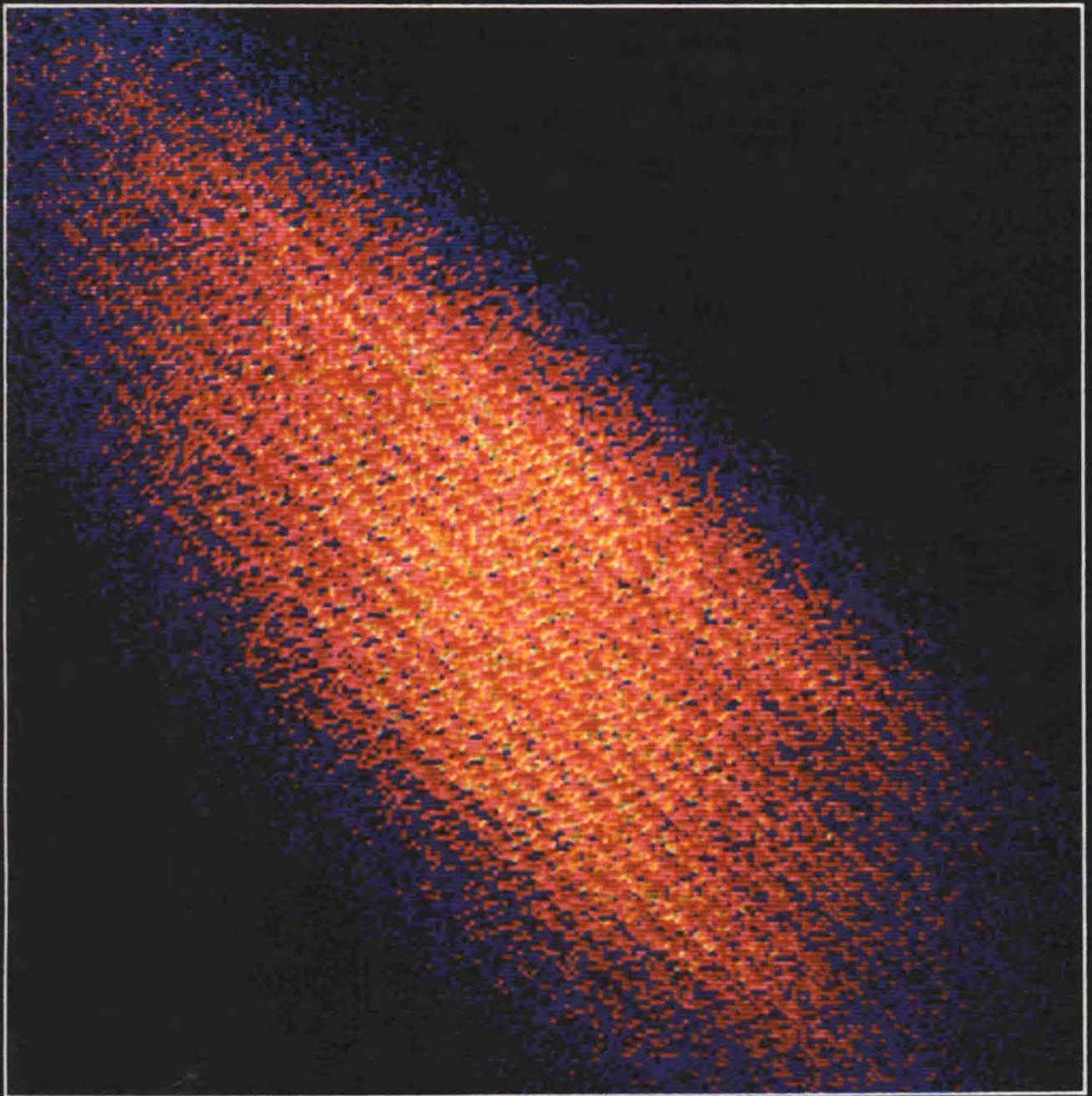
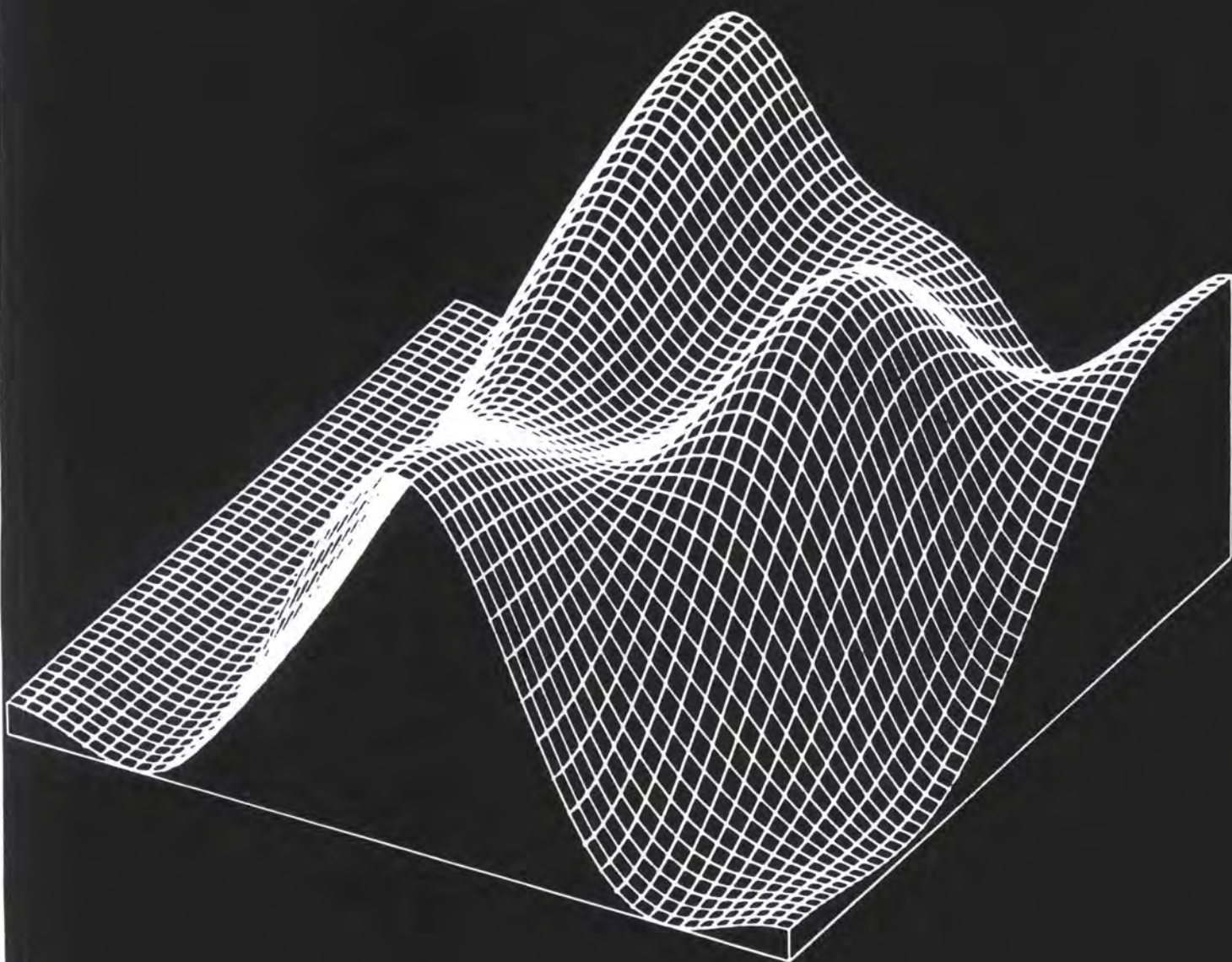


ANNUAL REPORT 83

INSTITUT MAX VON LAUE - PAUL LANGEVIN - GRENOBLE - FRANCE



ILL



Rotational potential in $(\text{NH}_4)_2\text{SnCl}_6$ (measurements obtained on D10 by W. Prandl et al., Tübingen)

Applications for the use of the ILL facilities

All research proposals have to be submitted to the Scientific Council for approval. The Council meets twice each year and the closing dates for the acceptance of applications are:

February 15 and August 31.

The completed research proposal forms should be sent to:

The Scientific Coordination & Public Relations Office (SCAPRO)

Institut Max von Laue — Paul Langevin

156 X

38042 Grenoble Cedex

France

Tel. (76) 48.72.44 B. Maier

48.71.79 G. Briggs

48.70.41 K. Mayer-Jenkins (Secretary)

48.70.82 A. Taffut (Secretary)

Telex: 320621 F

(Appropriate application forms may be obtained on request from the above office).

Under normal circumstances the ILL makes no charge for the use of its facilities. However, special equipment (other than the existing instruments, counters, standard cryostats and shielding requirements) must be provided by the user. This applies particularly to the experimental samples which must, in all cases, be provided by the user. Chemistry and Biology laboratory facilities are available for any necessary sample preparation.

The ILL makes a limited contribution towards the travel and subsistence expenses for experimentalists coming from approved laboratories in the three member countries. (Details on request).

Commercially exploitable results

Visitors and ILL scientists may occasionally be involved in experiments which have possible commercial applications. If any scientist considers that this is the case, he should get in touch with the Scientific Secretary.

Other publications available

Neutron Research Facilities at the ILL High Flux Reactor, Edition 1983.

Information and Regulations for Reactor Users, Long-Term Visitors and New Scientific Staff, Edition March 1984
both available from SCAPRO

Experimental Reports and Theory College Activities 1983
available from the ILL Library.

Front Cover

Correlation matrix for time-of-flight (y-axis) versus kinetic energy (x-axis) of fission fragments from thermal neutron induced fission of ²³⁵Uranium. For a given fragment mass there is a one-to-one correlation between the time it takes a fragment to travel along a fixed flight-path and its kinetic energy. Individual fission fragment masses should appear in the figure as diagonal lines running from the top left (long time-of-flight or equivalent low velocity and low kinetic energy) to the bottom right (short time-of-flight and high energy) with the mass number increasing from bottom left to top right. Indeed, the data gather around those lines which shows that individual masses have been resolved.

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The Institut Max von Laue - Paul Langevin

The Institut Max von Laue-Langevin (ILL) at Grenoble was formally founded in January 1967, with the signature of an intergovernmental convention between France and the Federal Republic of Germany.

The aim was to provide the scientific community of the affiliated countries with a unique neutron beam facility applicable in fields such as the physics of condensed matter, chemistry, biology, nuclear physics and materials science. The construction of the Institut and its high flux reactor was undertaken as a joint French-German project, with a total capital investment of 335 million FF. The reactor went critical in August 1971 and reached its full power of 57 MW for the first time in December 1971.

The year 1972 saw the start-up of the cold and hot sources, the first instruments and the beginning of the experimental programme. On January 1, 1973 the United Kingdom joined the Institut as a third equal partner, contributing its share to the total capital investment.

The corresponding intergovernmental convention was formally signed in July 1974 by the pertinent ministers from the three affiliated countries.

On December 9, 1981 a protocol was signed by representatives from the three member countries which extended the life of the ILL until December 31, 1992.

The ILL is a non-trading company under French civil law.

The three countries are represented by the following Associates:

- Kernforschungszentrum Karlsruhe GmbH, Germany
- Centre National de la Recherche Scientifique, France
- Commissariat à l'Énergie Atomique, France
- Science and Engineering Research Council, United Kingdom.

These Associates are represented on a Steering Committee, which establishes the general rules of the management of the ILL. The Institut is headed by a Director and two Assistant Directors, all with a five year tenure, the former to be nominated alternately by the German and the British Associates, the other two by the remaining Associates.

A Scientific Council, nominated by the Associates, advises the Directors on the scientific programme and on practical aspects relating to its operation.

The scientific users' community of the ILL is represented in 8 subcommittees of the Scientific Council, which meet twice a year to select those research proposals which are to be carried out at the neutron beam facilities of the ILL. A further Subcommittee of the Scientific Council deals with questions of instrumentation, serving as a discussion platform between the ILL and its external users.

The purpose of the ILL thus differs from other research institutes in so far as it is a central facility created so that chemistry, solid state physics, fundamental and nuclear physics, biology and metallurgy specialists from laboratories in the partner countries can use the unique power of neutron techniques to broaden the attack on their problems.

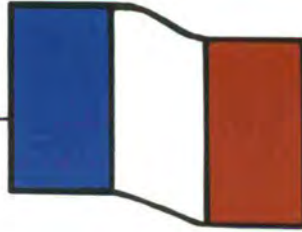
Designing and operating instruments and helping the visiting users to carry out their experiments is thus the principal task of the Institut's own scientists. The experimental use of the instruments by ILL staff is subject to the same approval system as their use by external teams.

External Organisation of the Institut Laue-Langevin 1983

Associates of the Institut



Science and Engineering
Research Council (SERC)



Commissariat à l'Énergie
Atomique (CEA)
Centre National de la Recherche
Scientifique (CNRS)



Kernforschungszentrum
Karlsruhe (KFK)

Steering Committee (at its last meeting)

Atkinson (SERC)	Cribier (CEA)	Blaesing (BMFT)
Hobbs (SERC)	Horowitz (CEA)	Hofbauer (BMF)
Leadbetter (SERC)	Lehmann (chairman) (CNRS)	Klose (KFK)
Otewill (Univ. of Bristol)	Miquel (CNRS)	Simon (Max-Planck-Ges.)

Audit Commission

Pettet	Polderman	Binder
Millington	Racine	Riess

Scientific Council (at its last meeting)

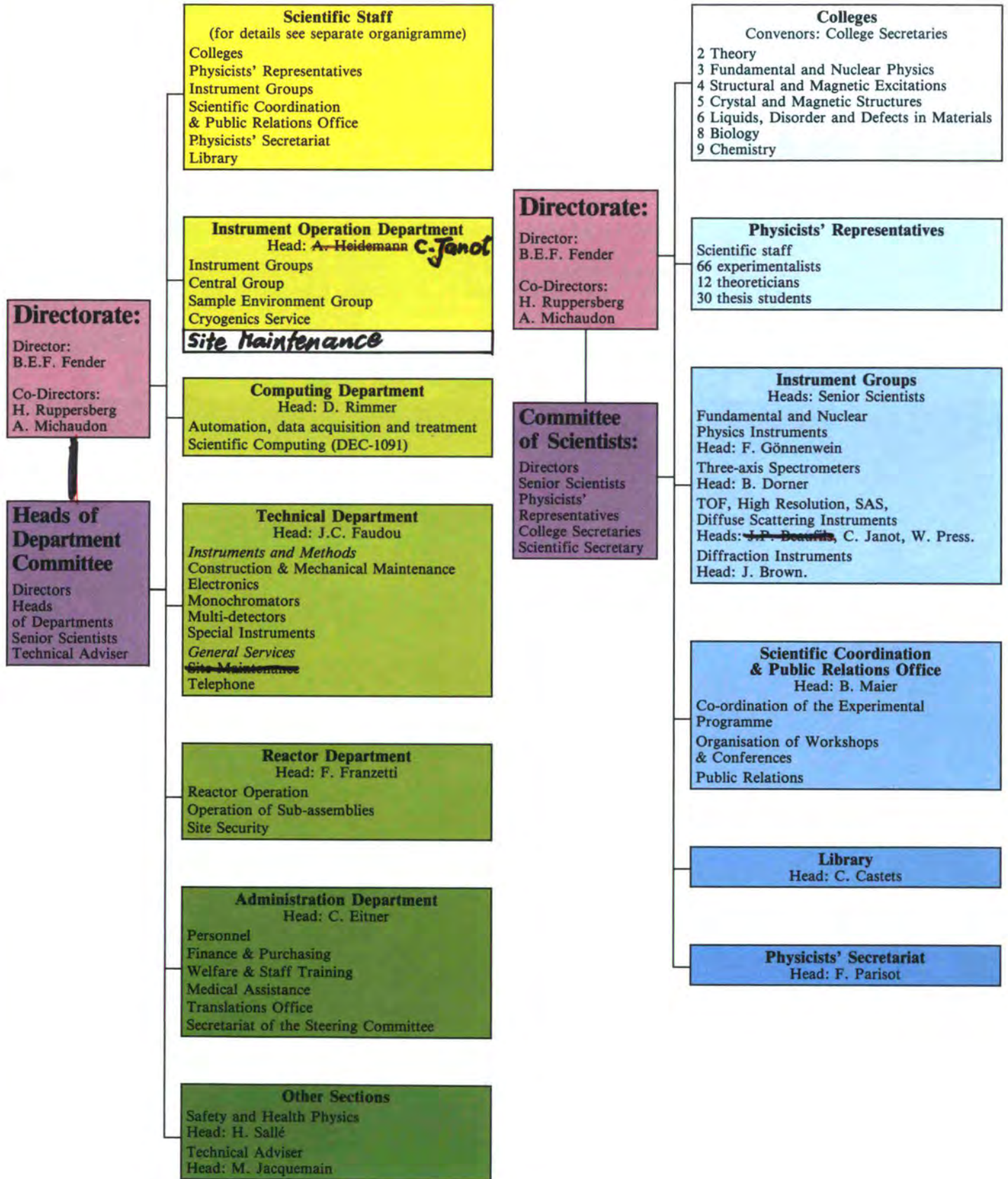
Armbruster — GSI Darmstadt	Enderby — Univ. Bristol	Maier — ILL
Bienfait — Univ. Marseille	Fender — ILL (Chairman)	Mampe — ILL
Blanquet — Ecole Polytech. Palaiseau	Franck — Univ. Karlsruhe	Miller — Univ. Oxford
Blundell — Birkbeck College, London	Hahn — TH Aachen	Nierhaus — MPI Berlin
Comes — Univ. Paris-Sud	Hart — London Univ.	Ruppertsberg — ILL
Cowley — Univ. Edinburgh	Hewat — ILL	Schatz — KFK Karlsruhe
Drifford — CEN Saclay	Horner — Univ. Heidelberg	Smith — Unilever Research
Eitner — ILL	Joly — CEN Saclay	Villain — CEN Grenoble
		Winter — ILL

Subcommittees of the Scientific Council

Fundamental and Nuclear Physics	Structural and Magnetic Excitations	Crystal and Magnetic Structures		Liquids, Disorders and Defects in Materials	Biochemistry	Chemistry		Instruments
						Large Molecules	Surfaces & Spectroscopy	
Lynn Schult Signarbieux Sinclair Specht Vinh Mau	Cowley Edwards Hanke Horner Lajzerowicz Lambert Rainford Rossat-Mignod Schatz	Coles Day Fuess Goodenough Plumier Prandl Souletie Zinn	Bronger Cheetham Fischer Galy Marezio Pouget Sim	Dupuy Durand Enderby Hensel Schilling Schofield Stewart Suck	Blundell Chabre Fuller Giège Janin Miller Nierhaus Saenger Schulz	Charvolin Cotton Hoffmann Kilian Otewill Richards Weill	Clough Conard Ehrhardt Forstmann Hueller Lassègues Thomas	Glaeser Nifenecker Pepy Press Rainford Renouprez Schatz Stewart Stirling

General Organigramme

Organigramme of the Scientific Section



Visits and Events in 1983

Visitors to the Institut in 1983 have included M. Lenz and M. Senard, co-ordinators of French-German cooperation; Mme Niblaeus, the Swedish Secretary of State at the Ministry of Research; M. Chabbal, President of the Scientific Mission of the Ministry of Industry and Research; M. Teillac, High Commissioner for the Atomic Energy Authority; M. Renon, Administrator-General of the CEA; M. Papon, Director General of the CNRS; Prof. Maier-Leibnitz; M. Laverie,

Deputy Head of the Central Nuclear Safety Commission; M. Lesgards and M. Chevillot (Cabinet of the Président de la République); Prof. Böhm (Executive Head of KFK Karlsruhe) and Prof. Treusch (President of the German Physical Society). Among the many groups visiting were the National Administrators of NATO and a groupe of 16-18 year old Germans who were prize winners in a nationally organised competition for scientific projects ("Jugend forscht").



Visits and Events in 1983



1. Prof. H. Maier-Leibnitz (second from left) during his visit to the ILL in September 1983. On this occasion he was presented with a photograph of himself (Dr. Fender, Director, at the right; Prof. Ruppertsberg, Co-Director, second from right; Dr. Heidemann, at the left).
2. Mrs. Niblaeus, Swedish Secretary of State, visited the ILL on 29 September 1983. In the picture she receives explanations on the ILL experimental activities from Dr. Fender and Prof. Ruppertsberg (in the middle: Dr. Comès from the CNRS and Dr. Heidemann, ILL).
3. The Swedish visitor was accompanied among others by Dr. Chabbal, President of the Scientific Mission of the French Industry and Research Ministry.
4. Prof. Böhm, Executive Head of the KFK Karlsruhe, visited the ILL on 25 November 1983. In the picture he (in the middle) is visiting the experimental hall of the HFR; on his tour he was accompanied by Prof. Ruppertsberg (left), Prof. Gönnerwein (right) and Dr. Maier.
5. The prize winners of the German competition for scientific projects "Jugend forscht" during their visit to the ILL in October 1983.
6. Prof. Treusch, Dortmund, the President of the German Physical Society (at the left), during his visit to the ILL on 22 November 1983. On the picture Mr. Kramer from the Reactor Department explains the storage procedure of fuel elements.
7. The members of the ILL Steering Committee visited the ILL on the occasion of their Autumn Meeting in Grenoble on December 2. In the picture are, from left to right, Dr. H. Atkinson, Prof. R. Ottewill, Dr. D. Schildt and Prof. A. Leadbetter during their visit to the test hall where they received explanations from Dr. R. Pynn on the new IN20.

Director's Report

I write this introduction for last year's activities with a record number of scientific proposals — 640 — piled on my desk. They cover the six month period April to October 1984 but only a fraction can be accommodated because the number of days asked for on neutron scattering instruments alone (5344) is 2.7 times larger than the number available.

Altogether there have been over 5300 proposals in the last five years — a remarkable demand in view of recent uncertainties in the reactor programme. There are also clear indications that, at this level of competition, good proposals are rejected and new users discouraged. This is especially the case in chemistry and biology, where the visiting researcher is nearly always also involved with other techniques in his home laboratory. It is also particularly true, of course, for applicants from non-member countries.

The strength of world-wide demand for the unique ILL facilities is shown by the fact that, out of the 640 proposals, nearly 90 involve scientists from outside the three member countries, including requests from Australia, Austria, Belgium, Bulgaria, Canada, Denmark, East Germany, Hungary, India, Ireland, Israel, Italy, Japan, the Netherlands, Norway, Poland, Sweden, Switzerland, USA, USSR and Yugoslavia.

Over 20 proposals include scientists from the United States, usually in collaboration with scientists from France, Germany or the U.K. The institutions involved are: Brookhaven National Laboratory, Argonne National Laboratory; Lawrence Livermore; Los Alamos National Laboratory; National Bureau of Standards, Washington; Oak Ridge National Laboratory; and among many universities: Cal Tech, Harvard, Illinois, Michigan, MIT and General Electric, Schenectady. There are applications from several Soviet laboratories including the Kurchatov Institute of Atomic Energy, Institute of Protein Research, and the Institute of Crystallography (all in Moscow); Leningrad Nuclear Physics Institute, Institute of Geology and Geophysics, Novosibirsk, and the Joint Institute for Nuclear Research at Dubna.

The mixing of nationalities, and thus of scientific cultures, is an important feature of the ILL; about a quarter of all experiments carried out involve two or more different countries. Even more important, the ILL stimulates inter-laboratory co-operation generally with nearly 60% of the experiments performed by collaborators from different laboratories. Naturally many of these (one-half) involve ILL scientists (not counting local contact participation) but quite apart from these obvious co-operations, it is clear the Institut catalyses a large number of other collaborations.

The role of the ILL as an advanced study institute emerges more and more clearly with a contribution much larger than simply the provision of neutron scattering or nuclear physics facilities. Even for Directors accustomed to a global view, the range of scientific activities is so diverse that an overall view can be elusive. How does one compare investigations on the foundations of quantum theory by neutron interferometry with studies on the dynamics of incommensurate structures on a triple axis spectrometer? Alternatively, can one judge between the relative importance of fundamental studies on creep in metals and the determination of the shape of individual protein molecules in ribosome? Yet the latter studies both compete for the same, scarce, small angle scattering time. What is clear is that even frequent visitors see the Institut largely as a reflection of their own interests while casual visitors often miss the depth of the contribution of neutron research to our general understanding of solids and liquids, to say nothing of its contributions to the understanding of nuclear fission, nuclear structure and fundamental physics.

To help readers of the Annual Report, we include the first of a series of reviews (this year on Incommensurate Structures by R. Currat) written by ILL scientists or visitors. Out of more than 450 publications (including 363 involving ILL staff) concerned with work at the ILL, I also draw attention to several general reviews which are given in the lists of publications:

- Neutron Scattering Studies of Virus Structure (*Cusack*);
- Concentrated Dispersions (*Ottewill*);
- Small Angle Neutron Scattering by Biological Systems (*Zaccai and Jacrot*);
- Establishment of Short-range Order during Nucleation and Growth of Precipitates within Amorphous Solids (*Wright et al*);
- Neutron Scattering Studies of Diffusion in Solids (*Lechner*);
- Magnetism in Solid ^3He (*Roger et al*);
- Neutron Optics (*Klein and Werner*);
- Neutron Spin Echo Ten Years After (*Mezei*).

Two ILL Workshops have also been published during the year: an International Conference on the Impact of Polarised Neutrons on Solid-State Chemistry and Physics (published by the *Journal de Physique*) and Position-Sensitive Detection of Thermal Neutrons (Eds. Convert and Forsyth, published by Academic Press). A Workshop on Reactor-Based Fundamental Physics will be published in the Spring of 1984.

Reactor Renewal Programme

The current aims of the reactor group are:

1. To complete the major programme of renewal centred around the beam tube replacement programme during the 1984/85 shutdown;
2. To replace and modernise control and measuring equipment associated with the reactor and health physics;
3. To install the new horizontal cold source in 1986;
4. To plan a renewal and maintenance programme which avoids, as far as possible, major interruptions to the reactor schedule.

The planning for the 1984/85 shutdown indicates a shutdown period running from October 1984 to the end of July 1985, with the most complicated task being the replacement of the beam tubes which serve the guide tubes. Since 1980 a major effort has gone into the design of the horizontal cold source; the timetable for its construction and installation involves the final designs being ready in mid-1984, construction to be completed by the beginning of 1986, and installation in mid-1986. The second guide hall is at present under construction.

Instruments and Methods

The Institut is in the middle of its most ambitious instrument building programme ever, which is possible because of the impetus given by the modernisation programme and by the experience gained in the first 10 years of operation. When completed, the effect on the Institut's programme will be little short of dramatic.

There are several ways of looking at this, but by 1986 the situation, compared with mid-1983, will be as follows:

- 5 new instruments (PN8, IN14, IN15, DB21, D22);
- 10 instruments with flux or rates of detection improved by a factor 5-10 (D2B, D20, D4B, D19, D9B, D7B*, IN1B, IN20*, IN4B, IN11B);

* Effectively new instruments

- 6 instruments with gains around a factor 2 (D11C, D16, D17, IN5, IN6, IN10B);
9 with significant improvements but less marked than above (PN1, PN2, PN3/4, D3, D10, D15, IN8, IN13).

It is also important to recognise that, apart from the normal, fully scheduled instruments, there will, by 1986, be nearly 40 other beam positions available for special beam experiments, tests or development projects. The degree to which these can be exploited, and indeed even whether the instrument programme can be kept to its tight schedule, will of course depend on the level of funding available over the next few years.

Apart from individual instruments, the development of neutron techniques and methods is of great importance both on the instrumental side and for sample environments. Among the highlights of the past year are:

Monochromators

The joint project with the MPI Stuttgart has now produced very good quality beryllium crystals in sufficient quantity to provide a focussing monochromator for the hot source single crystal diffractometer D9B, which will provide a factor two gain in flux over the present copper crystals. The MPI is clearly the only centre in the world capable of producing good quality beryllium monochromator crystals and several laboratories around the world have now agreed to participate in the more ambitious next stage of the collaboration.

Polarisers and mirrors

A new evaporator for producing polarisers and mirrors was delivered during the year. It has already been used to produce a new microguide in which the deflecting layers (Ni or Fe) are separated by a 4500 Å thick layer of aluminium. This is an important development because, in principle, it allows neutrons with a wavelength of 5 or 6 Å (or more) to be deflected through several degrees over only a short distance.

Sample Environments

The Sample Environments Service is absolutely vital for the successful conclusion of the majority of experiments. New experiments may also not be possible without the development of better equipment. Progress in 1983 included:

- the continued development of the dilution refrigerators which can be inserted in standard ILL cryostats (collaboration with the Technical University of Munich);
- the successful testing of a sophisticated temperature controller designed at the ILL;
- the first tests of equipment for the rapid stretching and relaxation of rubber polymers (collaboration with the University of Mainz);
- new pressure vessels made of high strength steel or non-magnetic materials (Cu-Be) have been tested successfully. Experiments under hydrostatic pressure (10 Kbar) and a magnetic field at very low temperature ($T < 300$ mK) are now feasible.

The sample environment group has benefited considerably from the modernisation programme, without which the Institut would not be in anything like such a strong position to provide the specialised environments now required.

Computing

Along with the staff of EDEX, front-line support for experiments is provided by the Department of Computing. The extreme pressure on instrument time demands sophisticated and reliable programs for the operation of instruments and the acquisition of data. Increasingly also, as we have observed, experiments are carried out by teams from different laboratories. The ILL acts thus as a meeting place for scientific discussions and for this to be fruitful some on-the-spot data treatment is also desirable. Within their resources the Department of Computing should be congratulated in trying to meet this goal.

Personnel

Directors are indebted to many people throughout a year. I thank particularly all those who made special efforts during the reactor shut-down; the Department of Administration for, among other tasks, preventing me from breaking too many laws; and the unions for their constructive approach to the new Collective Agreement signed in June. Finally I record with pleasure among the new arrivals: M. André Michaudon, the new French Director from the CEA; M. Christoph Eitner from the BMFT in Bonn, who replaced M. Grillo as Head of Administration in May; and M. Werner Press from Jülich, who took up a Senior Scientist position in November. M. Jacques Winter, the outgoing French Director, carries our every good wish next door to the CENG as the new Head of research. Our congratulations also go to Philippe Nozières on his appointment as "Professeur au Collège de France", and to Ferenc Mezei who will become Professor at the Technische Universität, West Berlin.

For 1984? I expect all ILL scientists, whether resident or visitor, to show that it can be fun as well as intellectually stimulating doing research at one of the world's outstanding research institutes. I hope for closer contacts between the ILL and researchers in the smaller European countries. I dream of new links between neutron studies and those using synchrotron X-radiation.

On the last point, the Institut will, early in 1984, present its proposals for locating the European Synchrotron Source at the ILL site.

B.E.F. Fender

Bericht des Direktors

Ich schreibe die Einleitung zum Jahresbericht mit einer Rekordzahl von wissenschaftlichen Experimentieranschlägen vor Augen, die sich auf meinem Schreibtisch stapeln. 640 Anträge sind es, die für den Zeitraum von April bis Oktober 1984 gestellt wurden und die nur zu einem Bruchteil genehmigt werden können. Allein für die Neutronenstreuinstrumente wurden 5344 Tage beantragt, das sind 2,7 mal mehr als wir vergeben können. Während der letzten fünf Jahre wurden insgesamt 5300 Experimentieranschläge eingereicht — eine bemerkenswerte Nachfrage in Anbetracht der mit dem Erneuerungsprogramm des Reaktors verbundenen Unsicherheiten. Es gibt deutlich Anzeichen dafür, dass aufgrund dieses starken Wettbewerbs selbst gute Experimentieranschläge abgelehnt und neue Reaktorbenutzer entmutigt werden. Das gilt vor allem für Chemie und Biologie, wo die Gastwissenschaftler in ihren Heimatinstitutionen fast immer mit anderen Methoden arbeiten, sowie für Experimentieranträge, die nicht aus den Mitgliedsländern stammen.

Wie stark weltweit die Nachfrage für die einzigartigen Experimentiereinrichtungen des ILL ist, wird dadurch illustriert, dass von den 640 Experimentieranschlägen nahezu 90 aus Nicht-Mitgliedsstaaten stammen, darunter Anträge aus Australien, Belgien, Bulgarien, Dänemark, der DDR, Indien, Irland, Israel, Italien, Japan, Jugoslawien, Kanada, den Niederlanden, Norwegen, Österreich, Polen, Schweden, der Schweiz, Ungarn, den USA, und der UdSSR.

An über 20 Forschungsprojekten sind Wissenschaftler aus den Vereinigten Staaten beteiligt, im allgemeinen zusammen mit Forschern aus Frankreich, der Bundesrepublik oder Grossbritannien. So liegen Anträge aus folgenden amerikanischen Forschungseinrichtungen vor: Brookhaven National Laboratory, Argonne National Laboratory; Lawrence Livermore; Los Alamos National Laboratory; National Bureau of Standards, Washington; Oak Ridge National Laboratory; und von vielen Universitäten, darunter: Cal. Tech, Harvard, Illinois, Michigan, MIT und Yale, sowie von Bell Laboratories, RCA Princeton und General Electric, Schenectady. Forschungsanträge gibt es auch von mehreren sowjetischen Laboratorien, so vom Kurchatov Institut für Atomenergie, vom Institut für Proteinforschung, vom Institut für Kristallographie (alle in Moskau); vom Institut für Kernphysik in Leningrad, vom Institut für Geologie und Geophysik in Nowosibirsk und vom Gemeinschaftsinstitut für Kernforschung in Dubna.

Mischung von Nationalitäten und damit von wissenschaftlichen Kulturen gehört zu den Hauptaspekten des ILL. Bei etwa einem Viertel aller Experimente sind zwei oder mehr Nationalitäten beteiligt. Fast noch wichtiger ist jedoch die Förderung der Zusammenarbeit verschiedener Laboratorien. Fast 60% der Experimente sind Gemeinschaftsvorhaben mehrerer Forschungseinrichtungen. Es liegt auf der Hand, dass hierbei die Beteiligung von ILL-Wissenschaftlern besonders hoch ist (etwa bei der Hälfte, ohne die üblichen Dienstleistungen der "local contacts" zu zählen). Ganz abgesehen von diesen offensichtlichen Kooperationen ist es ganz klar, dass das Institut schlechthin Katalysator für Zusammenarbeiten ist.

Es zeigt sich immer deutlicher, dass das ILL nicht nur einfache Vorrichtungen für Neutronenstreuung oder Kernphysik bereitstellt, sondern zunehmend anfängt, die Rolle eines "advanced study"-Instituts zu spielen. Die wissenschaftlichen Aktivitäten sind dabei so vielfältig, dass es selbst einem Direktor, der an übergreifende Beurteilungen gewöhnt ist, schwerfällt, einen zutreffenden Gesamteindruck zu vermitteln. Wie etwa soll man mit Neutroneninterferometrie erhaltene Informationen über Grundlagen der Quantentheorie vergleichen mit Untersuchungen über die Dynamik inkommensurabler Phasen an einem Dreiachsenspektrometer? Oder wie soll man die Bedeutung grundlegender Untersuchungen über das Kriechen von Metal-

len gegenüber der Bestimmung der Form einzelner Proteinmoleküle in Ribosomen abwägen? Und dennoch konkurrieren die letztgenannten Methoden beide um die gleiche knapp bemessene Kleinwinkelstreuzeit. Es ist klar, dass selbst häufige Besucher das Institut im wesentlichen nur im Spiegel ihrer eigenen Interessen sehen, während gelegentliche Besucher sich oft nicht der Breite des Beitrages der Neutronenforschung für das allgemeine Verständnis von Festkörpern und Flüssigkeiten bewusst werden, geschweige denn ihres Anteils an der Erforschung der Kernspaltung, der Kernstruktur und an der Lösung von Problemen der Grundlagenphysik.

Um den Lesern des Jahresberichtes zu helfen, enthält dieser den ersten von einer Serie von Übersichtsartikeln (diesmal von R. Currat über inkommensurable Strukturen), die von ILL-Wissenschaftlern oder Besuchern verfasst wurden. Ich möchte Sie weiter darauf aufmerksam machen, dass es unter den mehr als 450 Veröffentlichungen über Arbeiten am ILL (davon 363 mit Beteiligung von ILL-Mitgliedern) die folgenden allgemein gehaltenen und in der Publikationsliste näher bezeichneten Übersichtsartikel gibt:

- Neutron Scattering Studies of Virus Structure (*Cusack*);
- Concentrated Dispersions (*Ottewill*);
- Small Angle Neutron Scattering by Biological Systems (*Zaccai and Jacrot*);
- Establishment of Short-range Order during Nucleation and Growth of Precipitates within Amorphous Solids (*Wright et al*);
- Neutron Scattering Studies of Diffusion in Solids (*Lechner*);
- Magnetism in Solid ^3He (*Roger et al*);
- Neutron Optics (*Klein and Werner*);
- Neutron Spin Echo Ten Years After (*Mezei*).

Im Laufe des Jahres sind auch Berichte zu zwei ILL-Workshops erschienen: "International Conference on the Impact of Polarised Neutrons on Solid State Chemistry and Physics" (Journal de Physique) und "Position Sensitive Detection of Thermal Neutrons" (Academic Press, Eds. Convert and Forsyth). Ein Workshop über "Reactor-based Fundamental Physics" wird im Frühjahr 1984 veröffentlicht.

Erneuerungsprogramm für den Reaktor

Es bestehen folgende Ziele:

1. Der wesentliche Teil des Erneuerungsprogramms, in dessen Mittelpunkt der Austausch der Strahlrohre steht, soll während des Reaktorhalts 1984/85 abgeschlossen werden.
2. Kontroll- und Messeinrichtungen, die dem Reaktorbetrieb und dem Strahlenschutz dienen, sollen ersetzt und modernisiert werden.
3. 1986 soll die neue horizontale kalte Quelle installiert werden.
4. Es soll ein Erneuerungs- und Wartungsprogramm ausgearbeitet werden, das in Zukunft grössere Unterbrechungen des normalen Reaktorbetriebs so weit wie möglich vermeidet.

Der lange Reaktorhalt 1984/85 fällt wahrscheinlich in die Zeit von Oktober 1984 bis Juli 1985. Die schwierigste Aufgabe ist der Ersatz der kombinierten Strahlkanäle für die Neutronenleiter. Seit 1980 wird mit erheblichem Aufwand an der Konstruktion der horizontalen kalten Quelle gearbeitet. Der Zeitplan sieht vor, dass diese Aufgabe Mitte 1984 abgeschlossen ist. Die Fertigung wird Anfang 1986 und der Einbau Mitte 1986 abgeschlossen sein. Die zweite Neutronenleiterhalle ist gegenwärtig im Bau.

Instrumente und Methoden

Das Institut steht mitten in der Abwicklung seines äusserst ehrgeizigen Instrumentenbauprogramms, das durch die Impulse des Modernisierungsprogramms und durch die während der vergangenen zehn Jahre gesammelten Erfahrungen möglich geworden ist. Nach seinem

Abschluss wird es sich auf das wissenschaftliche Programm des Instituts in geradezu spektakulärer Weise auswirken. Man kann das von verschiedenen Gesichtspunkten aus betrachten ; die Situation Mitte des Jahres 1986 verglichen mit der Mitte 1983 wird jedenfalls folgendermassen aussehen :

- 5 neue Instrumente (PN8, IN14, IN15, DB21, D22)
- 10 Instrumente mit fünf bis zehnmal höherem Fluss bzw. Nachweisrate (D2B, D20, D4B, D19, D9B, D7B*, IN1B, IN20*, IN4B, IN11B).
- 6 Instrumente mit annähernd verdoppeltem Gewinn (D11C, D16, D17, IN5, IN6, IN10B).
- 9 Instrumente mit bedeutenden, aber weniger augenscheinlichen Verbesserungen (PN1, PN2, PN3/PN4, D3, D10, D15, IN8, IN13).

* praktisch neue Instrumente.

Wichtig ist ferner, dass neben den normal programmierten Instrumenten 1986 nahezu 40 weitere Strahlpositionen für spezielle Experimente, Test- und Entwicklungsprojekte zur Verfügung stehen. Bis zu welchem Grad diese Möglichkeiten ausgenutzt werden können, und ob das Instrumentenbauprogramm überhaupt planmässig durchgeführt werden kann, wird natürlich von den während der nächsten Jahre verfügbaren finanziellen Mitteln abhängen.

Neben der Konstruktion einzelner Instrumente ist die Entwicklung von Neutronentechniken und -methoden von grosser Bedeutung sowohl im Hinblick auf die Instrumente selbst als auch für die Probenumgebung. Aus den im letzten Jahr in diesem Bereich unternommenen Aktionen ragen die folgenden heraus :

Monochromatoren

In Zusammenarbeit mit dem MPI Stuttgart wurden jetzt hinreichend viele hochwertige Berylliumkristalle hergestellt, um für das an der heissen Quelle stehende Einkristalldiffraktometer D9B einen fokussierenden Monochromator zu bauen. Ein Ersatz des gegenwärtigen Kupfermonochromators wird den Neutronenfluss verdoppeln. Das MPI ist ohne Zweifel weltweit das einzige Labor, das hochwertige Monochromatorkristalle aus Beryllium herstellen kann, und mehrere Forschungszentren in aller Welt haben sich jetzt bereit erklärt, an einer Zusammenarbeit mit noch höher gesteckten Zielen teilzunehmen.

Polarisatoren und Superspiegel

Im Frühjahr ist ein neues Aufdampfgerät zur Herstellung von Polarisatoren und Superspiegeln geliefert worden. Das Gerät wurde bereits dazu benutzt, einen neuartigen Mikroleiter herzustellen, bei dem die ablenkenden Schichten (Nickel oder Eisen) durch eine 4500 Å dicke Schicht von Aluminium getrennt sind. Diese Entwicklung ist wichtig, da dadurch Neutronen mit einer Wellenlänge zwischen 5 und 6 Å (oder länger) über eine kurze Strecke eine Ablenkung von mehreren Grad erfahren können.

Probenumgebungen

Für die erfolgreiche Abwicklung der meisten Experimente leistet die Abteilung "Probenumgebung" unerlässliche Hilfe. Neue Experimente sind häufig nicht denkbar ohne die Entwicklung besserer Ausrüstungen. Fortschritte wurden 1983 insbesondere auf folgenden Gebieten erzielt :

- In Zusammenarbeit mit der Technischen Universität München wurden Entmischungskühlgeräte weiterentwickelt, die in die Standard-ILL-Kryostaten eingebaut werden können.
- Die Erprobung eines hochentwickelten, am ILL entworfenen Temperaturreglers verlief erfolgreich.
- Erste Versuche mit einer Vorrichtung zur schnellen Dehnung und

- Entspannung von Gummi-Polymeren wurden in Zusammenarbeit mit der Universität Mainz durchgeführt.
- Neue Druckbehälter aus hochfestem Stahl oder nichtmagnetischen Werkstoffen (Cu-Be) sind erfolgreich erprobt worden. Experimente unter hydrostatischem Druck (10 Kbar) und einem Magnetfeld bei einer sehr niedrigen Temperatur ($T < 300$ mK) sind jetzt durchführbar.

Der Gruppe "Probenumgebung" ist das Modernisierungsprogramm sehr zugute gekommen. Ohne dieses wäre das Institut nicht entfernt in der Lage, den jetzt gewünschten hohen Anforderungen an Probenumgebungen zu genügen.

Informatik

Die Informatik arbeitet ebenso wie die Belegschaft der Abteilung "Instrumentenbetrieb" an vorderster Front bei der Unterstützung der Experimente. Der unerhörte Druck auf Instrumentenzeit erfordert hochentwickelte und zugleich zuverlässige Programme für die Instrumentensteuerung und für die Datenerfassung. Wie erwähnt, werden obendrein zunehmend Experimente von Gruppen aus verschiedenen Laboratorien durchgeführt. Das ILL wird auf diese Weise zum Treffpunkt der Wissenschaftler, deren Zusammenarbeit allerdings nur dann optimal ist, wenn Daten schon sofort vor Ort verarbeitet werden können. Im Rahmen ihrer Möglichkeiten versucht die Informatikabteilung diesem Bedarf zu entsprechen und kann für die erzielten Ergebnisse nur beglückwünscht werden.

Personalangelegenheiten

Als Direktor hat man für ein ganzes Jahr vielen Menschen zu danken. Speziell bin ich den Mitarbeitern verpflichtet, die sich während des langen Reaktorhalts besonders eingesetzt haben, sowie der Verwaltung neben anderem dafür, dass sie mich davor bewahrte, allzu viele Gesetze zu missachten. Den Gewerkschaften danke ich für ihre konstruktive Zusammenarbeit bei der Ausarbeitung des im Juni unterzeichneten Betriebstarifvertrages.

Abschliessend begrüsse ich mit Freude unter den neu zu uns gekommenen : Dr André Michaudon vom CEA, neuer französischer Direktor des Instituts ; Christoph Eitner vom BMFT in Bonn, der im Mai die Leitung der Verwaltungsabteilung als Nachfolger von Dr Wolfgang Grillo übernahm ; und Dr Werner Press aus Jülich, der im November eine Stelle als Senior Scientist antrat. Den scheidenden französischen Direktor, Dr Jacques Winter, begleiten unsere besten Wünsche für seine Tätigkeit als Forschungsdirektor im benachbarten Centre d'Etudes Nucléaires de Grenoble (CENG). Unser Glückwunsch geht auch an P. Nozières zu seiner Ernennung als Professor am "Collège de France" und an F. Mezei, der eine Stelle als Professor an der TU-Berlin antreten wird.

Meine Erwartungen für 1984 ? Ich denke, alle ILL-Wissenschaftler, ob angestellt oder Besucher, werden unter Beweis stellen, dass Forschen an einem der angesehensten Institute der Welt geistig stimuliert und obendrein Spass macht. Ich hoffe auf engere Kontakte zwischen dem ILL und Forschern aus den kleineren europäischen Staaten. Und ich träume von neuen Bindungen zwischen Arbeiten mit Neutronen und Synchrotron-Röntgenstrahlung.

Was den letzten Punkt betrifft, wird das ILL im Frühjahr 1984 seinen Vorschlag zum Bau der Europäischen Synchrotronquelle auf dem ILL-Gelände unterbreiten.

B.E.F. Fender

Rapport du Directeur

En écrivant cette introduction aux activités de l'année écoulée, j'ai un nombre record (640) de propositions d'expériences empilées sur mon bureau, et ceci seulement pour la période de six mois, d'avril à octobre 1984. Toutes ne pourront pas être acceptées puisque le nombre de jours demandés, (5 344), uniquement pour les instruments de diffusion neutronique est 2,7 fois plus important que le nombre de jours disponibles. Pendant les cinq dernières années l'Institut a reçu plus de 5 300 propositions d'expériences, ce qui est remarquable, compte tenu des incertitudes sur le fonctionnement du réacteur. Il est à craindre que, à ce niveau de concurrence, de bonnes propositions seront rejetées et de nouveaux utilisateurs risquent d'être découragés. Ceci est notamment le cas en chimie et en biologie, où le chercheur invité est presque toujours impliqué dans d'autres techniques dans son laboratoire d'origine. Ceci est vrai aussi pour les propositions provenant de pays autres que les pays membres.

L'importance de la demande mondiale pour l'utilisation des moyens uniques de l'Institut est indiquée par le fait que, sur ces 640 propositions, presque 90 impliquent des physiciens de pays autres que les trois pays membres, tels que : Allemagne de l'Est, Australie, Autriche, Belgique, Bulgarie, Canada, Danemark, Hongrie, Inde, Irlande, Israël, Italie, Japon, Norvège, Pays-Bas, Pologne, Suède, Suisse, URSS, USA et Yougoslavie.

Une bonne vingtaine de propositions émanent de scientifiques américains, généralement en collaboration avec d'autres scientifiques du Royaume-Uni, de la RFA ou de la France. Les établissements concernés sont les suivants : Brookhaven National Laboratory, Argonne National Laboratory, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, National Bureau of Standards, Oak Ridge National Laboratory, ainsi que de nombreuses universités : California Institute of Technology, Harvard, Illinois, Michigan, MIT et Yale ; y figurent également Bell Laboratories, RCA Princeton et General Electric (Schenectady).

Des propositions ont été reçues de plusieurs laboratoires soviétiques, y compris l'Institut Kurchatov de l'Energie Atomique, l'Institut de Recherche Protéique et l'Institut de Cristallographie (tous à Moscou) ; l'Institut de Physique Nucléaire de Leningrad, l'Institut de Géologie et de Géophysique à Novosibirsk et le Centre d'Etudes Nucléaires de Dubna.

Le mélange des nationalités, et donc des cultures scientifiques, est une caractéristique importante de l'ILL ; environ 25% de toutes les expériences faites ici concernent chacune deux ou plusieurs pays. Plus important encore, l'Institut stimule la collaboration entre laboratoires, près de 60% des expériences étant en général partagées par des collaborateurs de différents laboratoires. Naturellement beaucoup (environ la moitié) de ces collaborations impliquent des physiciens ILL (non compris la participation des "local contacts"), mais même si l'on écarte ces cas, il est certain que l'Institut agit comme catalyseur de nombreuses autres collaborations.

Le rôle de l'ILL comme institut d'études avancées se dégage de plus en plus clairement, avec une contribution beaucoup plus large que la simple fourniture d'instruments de diffusion neutronique ou de physique nucléaire. Même pour une Direction habituée à une vue globale des choses, la gamme des activités scientifiques couvre un spectre si large qu'une vue d'ensemble est difficile à saisir. Comment comparer des études fondamentales telles que la théorie quantique par interférométrie neutronique avec l'examen de la dynamique des structures incommensurables en utilisant un spectromètre à trois axes ? De même, comment juger l'importance relative d'études fondamentales du fluage dans les métaux et celle de la structure des molécules protéiques dans le ribosome ? Ces dernières études sont cependant concurrentes pour le même temps (rare) de mesures sur les instru-

ments à diffusion à petits angles. Il est évident que pour les chercheurs en visites fréquentes, l'Institut agit surtout comme une continuation de leurs propres intérêts, tandis que les visiteurs occasionnels ignorent souvent la profondeur de la contribution de la recherche neutronique à notre connaissance des solides et des liquides, sans parler de la fission nucléaire, de la structure nucléaire et d'autres aspects de la physique fondamentale.

Afin de faciliter la lecture du Rapport Annuel, signalons que celui-ci comprend cette année un article général sur les structures incommensurables (R. Currat) qui sera suivi les prochaines années par d'autres articles généraux rédigés par des chercheurs ILL ou invités. Sur plus de 450 publications (dont 363 avec la participation d'agents ILL) au sujet des travaux à l'Institut, j'attire également l'attention sur quelques rapports généraux mentionnés dans les listes des publications :

Neutron Scattering Studies of Virus Structure (*Cusack*) ;

Concentrated Dispersions (*Ottewill*) ;

Small Angle Neutron Scattering by Biological Systems (*Zaccai and Jacrot*) ;

Establishment of Short-range Order during Nucleation and Growth of Precipitates within Amorphous Solids (*Wright et al*) ;

Neutron Scattering Studies of Diffusion in Solids (*Lechner*) ;

Magnetism in Solid ^3He (*Roger et al*) ;

Neutron Optics (*Klein and Werner*) ;

Neutron Spin Echo Ten Years After (*Mezei*).

Deux "Workshops" à l'ILL ont également été publiés pendant l'année : un congrès international sur l'"Impact of polarised neutrons on solid-state chemistry and physics" (publié par le Journal de Physique) ainsi que "Position-sensitive detection of thermal neutrons" (rédigé par Convert et Forsyth, publié par Academic Press). Un "Workshop on Reactor-based fundamental physics" sera publié au printemps 1984.

Programme d'amélioration du réacteur

Les buts actuels du Département Réacteur sont les suivants :

1. Terminer le programme important de modernisation centré sur l'échange des canaux pendant l'arrêt 1984/85.
2. Remplacer et moderniser le matériel de contrôle et mesure associé au réacteur et à la radioprotection.
3. Installer la nouvelle source froide horizontale en 1986.
4. Prévoir un programme de renouvellement et d'entretien qui évite dans la mesure du possible des interruptions importantes dans le planning d'utilisation du réacteur.

Le programme de travail pour l'arrêt 1984/85 prévoit une interruption d'octobre 1984 à fin juillet 1985, la tâche la plus compliquée étant l'échange des canaux qui alimentent les guides. Depuis 1980 un grand effort a été consacré à l'étude de la source froide horizontale ; le planning de sa construction et de son installation impose l'établissement des plans définitifs à la mi-1984, l'achèvement de la construction au début 1986 et l'installation en mi-1986. La construction du deuxième hall des guides de neutrons est actuellement en cours.

Instruments et Méthodes

L'Institut poursuit un programme de construction des instruments le plus ambitieux qu'il ait jamais connu, rendu possible par l'élan donné par le programme de modernisation et par l'expérience des dix premières années de fonctionnement. Une fois terminé il aura un effet spectaculaire sur le programme de l'Institut.

Une des façons de l'illustrer est de remarquer que la situation en 1986, comparée à la mi-1983, sera la suivante :

- 5 nouveaux instruments (PN8, IN14, IN15, DB21, D22)
- 10 instruments dont les flux ou les taux de détection seront améliorés d'un facteur 5 à 10 (D2B, D20, D4B, D19, D9B, D7B*, IN1B, IN20*, IN4B, IN11B).
- 6 instruments améliorés d'un facteur 2 environ (D11C, D16, D17, IN5, IN6, IN10B).
- 9 instruments améliorés de façon significative mais moins que ceux cités ci-dessus (PN1, PN2, PN3/4, D3, D10, D15, IN8, IN13).

* en fait de nouveaux instruments.

Par ailleurs il faut reconnaître que, en dehors des instruments dont le temps de mesure complet est programmé, il y aura d'ici 1986 presque 40 autres positions de faisceaux disponibles pour des expériences spéciales, des essais ou des projets de développement. Le taux d'exploitation de celles-ci, et même la possibilité de maintenir le programme d'expériences avec son planning serré, dépendront bien sûr du niveau de financement dans les années à venir.

Outre les instruments eux-mêmes, le développement des techniques neutroniques et des méthodes est très important tant pour les instruments que pour l'environnement des échantillons. Parmi les points forts de l'année écoulée on peut citer :

Monochromateurs

Le projet commun avec le MPI Stuttgart a désormais permis d'obtenir des cristaux de béryllium de très bonne qualité et en quantité suffisante pour fournir un monochromateur focalisant associé au diffractomètre D9B à monocristal sur la source chaude, avec pour conséquence une amélioration d'un facteur 2 sur le flux par rapport aux cristaux actuels de cuivre. Il est clair que le MPI est le seul institut au monde capable de fournir des cristaux monochromateurs de béryllium de bonne qualité et plusieurs laboratoires au niveau mondial sont maintenant d'accord pour participer à la prochaine étape plus ambitieuse de la collaboration.

Polariseurs et miroirs

Un nouvel évaporateur pour la fabrication de polariseurs et de miroirs a été livré pendant l'année. Il a déjà été mis en service pour fabriquer un nouveau micro-guide dans lequel les couches réfléchissantes (de Ni ou Fe) sont séparées par une couche d'aluminium de 4500 Å d'épaisseur. Il s'agit d'une évolution importante puisque celle-ci permet, en principe, aux neutrons d'une longueur d'onde de 5 ou 6 Å (ou d'avantage) d'être déviés de plusieurs degrés sur une courte distance.

Environnement des Echantillons

Le Service "Environnement des Echantillons" est absolument vital pour le succès d'une majorité d'expériences. Certaines nouvelles expériences ne pourront pas aboutir sans le développement d'un matériel perfectionné. Parmi les progrès accomplis en 1983 citons :

- poursuite du développement des cryostats à dilution qui peuvent être insérés dans les cryostats standards ILL (collaboration avec l'Université de Munich)
- essais réussis d'un contrôleur de température perfectionné de conception ILL
- premiers tests d'un dispositif d'extension et de relâchement rapides des polymères de caoutchouc (collaboration avec l'Université de Mayence).
- essais réussis sur de nouvelles enceintes de pression en acier à résistance élevée ou en matériau non magnétique (Cu-Be). Des expériences sous pression hydrostatique (10 Kbar) et champ magnétique à très basse température ($T < 300$ mK) sont désormais possibles.

Le service environnement des échantillons a beaucoup bénéficié du programme de modernisation, sans lequel l'Institut serait dans une situation beaucoup moins favorable pour assurer les environnements spécialisés actuellement exigés.

Informatique

Le Département Informatique fournit, avec le personnel du Département Exploitation des Instruments, un soutien de première ligne aux expériences. La demande très forte de temps de mesure exige de programmes perfectionnés et fiables pour l'exploitation des instruments et l'acquisition des données. Il y a également une tendance croissante, comme nous l'avons remarqué, pour des expériences faites par des équipes en provenance de plusieurs laboratoires différents. L'ILL sert donc de lieu de rencontre pour les discussions scientifiques et, pour qu'elles soient profitables, il est souhaitable qu'un traitement de données, même limité, puisse être effectué sur place. Le Département Informatique doit être félicité de son effort dans cette direction et ceci, en utilisant au mieux les moyens qui lui ont été affectés.

Personnel

Les directeurs sont redevables à de nombreuses personnes pour le travail accompli dans l'année écoulée. Je remercie notamment tous ceux qui ont fait des efforts particuliers pendant l'arrêt du réacteur ; le Département Administratif et Financier (DAF), qui entre autres tâches, m'a empêché d'enfreindre trop de règlements ainsi que les syndicats pour leur attitude constructive à l'élaboration de la nouvelle convention d'entreprise signée au mois de juin.

Enfin parmi les nouveaux arrivants, nous avons eu le plaisir d'accueillir : M. André Michaudon, le nouveau Directeur français venant du CEA ; M. Christoph Eitner du BMFT (Ministère de la Recherche et Technologie) à Bonn, qui a remplacé M. Grillo en mai comme Chef du DAF ; et M. Werner Press venant de Jülich, qui a pris ses fonctions de "Senior Scientist" au mois de novembre. M. Jacques Winter, le Directeur français sortant, nous quitte avec nos meilleurs vœux pour le CENG voisin, où il est le nouveau Chef du Département de Recherche Fondamentale. Nous félicitons également M. Philippe Nozières pour sa nomination de Professeur au Collège de France, ainsi que M. Ferenc Mezei, qui occupera un poste de professeur à la "Technische Universität" de Berlin-Ouest.

Et pour 1984 ? J'attends de tous les scientifiques travaillant à l'ILL, ceux de l'Institut et les invités, qu'ils montrent que c'est à la fois un plaisir et un défi intellectuel stimulant d'effectuer des travaux de recherche dans un des meilleurs Instituts de recherche au monde. J'espère voir des contacts plus étroits entre l'Institut et les chercheurs d'autres pays européens. Je rêve de nouveaux liens entre les études neutroniques et celles utilisant le rayonnement synchrotron. A ce propos l'Institut soumettra début 1984 ses propositions pour l'implantation de la Source Européenne Synchrotron sur le site de l'ILL.

B.E.F. Fender



COLLEGE 2

Theory

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COLLEGE 3

**Fundamental
and Nuclear Physics**

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COLLEGE 4

**Structural
and Magnetic Excitations**

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COLLEGE 5

**Crystal
and Magnetic Structures**

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COLLEGE 6

**Liquids, Disorder
and Defects in Materials**

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COLLEGE 8

AND EMBL GRENoble

Biochemistry

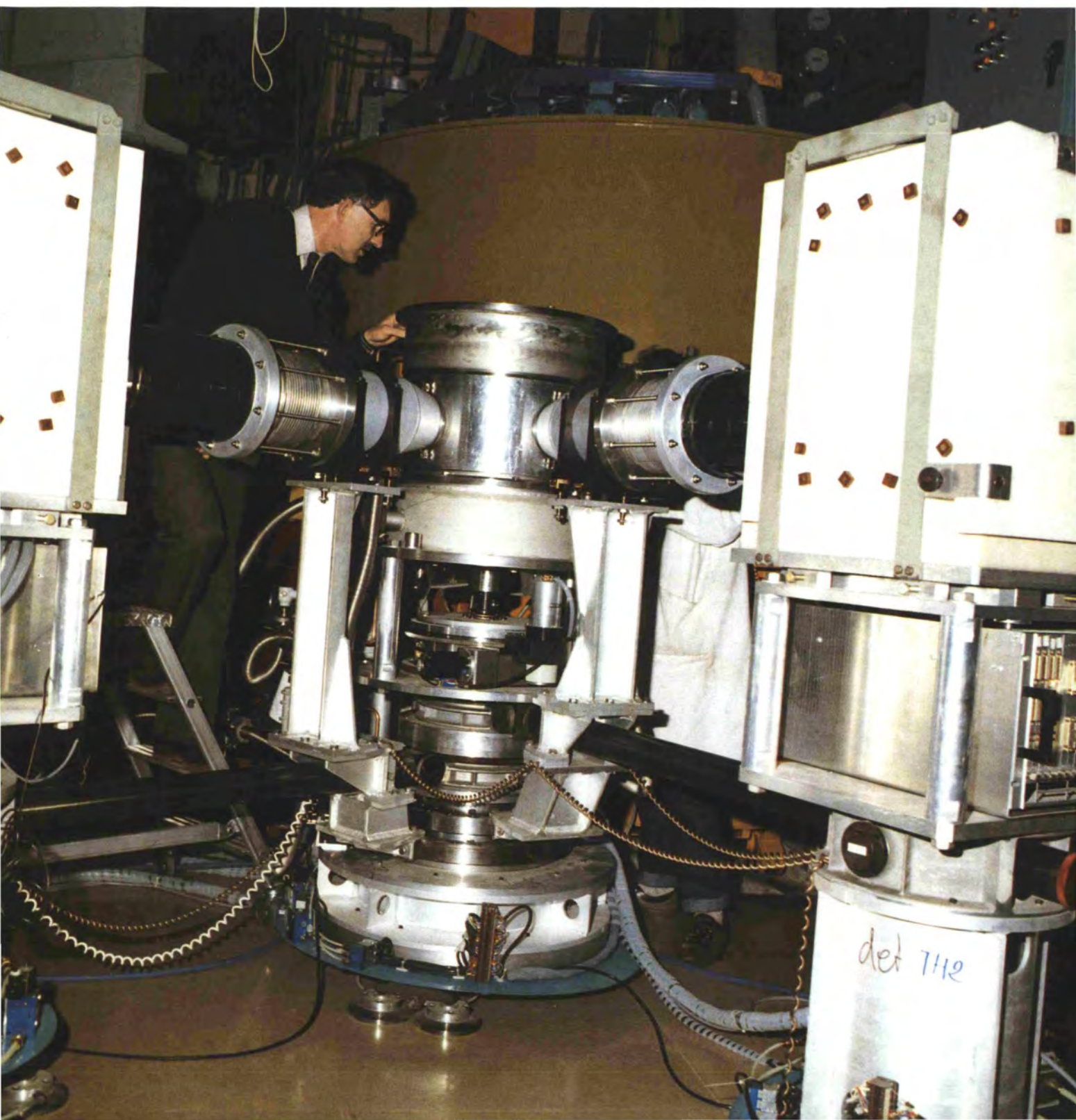
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COLLEGE 9

Chemistry

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COLLEGES



Introduction

All the internal scientific activity of the Institut is grouped into "colleges" with particular scientific interests.

The following is the current list of colleges:

College 2: Theory.

College 3: Fundamental and Nuclear Physics.

College 4: Structural and magnetic excitations.

College 5: Crystal and magnetic structures.

College 6: Liquids, disorders and defects in materials.

College 8: Biochemistry.

College 9: Chemistry.

Each College corresponds to a Subcommittee of the Scientific Council

of the ILL, which advises the Directors on the scientific programme. New research proposals submitted to the ILL will first be examined by the Colleges with respect to their technical feasibility and then be presented to the Council Subcommittees. A further task of the College is to contribute to a smooth carrying-out of the experiments by appointing local contacts and by advising the instrument responsible as well as the Scientific Secretary on the time schedules for the various instruments. The College Secretaries are normally elected for a 2 year term and have regular meetings with the Directors and Senior Scientists to ensure the flow of information on all matters concerning the scientific activity of the Institut.

Einleitung

Die gesamte wissenschaftliche Tätigkeit des Instituts ist in Kollegien mit spezifischen wissenschaftlichen Interessen aufgeteilt.

Zur Zeit sind folgende Kollegien am Institut tätig :

Kollegium 2 : Theorie.

Kollegium 3 : Grundlagen- und Kernphysik.

Kollegium 4 : Strukturelle und magnetische Anregungen.

Kollegium 5 : Kristallographische und magnetische Strukturen.

Kollegium 6 : Flüssigkeiten, Unordnungen und Fehlstellen in Substanzen.

Kollegium 8 : Biochemie.

Kollegium 9 : Chemie.

Jedes Kollegium entspricht einem Unterausschuss des Wissenschaftlichen Rates des ILL, der die Direktion in Fragen des wissenschaftli-

chen Programms berät. Die Kollegien prüfen als erste dem ILL unterbreitete Vorschläge zu neuen Forschungsvorhaben im Hinblick auf ihre technische Realisierbarkeit. Daraufhin werden sie den Unterausschüssen vorgelegt. Eine weitere Aufgabe der Kollegien ist es, zu einem reibungslosen Ablauf der Experimente beizutragen : Sie stellen den Gastforschern wissenschaftliche Hilfe vor Ort und beraten den Verantwortlichen der Experimentiereinrichtung und den Wissenschaftlichen Sekretär über die Zeiteinteilung für die Experimente an den verschiedenen Instrumenten. Die Sekretäre der Kollegien werden normalerweise für 2 Jahre gewählt, und halten mit der Direktion und den "Senior Scientists" regelmässige Sitzungen ab, um den notwendigen und alle wissenschaftlichen Tätigkeiten des ILL betreffenden Informationsfluss zu gewährleisten.

Introduction

L'ensemble de l'activité scientifique de l'Institut est réparti en collèges avec des intérêts scientifiques spécifiques.

La liste actuelle des collèges se compose comme suit :

Collège 2 : théorie.

Collège 3 : physique fondamentale et nucléaire.

Collège 4 : excitations structurelles et magnétiques.

Collège 5 : structures cristallographiques et magnétiques.

Collège 6 : liquides, désordres et défauts dans les matériaux.

Collège 8 : biochimie.

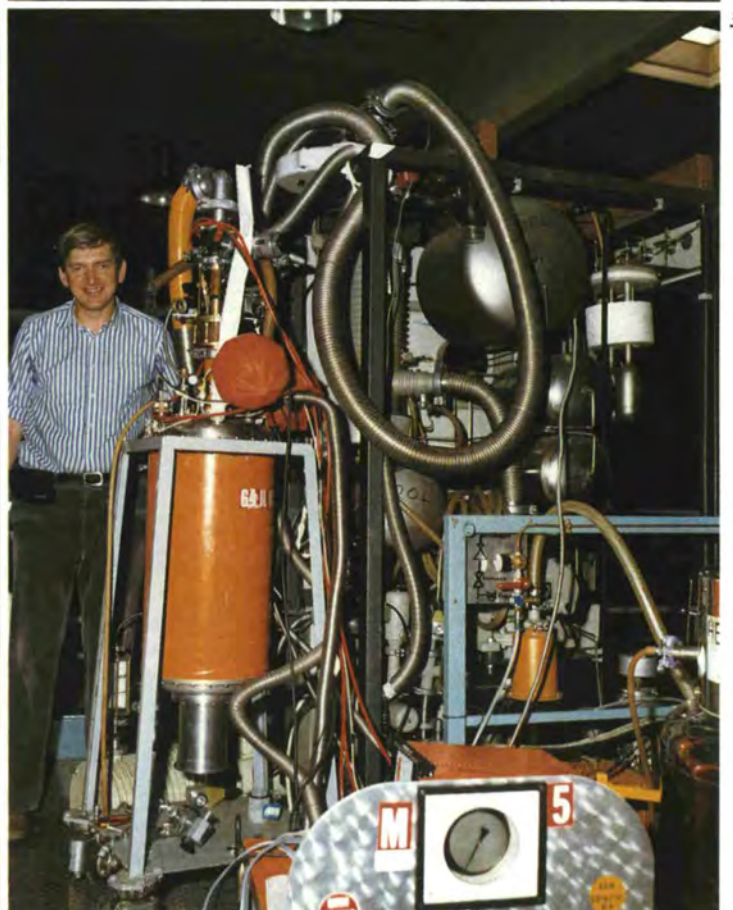
Collège 9 : chimie.

Chaque collège correspond à un sous-comité du Conseil Scientifique de l'ILL, qui conseille la Direction en matière de programmes scien-

tifiques. Les collèges examinent d'abord la faisabilité technique des propositions de recherche soumises à l'ILL. Elles sont ensuite présentées aux sous-comités du Conseil Scientifique. Les collèges contribuent également au bon déroulement des expériences en proposant des collaborateurs locaux aux chercheurs invités, et en conseillant le responsable d'instrument ainsi que le Secrétariat Scientifique de la répartition du temps d'expérience sur les différents instruments. Les Secrétaires de Collège sont normalement élus pour 2 ans et se réunissent régulièrement avec la Direction et les "Senior Scientists" dans le but d'assurer une bonne circulation de l'information dans tous les domaines d'activité scientifique de l'Institut.



1. A view of the crowded experimental area around the guides H23, H24 and H25 in the Guide Hall.
 2. Prof. Ottewill, Chairman of the British Neutron Beam Research Committee and member of the ILL Steering Committee, comes regularly to the ILL as a user. In the picture he and his assistant are seen at data treatment work.
 3. Dr. Neumaier, Meissner Institut Garching, with his complex cryogenics set-up on top of IN13 during an experimental run on tunneling motions of methyl groups in Mn-Acetate at temperatures down to 50 mK (November 83)





COLLEGE 2 THEORY

Membership 1983

1. ILL Members

P. Nozières
P. Becker
B. Desplanques
D. Grempel
R. Hasse
S. Hess
D. Newns
H.J. Schulz
H.J. Sommers
M. Uwaha
T.A.L. Ziman

2. Long term visitors

D. Baals
R. Beddell
C. Bourbonnais
P. Coppens
W. Dupont
K. Makoshi
C. Nemes
S. Noguera
N. Read
J. Solyom
M. Stroth
J. Treiner
J. Voit
M. Walker

INTRODUCTION

The Theory College has been active in various fields of Condensed matter and Nuclear Physics research and many collaborations with the experimental groups of the Institute have been developed.

P. Nozières has become "Professeur at the Collège de France". H.J. Schulz has been awarded the Humboldt prize for scientific collaboration between Germany and France.

The College has been in charge of the General Colloquia (Ziman) and the weekly theory seminar which has attracted this year a large group of scientists from the Grenoble area. A series of lectures on the dynamics of liquids has been organized with College 6: S. Hess has developed the theoretical aspects and several experimental contributions will be presented in the near future. This type of collaboration with experimental groups seems quite satisfactory and the theory college intends to initiate similar projects on "hot spots" in Physics during the shut-down of the reactor in 1985.

P. Nozières has given an advanced course on quantum liquids and solids, that has been attended by a large audience of either experimentalists or theorists. P. Becker is currently giving a Course of Troisième Cycle on the theory of X-ray and neutron scattering and applications to condensed matter.

Desplanques was one of the organisers of an International Workshop on "Reactor-based Fundamental Physics".

SCIENTIFIC ACTIVITIES IN 1983

1. Magnetism

— Sommers made several new contributions to the theory of spin glasses. In the case of uniaxial anisotropy, easy axis systems show Ising-type behaviour, though easy plane systems can change from X-Y type to a non magnetic singlet ground state for $S = 1$. He derived equations for order parameter and local field distribution within the Sherrington-Kirkpatrick model (with Dupont). A collaboration with de Dominicis and Gabay clarified the origin and meaning of the continuous set of spin glass order parameters.

— Ziman has continued his collaboration with Solyom concerning one-dimensional quantum Heisenberg ferro- and antiferromagnets with axial anisotropy (such as CsNiF_3). An exact diagonalisation for a finite chain bypasses the drawbacks of mean field and perturbation approaches. Phase diagrams are obtained for $S = 1/2, 1, 3/2$. This work is being extended to longer chains with H.J. Schulz.

In collaboration with Lindgaard, Ziman calculated the low temperature dynamic structure factor for incommensurably modulated magnetic structures (such as neodymium or praseodymium) where the modulation of the magnetisation is longitudinal. This work explains the experimental observations and is presently extended towards rare earths in general.

— After the thèse d'Etat of B. Gillon (directed by Becker) on the spin properties of crystalline radicals, a comparison between LCAO and local density approaches to spin density has been performed with Delley: the differences between the two approaches suggest a careful study of the approximations implied in the various models. A collaboration with Coppens led Becker to look simultaneously at charge and spin densities in transition metal compounds, which leads to contradictions with simple ligand field models. A Nato research grant was obtained for this type of study in the case of metalloporphyrins.

— Newns and Read performed a large N expansion of the intermediate valence problem (N: degeneracy of the magnetic state of rare earth impurity ions): the thermodynamic properties tend towards those of the impurity. The comparison with the exact solution of the impurity problem and with experimental measurements is successful.

2. Phase transitions

— Schulz studied the influence of long range Coulomb interactions in quasi-one-dimensional conductors: the metallic region is not affected by Umklapp processes. Such a metallic region seems not to exist in $(\text{TMTSF})_2\text{X}$, which is still not very clear. The influence of quantum fluctuations on the superconductivity in quasi-one-dimensional conductors has been investigated by Schulz from a microscopic viewpoint and their



crucial influence on the properties of $(\text{TMTSF})_2\text{X}$ is evidenced: most anomalies are explained by this theory.

— Ziman has developed an approach of Anderson localisation of excitations in disordered crystals, including the coupling to spin degree of freedom, with allowance for spin-orbit coupling — the model is capable of matching the two extreme regions of perturbation and strong disorder.

— The γ -ray diffraction study of ferroelectric-ferroelastic transition in RbDP has been successfully interpreted in terms of the extinction theory of Becker and led him with Bastie to connect the “extinction parameter” with Landau type parameters. A generalisation of this approach is being started, together with a possibility of testing Kato’s theory of multiple scattering.

3. Surface physics

Schulz has developed a theory for the phase transitions in adsorbed layers when commensurate and uniaxially incommensurate phases exist: the transition occurs via an intermediate fluid phase, in which there is a “disorder line” when the correlations acquire an oscillating component. For highly degenerate commensurate phases, melting occurs through a floating phase that is modulated.

Newns and Makoshi made a quasi-classical adiabatic theory of the $\text{He}(1120) \rightarrow \text{He}^+$ process at an alkali covered Cu phase: the comparison with experiments at Saclay is fair. The work is continued with better Hamiltonians.

4. Molecular physics

Becker, with Lehmann and C. Cohen-Addad, has completed a study on the charge density in compounds with short O-S...O interactions. Parallel to the X-N study, a theory was developed that explains the shortening of X-S...O in terms of the interactions of X-S antibonding levels with O lone pairs. This work is being continued on a very short O-S-O contact.

5. Physics of liquids

Hess, with Hanley, studied the transport properties and structure of liquids and colloidal solutions subjected to high shear rates: calculation of time dependent pair-correlation function, application to non linear viscous behaviour. He calculated the elastic properties of some liquids and cubic crystals, including point defects and uniaxial or biaxial deformations. Hess also made an interesting study of the decay of crystalline and bond orientational order into a liquid, using a dynamic Ginzburg-Landau approach. He performed a theoretical investigation of flow alignment and viscosity of molecular liquids, liquid crystals and polymers, the applications of which are quite broad: this includes a simulation program for non spherical entities of fixed orientation.

6. Quantum solids and fluids

— Uwaha and Nozières have developed a detailed theory for ^4He crystal growth: the superfluidity allows for non dissipative transport of heat and matter, there is high mobility of steps or kinks and the crystallisation is very fast: facets even appear above the roughening transition. Dissipation mechanisms near the interface are very important: intrinsic dissipation due to step mobility, volume dissipation due to reflexion of phonons and rotons.

— Uwaha (with G. Baym) finished his work on sound attenuation in electron-hole liquids, using multicomponent kinetic equations with a single deformation potential: this eliminated the existing discrepancy between theory and experiment in Ge.

— Nozières studied the transition between the two regions of strong coupling (ideal Bose gas) and weak coupling (BCS) in a gas of attractive fermions.

7. Nuclear theory

Desplanques and Noguera made important contributions to the parity non conservation in nuclear forces. The study was motivated by experiments at ILL and in other places. The study aims to understand the precise origin of parity violation in very low energy neutron-nucleus scattering. Work on weak interaction decays of hyperons and magnetic properties of nuclei has also been done in collaboration with physicists at Valencia and Orsay.

Desplanques and Noguera also studied the quenching of Gamow-Teller and M1 transitions in various processes. Its source, size and relation to the $\text{Su}(4)$ breaking part of the nucleon-nucleon interaction have been particularly investigated.

Hasse has extended his work on semi-classical nuclear physics to the optical potential. The imaginary part of the potential is used to calculate the real part via the dispersion relation, and to obtain quasi-particle lifetimes as well as widths of giant resonance excitations. Response of collective excitations is also obtained.

A collaboration with college 3 led Hasse to investigate “cold fission”. He computed potential energy surfaces from saddle to scission. A quantum wave packet representing the probability of events with certain deformation can tunnel through the ridge, yielding cold fission events.

The topics of interest to the theory college are very broad and one can easily see that the main problems studied this year are closely connected with real questions arising from recent experiments. The increased stability of the college composition during the last two years may be responsible for this closer interaction.

Secretary:
P. BECKER

COLLEGE 3 FUNDAMENTAL AND NUCLEAR PHYSICS

Members of the college

I. Internal members

J. Bartel
H.G. Börner
F. Blönnigen
R. Brissot
G. Colvin
B. Desplanques
H.R. Faust
F. Gönnenwein
B. Heckel
R.W. Hasse
F. Hoyler
C. Jewell
S.A. Kerr
W. Mampe
P. Miranda
B. More
S. Noguera
J. Pannicke
B. Pfeiffer
K. Schreckenbach
U. Stöhlker
H. Weikard

II. External Members

M. Avenier (ISN)
G. Bagieu (ISN)
W. Gelletly (Manchester)
J. Green (NBS)
P. Liaud (Chambéry)
N. McLeish (Manchester)

E. Monnard (CENG)
P.E.J. Perrin (CENG)
C. Ristori (CENG)

III. Visiting Members

E. Aker (Karlsruhe)
C. Botty (Rutherford)
J. Chauvin (ISN)
R. Deslattes (NBS)
D. Dubbers (Heidelberg)
D. Engelhardt (Karlsruhe)
P. Geltenbort (Tübingen)
R. Golub (München)
K. Gern (Rutherford)
W.D. Hamilton (Sussex)
P. Heeg (Darmstadt)
E. Kessler (NBS)
E. Krüger (PTB Braunschweig)
B. Leroux (Bordeaux)
J. Morse (Rutherford)
W. Nistler (PTB Braunschweig)
R. Olivier (ILL)
J.M. Pendlebury (Sussex)
N. Ramsay (Harvard)
P. de Saintignon (ISN)
A. Steyerl (München)
G.P. Theobald (Darmstadt)
B. Vignon (ISN)
W. Weirauch (PTB Braunschweig)
R. Wilson (Harvard)

Collaboration of College 3 with Institutes and Universities in 1983

Fission

Darmstadt GSI
Darmstadt TH
Grenoble CEN
Grenoble University
Geel JRC
Gent
Bordeaux
Mainz
München

ISPRA
Tübingen
Lyon

EDM-Experiment

Sussex
Harvard
Oak Ridge Nat. Lab.
Rutherford Lab.

UCN Research

Lancaster
Sussex
München

Nuclear Spectroscopy

Köln
Belgrade
Sussex
Glasgow
München
Manchester
Maryland
Giessen
Fribourg
Braunschweig
Göttingen
Mol
Brookhaven Nat. Lab.
Grenoble CEN
Livermore LL
Leningrad
Jülich KFA
Buenos Aires CNEA
Nice
Surrey
Nat. Bureau Standards
Ottawa NRC

Weak-Nucleon-Nucleon Force

Spin rotation:
Harvard
Rutherford
Ispra
Sussex
n, p capture:
Grenoble ISN
Harvard

Theoretical Physics

Bordeaux
München
Lyon
Grenoble CENG
Grenoble ISN
Orsay IPN
Orsay CSNSM
Regensburg

Fundamental Constants

Braunschweig PTB

n-decay

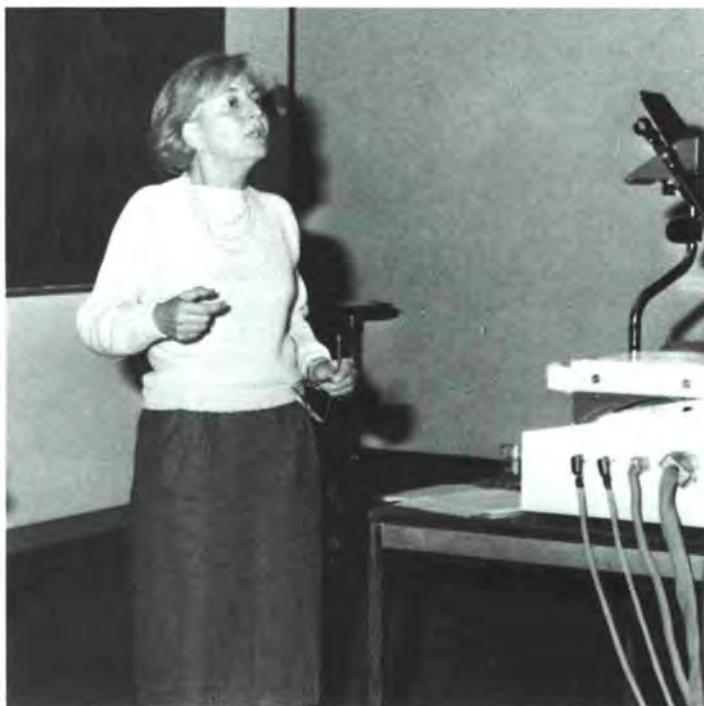
Bonn
Heidelberg
Argonne
Los Alamos



The Workshop on "Reactor-Based Fundamental Physics" was a great success. The world's most outstanding researchers gathered for this event at the ILL.



R. Mössbauer (München) during his lecture on neutrino oscillations.



Mrs. Baldo-Ceolin (Padua) impressed with her talk on $n-\bar{n}$ oscillations.

GENERAL SUMMARY

The work performed in College 3 during the three reactor cycles available in 1983 can be broadly grouped into the following categories:

1) **Nuclear Structure Studies** have been performed by the instruments PN2-electron spectrometer (BILL), PN3-curved crystal spectrometers (GAMS), PN4-pairspectrometer, PN6-on-line mass separator for fission products (OSTIS) and H22F — the γ - γ correlation facility.

The unique advantages of the high fluxes available at BILL, GAMS and PN4 have enabled nuclei produced by double neutron capture (where cross-sections are favourable), and low cross-section odd-odd nuclei to be investigated. Tests of the Interaction Boson Approximation model (IBA) have continued, particularly concerning multipole mixing ratios, which until recently have been rarely studied. A thorough study of low lying levels in Se have concluded that there is evidence for a $\Delta N = 2$ term in the E2 operator, which has not yet been included in IBA calculations.

2) **Fission** induced by thermal neutrons was studied at the parabola spectrometer PN1 (LOHENGRIN), the double torus ionisation chamber at H22E (DIOGONES) and at the neutron guide H22D. The LOHENGRIN spectrometer was recommissioned in August, and work has started on the determination of isomeric yield ratios of the heavy mass group in ^{236}U fission. Measurements on the reaction $^{238}\text{U}(n_{\text{th}}, F)$ at H22D have resulted in a preliminary fission cross-section value, whilst ternary fission in ^{241}Am has also been studied at this position. The double torus ionisation chamber DIOGENES installed at H22E has continued work on ^{235}U and is now studying ternary fission in ^{242}Pu .

The final test phase on the fission fragment spectrometer COSI FAN TUTTE has been successfully completed and has shown that this instrument will be a useful addition to the fission studies done at the ILL. Proposed experiments include the (n,f) reaction on ^{229}Th , ^{241}Pu , 245 , ^{247}Cm and ^{249}Cf .

3) **The Ultra-cold Neutrons (UCN)** from PN5 continued to be used in the search of the electric dipole moment (EDM) of the neutron and also for a study of the characteristics of the first concave mirror of the neutron microscope. The superthermal UCN source H17 is now operational with an improved neutron containment lifetime in order to allow the temperature dependence of the scattering cross-section of helium-4 to be studied.

4) **The Neutron-antineutron Oscillation** experiment at H18 was concluded at the beginning of 1983. A preliminary analysis of the results give a lower limit of 10^6sec for the oscillation time of a free neutron. A larger scale experiment, aiming at a sensitivity of 10^8sec is under discussion for the second cold source at the ILL.



5) A **Neutrino Physics** experiment was performed at the beta spectrometer BILL in order to determine the extent of massive neutrino mixing present in nuclear beta-decay. This comparative experiment performed on ^{64}Cu decay resulted in an upper limit of $\sin^2\theta = 3.5 \times 10^{-3}$ as the best value achieved.

6) **Special beam experiments** comprise a preliminary test on the viability of neutron tomography carried out on H22F, determination of rare earth concentrations in geological materials by neutron activation analysis and the set-up of a new beam (HI42) for the measurement of the lifetime of the free neutron. At H22D, systematic studies of (n_{th}, p) and (n_{th}, α) reactions were continued. The studies of (n_{th}, α) on ^{32}S , ^{35}S and ^{65}Zn , and $(n_{\text{th}}, \gamma\alpha)$ on ^{33}S have now been finalised.

7) **Theory** studies have concentrated on semiclassical evaluations of fission barriers and the imaginary part of the optical potential.

SCIENTIFIC TRENDS AND HIGHLIGHTS IN 1983

Nuclear Structure

The low lying levels in ^{75}Se and ^{77}Se have been investigated at GAMS, BILL and PN4 within the framework of the truncated quadrupole phonon model (TQM). There, nuclei lie in a region of the nuclear chart in which even-even nuclei of seemingly vibrational character have unusually low 0^+ levels, and where odd-mass nuclei with only a $g_{9/2}$ orbital available for positive parity states have low energy $5/2^+$ and $7/2^+$ levels. Calculations of energy levels in these two nuclei have been performed in the SU(6) particle-vibration mode. Results suggest that there is evidence for another term ($\Delta N=2^*$) in the E2 operator which is at present not included in TQM and IBA calculations. For example, the $5/2^+ \rightarrow 9/2^+$, E2-transition in ^{77}Se amounts to a $\Delta N=2$ contribution of more than 99% of the overlap between wavefunctions of these two states. Further tests on the IBA model have been carried out at the beta spectrometer BILL in which multipole mixing ratios (^{168}Er), and in particular E0 components were measured (^{124}Te and ^{150}Sm). In terms of the IBA model, the E0 pattern provides detailed information on the wave functions of the nucleus. Thus the Su(5)-O(6) transition region (represented by ^{124}Te) and the Su(5)-Su(3) transition region (represented by ^{150}Sm) can be investigated using this information. These experiments complement earlier work on E0 transitions in the Pt, Os and Ba isotopes.

Some interesting results are emerging from the systematic measurements performed on the Dy nuclei. In particular for the case of even-even isotopes, double neutron capture has enabled the previously unknown level scheme of ^{166}Dy to be constructed from BILL, GAMS and PN4 measurements (aided by the difference in neutron flux rates between the spectrometers), which to date include the ground and gamma bands (Fig. 1). As a consequence, it has been shown that maximum deformation of Dy occurs at $N=98$, which is before the neutron shell $N=82-126$ is half filled (see Fig. 2).

For the odd-even dysprosia, and in particular ^{163}Dy , recent results have enabled the identification of a number of excited bands as being single particle (Nilsson) states, coupled to vibrational modes of the even-even core (e.g. $2^+ \otimes 5/2$ [642], $2^+ \otimes 5/2$ [523] and $2^- \otimes 5/2$ [523]).

Detailed structure studies on actinide nuclei were continued with ^{231}Th and ^{244}Cm . In this latter nucleus, levels populated by the beta-decay of 10 hour ^{244g}Am and ^{244m}Am have been observed, in which new gamma transitions have been assigned including a prominent E0 transition depopulating the first excited 0^+ state of ^{244}Cm .

* where N is the phonon number of the quadrupole vibration.



The measurements made at the mass separator for fission fragments (OSTIS) continued with the systematic study of nuclear shape changes in the transitional region around mass number 100. The gross beta-decay properties, half-lives and neutron emission probabilities of mass $^{96-100}\text{Rb-Sr-Y}$ precursors were determined by simultaneous beta and neutron multiscaling, whilst detailed γ -spectroscopic work was performed on $^{98-100}\text{Rb-Y}$. From these data, level systematics and further information on the rapid change from spherical to strongly deformed nuclear shapes were derived. Of special interest in this context are the $N=60$ isotones ^{98}Sr and ^{100}Zr , whose low-lying excited states may be interpreted as arising from the coexistence of deformed and spherical shapes. For the decay of ^{99}Rb , a groundstate band built on the $3/2$ [411] Nilsson state was observed as well as two excited bands based on the $5/2$ [413] and $3/2$ [422] neutron configurations. From combined γ - γ and n - γ spectroscopy, the beta strength function $S_\beta(E)$ of ^{99}Rb decay was deduced up to an energy of 8 MeV. The fast decay rates to low-energy levels can in general be understood within the framework of a Random Phase Approximation [RPA] shell model. A first on-line test with the new negative ion-source has revealed an interesting result on heavy Br isotopes. From a comparison of the experimental beta-branching patterns of $^{90, 91}\text{Br}$ with RPA predictions, it is evident that in contrast to $Z > 37$ elements, nuclear deformation related changes in the shape of $S_\beta(E)$ of $Z=35$ isotopes seem to set in at $N=55, 56$ and not $N=60$. This effect of a weakening of the spherical sub-shell effect at $N=56$, combined with the occurrence of nuclear deformation for these isotones, has been previously predicted.

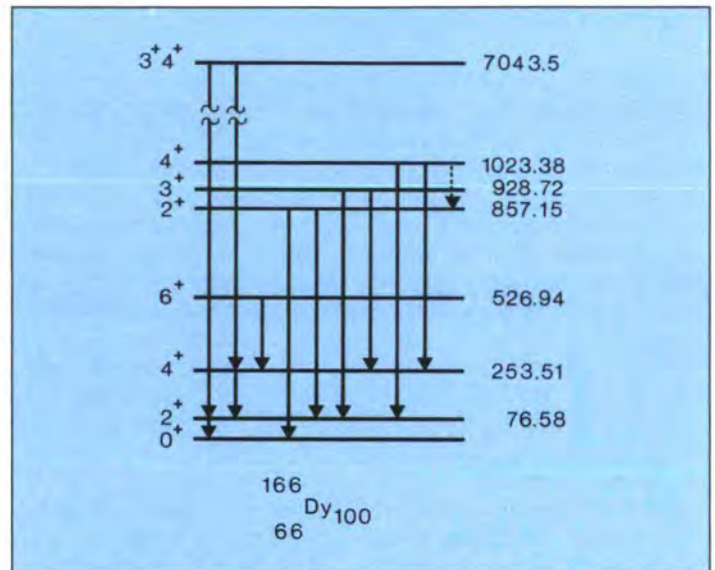


Figure 1: The level scheme of ^{166}Dy obtained from BILL, GAMS and PN4 measurements.

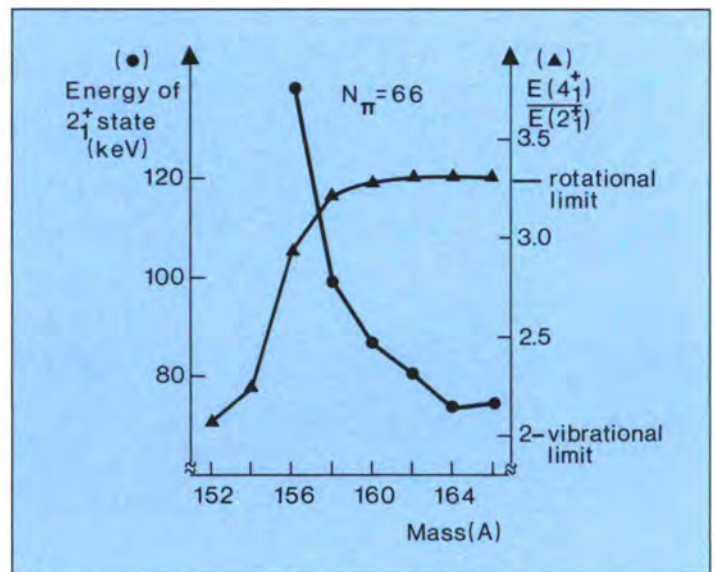


Figure 2: Systematics of even-even Dy isotopes showing that minimum deformation occurs at $N=98$ ($A=164$).



Thermal Neutron induced fission

The reinstallation of the parabola fission spectrometer PN1 (LOHENGRIN) was completed in August 1983. The first available reactor cycle was used for beta-gamma spectroscopic work by the Braunschweig group to determine Q_{β} -values in neutron-rich nuclei. The Mainz collaboration performed gamma decay measurements on several mass chains populated in the fission of ^{235}U , in order to determine yields and yield ratios in the heavy mass group. Both collaborations profited from the improved stability of the high tension achieved by the modification of the regulation unit (Giessen).

The recent commissioning of the fission fragment spectrometer COSI FAN TUTTE (PN8) allowed its first study (on $^{235}\text{U}(n,f)$) to get underway. The fission reactions which are proposed for the near future are $^{229}\text{Th}(n,f)$, $^{241}\text{Pu}(n,f)$, $^{245,249}\text{Cm}(n,f)$ and $^{249}\text{Cf}(n,f)$.

At the H22E beam position, multiparameter measurements of ternary fission of ^{235}U (see Fig. 3) has been achieved using the double torus ionisation chamber DIOGENES. The extension of this type of measurement to ternary fission of ^{241}Pu is under way. Further measurements were performed at H22D on $^{238}\text{U}(n_{th},f)$, resulting in a preliminary fission cross-section of $10 \mu\text{barns}$. Finally, a study of the yields and energy distributions of the light charged particles emitted during the thermally induced ternary fission of ^{241}Am has been started.

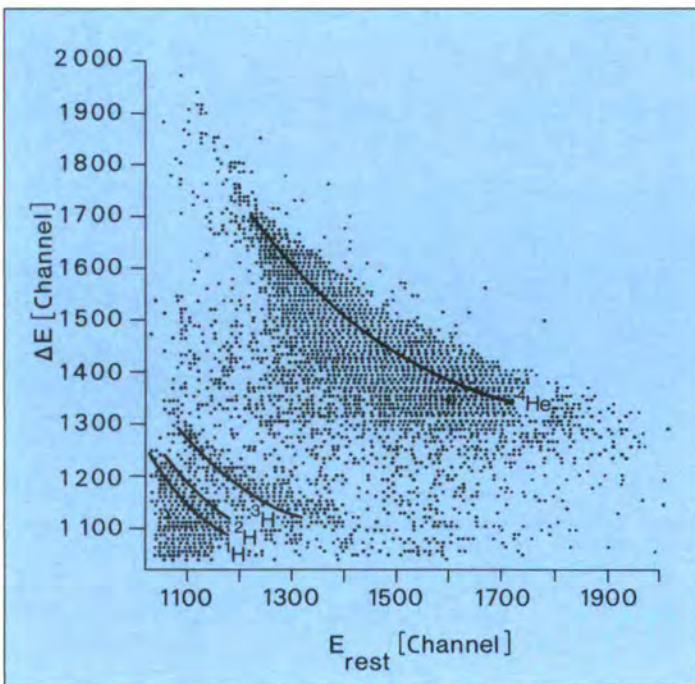


Figure 3: $\Delta E/E$ spectrum of the light particle emission following fission of ^{235}U . The dark lines are calculated values.



V. Nazarenko and A. Serebrov (Gatchina) at the workshop on Reactor-based fundamental physics.



R. Delattes (Washington) exchanges information with B.E.F. Fender (Director of the ILL) at the workshop on Reactor-based fundamental physics.

Properties of the neutron

The Sussex-Harvard-RAL-ILL collaboration to search for a neutron dipole moment (EDM), situated on SN5, has produced a preliminary value of $(0.3 \pm 4.8) \times 10^{-25} \text{e.cm}$. The actual limit is a consequence of counting statistics, whereas magnetic field stability and homogeneity, leakage currents and the conservation of polarisation are not currently restrictive. This experiment, based on the observation of the magnetic resonance of bottled UCN in a static field by looking for a possible shift in the resonance frequency when an electric field is applied, should undergo future developments leading to a factor 5 improvement over the current system.

The neutron microscope on SN5 is currently being used to study the characteristics of the first concave mirror only, due to adjustment problems of the two mirror system caused by low counting rates. An image magnification of 25 has been obtained.

The neutron-antineutron oscillation experiment on H18 (CERN-Padua-Sussex-RAL-ILL collaboration) was concluded at the beginning of 1983, and the data evaluation of two phases (from a total of three) has been completed in CERN and Padua. As a result, the lower limit of the oscillation time of a free neutron is $0.8 \times 10^6 \text{s}$ with a 90% confidence limit. A second experiment of a much larger scale is currently under discussion for the second cold source at the ILL.

Fundamental Physics

Parity violation in the weak nucleon-nucleon force is being examined on SN7 through investigations into the gamma-ray asymmetry (A_γ) following polarised neutron capture by protons. The parity violating contribution of the weak neutral current between nucleons is poorly understood in contrast to the structure of the parity conserving forces. The most reliable theoretical predictions are in the region $A_\gamma = 10^{-7}$ to 10^{-8} , thus the measured values of $A_\gamma < 1.5 \times 10^{-8}$ for the empty targets' asymmetry (assuming a signal/noise ratio of 10) and an unoriented ^{60}Co source tested to an accuracy of $< 1.1 \times 10^{-8}$, lie within this sensitive range. Calibration of the apparatus with the ^{35}Cl reaction yielded a result which was in agreement with previous measurements.

A comparative measurement of the β^+ and β^- spectral shape of the ^{64}Cu decay (done at BILL) allowed a sensitive search for heavy neutrino branches in nuclear beta-decay. Approximately 3×10^8 events were recorded for both spectra. A heavy neutrino branch would appear as a "kink" in both spectra at corresponding energies of m_ν below their end-point energies. Although no evidence could be found for such massive branches, stringent limits could be established. (See Fig. 4). A sensitivity close to that of the best appearance experiments (at accelerators) was achieved, but with a more general limit, namely that it is valid for any kind of massive neutral particle emitted in beta-decay.

Special beam experiments

At the H22F neutron guide some preliminary studies were performed to investigate some fundamental aspects of neutron tomography. Imaging with neutrons is a novel technique, analogous to that employed in X-ray tomographic scanners. Results from these measurements indicate that a spatial resolution of approximately 1 mm is achievable with the technique, and would be improved upon. (See Fig. 5).

The neutron activation analysis facility continued to operate in 1983. Studies were performed to determine rare earth and trace element concentrations in 2.8 million year dioritic rocks from the Greenland

Craton, which showed three distinct magma pulses in these highly metamorphosed rocks. A series of oceanic granites of Devonian age from the Massif Central were also studied and work was continued on the Hercynian intrusives of the external alps.

The systematic studies on the (n_{th}, p) and (n_{th}, α) reactions at H22D were continued. The results from the reaction (n_{th}, α) on the isotopes ^{32}S , ^{33}S , ^{65}Zn and the reaction $(n_{\text{th}}, \gamma\alpha)$ on ^{33}S have now been finalised.

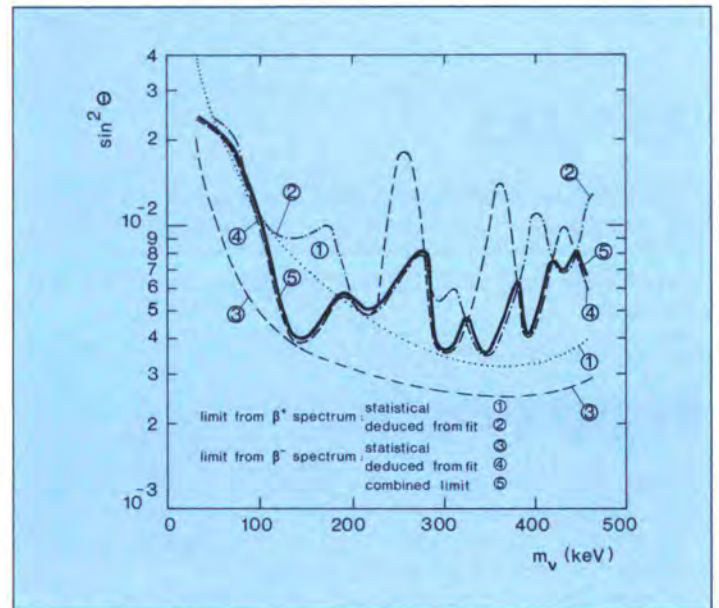


Figure 4: Exclusion plots for massive neutrino branches, deduced from the present measurements. The solid line shows the achieved limits, combining the results from the analysis of the β^+ and β^- spectrum (90% confidence limit). The region above this curve is excluded by either β^+ or β^- decay experiments.

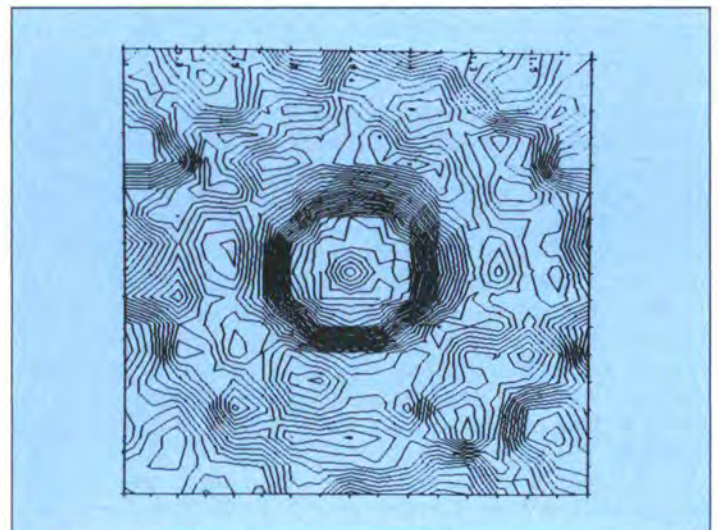


Figure 5: An iso-attenuation contour map constructed from a neutron tomogram of concentric cylinders of iron (centre), ceramic and nickel.



Theory

Two main areas concerning semiclassical physics have been studied by the theoretical group. There were the influence of the fission barrier's curvature terms on the potential slope from saddle to scission and an evaluation of the imaginary part of the optical potential, of which a constant expansion in powers of n has been performed revealing deviations from the literature.

SEMINARS

The seminar programme has invited 23 speakers who presented a wide range of subjects relevant to the work done by the college. Some interesting related topics were also included in order to appreciate more other fields of physics outside of the ILL's experience.

WORKSHOPS

In 1983, three workshops concerning fundamental and nuclear physics were organised at the ILL. In all cases, these workshops have been very successful in their aims and have provided a good platform for fruitful discussions.

Chronologically, these workshops were as follows:

a) "Workshop on COSI FAN TUTTE" (Organised by F. Gönnerwein) held on 8th February — with the testing period on the fission fragment spectrometer "COSI FAN TUTTE" coming to an end, the aim of the workshop was to inform potential users on the performance achieved and the choice of measuring configurations and targets available. Some 20 scientists attended. At the instigation of the subcommittee for fundamental and nuclear physics, collaborations between different laboratories were established which could keep COSI FAN TUTTE busy for up to three years.

b) "Lectures on the IBA model" (organised by K. Schreckenbach) held on 10th-11th May. The aim of this series of lectures was primarily educational for the 40 participants, all frequent users of the I.L.L. facilities. Six invited speakers (A.E.I. Dieperink, A. Evans, W. Gelletly, K. Heyde, P. Schuck and D.D. Warner) presented varying viewpoints ranging from theoretical aspects to experimental tests on the Interacting Boson Approximation model. Ample room was given to further discussions concerning this currently popular description of the nucleus.

c) "Workshop on Reactor-based Fundamental Physics" (organised by B. Desplanques, F. Gönnerwein and W. Mampe) held on 7th-9th November. This International Workshop, attended by approximately 100 scientists proved

to be very lively and stimulating for all participants. A distinguished series of invited speakers (M. Baldo-Ceolin, J. Bernabeu, J. Byrne, B. Desplanques, E. Fiorini, H. Fritsch, R.P. Mössbauer, V. Nazarenko, N. Ramsey, H. Rauch and A. Steyerl) and a good selection of presented papers produced a successful three days. Those topics discussed included neutron properties, reactor based neutron physics, nucleon decay, neutron interferometry and wave optics, $n\bar{n}$ measurements and parity non-conservation in neutron interactions.

Secretary :
G. COLVIN



Snapshots from the workshop on "Reactor-based fundamental physics":

1. G. Petrov, A. Serebrov and A. Sumbaev (Gatchina) (from left to right).
2. R. Ringo (Argonne) and N. Ramsay (Harvard) (from left to right).
3. B. Vignon (Grenoble).
4. From left to right: O.W.B. Schult (Jülich), F. Gönnenwein (ILL), N. Ramsay (Harvard) and G. Petrov (Gatchina) exchanging preprints and data.



Cold Fragmentation

Nuclear Fission is a process where large amounts of nuclear binding energy are converted into kinetic and excitation energy of the outgoing reaction products. Let us consider the thermal neutron induced fission of ^{235}U as an example. Upon capture of a neutron a ^{236}U compound nucleus is formed, with the binding energy of the neutron heating up the compound system to an excitation energy of 6.5 MeV. In terms of the nucleus as a liquid drop, fission may be visualized as a process where an originally spherical drop is deformed into a spheroidal (or even more complicated) shape, which becomes more and more elongated and eventually breaks apart into two pieces, the fission fragments. Plotting the potential energy of the liquid drop versus deformation, a potential barrier shows up, which normally ensures the stability of nuclei against fission. The height of this barrier for the ^{236}U nucleus is 5.6 MeV. Therefore, after neutron capture by ^{235}U the excitation energy of the ^{236}U compound system may allow the nucleus to overcome the barrier, and fission will compete with other decay modes. The excitation energy left to the nucleus at the potential barrier, or "saddle point", is 0.9 MeV. Once the barrier has been passed, nuclear matter slopes down the potential hill and finally reaches the point of fragmentation, the "scission point". At this point, at least one, if not both of the nascent fragments are heavily deformed. The strong electrostatic repulsion between the two fragment nuclei will accelerate them into opposite directions and impart to them a high kinetic energy. The lion's share of the energy available in the fission process goes into the total kinetic energy TKE of the fragments. In the case of $^{235}\text{U}(n,f)$ the TKE equals 170.4 MeV on the average. Some 28 MeV of energy stay on the average with the fragments as internal excitation or — at the scission point — as energy tied up in deformation. However, once the fragments have separated the deformation will induce a collective oscillation, and frictional forces will transfer this collective energy into heat, which has to be added to the internal excitation already present. The heat is released by the fragments through neutron evaporation and γ -emission. In the $^{235}\text{U}(n,f)$ reaction the total of 2.4 evaporated neutrons take away binding energy (17.5 MeV) and kinetic energy (2.9 MeV), while the γ 's carry 7.6 MeV of energy. The fragments will by now (in the majority of cases 10^{-12} s after neutron capture) have reached their ground states. They are, though, not stable against β -decay. The energy release accompanying β -decay will contribute another 14.5 MeV per fission of useful energy to the power output of a reactor.

It should again be stressed that all the quoted figures are average values. Within the constraints of energy conservation some of the excitation or deformation energy present

at the scission point may be shuffled into the kinetic energy of the fragments and vice versa. For example, even for a given fragmentation of the compound nucleus (i.e. the fragment masses and so the Q-value of the reaction being fixed) one observes a distribution of the TKE of fragments with a width of about 20 MeV (FWHM). Surprisingly enough, it was discovered more than two decades ago that there are (though rare) fission events, where the TKE comes rather close to the Q-value of the reaction ⁽¹⁾. As a corollary to that, not sufficient excitation energy is left to emit neutrons and, in fact, it is known that for $^{235}\text{U}(n,f)$ in 3.1% of all cases fission proceeds with no neutron emission at all. This limiting case of nuclear fission, which is characterized by a TKE of the fragments nearly exhausting the Q-value and an excitation energy approaching within a few MeV zero, has been coined "cold fragmentation". Cold fragmentation has come back into focus in recent years ⁽²⁾, since it is felt that its study may give new insight into the fission process. Due to the low yields involved cold fragmentation is, however, difficult to tackle experimentally. Close to the Q-value the yields drop by an order of magnitude (from the 10^{-5} to the 10^{-6} level) upon increasing the TKE by only 1 MeV. A simple but very elegant method to search for high kinetic energy events, which is based on time-of-flight techniques, has been devised by C. Signarbieux ⁽²⁾. First experiments have been run at the ILL. Also the Lohengrin facility, with its outstanding capability to pick a few specified events out of a large background, is ideally suited to this type of research. Lohengrin offers the additional advantage that, besides the mass and energy of the fragments, it can also give information on their nuclear charge. Some first results have already been obtained ⁽³⁾.

Let us review some of the new features and questions concerning the fission process which have emerged from the above studies. Cold fragmentation is a quite general phenomenon, common to all masses with a high over-all yield (only those have been studied so far). More specifically this implies that the fission prone nuclear system follows enhancements of the Q-value, which are due to nuclear shell effects, down to very low residual excitation energies. In fact, at low excitation the mass yields are dominated by shell stabilized fragments. A closer inspection shows that the lowest excitation energies (below 1 MeV) are obtained for combinations of 2 "magic" fragments, one with a spherical shell and the other with a deformed shell. On the other hand, it is evident from the high TKE involved that cold fragmentation is a process where the rupture takes place close to the saddle point of deformation. In the picture of the liquid drop this would rather correspond to a necking-in mode near the saddle point than to an elongation mode from the saddle point onwards. Would this then prove that fragment properties become decisive at a very early stage of fission, as put




forward in some theoretical models? The next question is, how close to the Q-value can one come with the TKE for a given fragmentation. Can one really go with the excitation energy of the fragments below the excitation energy of the compound system at the saddle point (0.9 MeV in the case of $^{235}\text{U}(n,f)$)? That would be rather strange. In any case, near zero excitation of the fragments, one would expect to see the influence of individual excited states in the TKE, at least for some favorable nuclei with low level density. If this were to be observed, it would certainly not be a new tool for nuclear spectroscopy, but perhaps a means to study what types of nuclear states are reached in fission.

Another observation which has some bearing on cold fragmentation is the so-called "even-odd effect" for nuclear charge and neutron numbers of fission fragments. By "even-odd effect" is understood the fact that for a fissioning even-even compound nucleus (like in $^{235}\text{U}(n,f)$) one finds more fragments with an even charge number (and to a lesser extent also with an even neutron number) than with odd ones. For example, the ratio R of even to odd proton numbers in the fragments from $^{235}\text{U}(n,f)$ induced by thermal neutrons is $R = 1.6$ if one averages over all fragmentations. The preponderance of even charge numbers has to be traced back to nuclear pairing forces. The typical energy to break a pair and create a 2 quasi-particle excitation in a fragment is about 2 MeV. The mere fact that pairing survives — at least partly — fission then means that the internal heat generated during the fission process cannot be high. Stated otherwise, the radical rearrangement of nuclear matter in fission proceeds with low dissipation of energy. This is in keeping with the findings on cold fragmentation and has even prompted ideas of fission to be a superfluid mode. One would conjecture that a superfluid mode should become dominant at low internal excitation energies of the fragments, i.e. for cold fragmentation. Low count rates prevented, however, so far nuclear charge distributions to be studied at true cold fragmentation. In the meantime, the detecting techniques have been developed further and the data under question should become available in the near future. For the moment there is only one set of data for $^{235}\text{U}(n,f)$ at a TKE of fragments just high enough to preclude any neutron emission. The even-odd ratio found for protons is $R = 2.7$, while for neutrons it is $R = 1.25$. These figures are at variance with superfluidity or perfect pairing. A similar conclusion may be drawn upon closer inspection of the cold fragmentation data. The even-odd staggering of the Q-values versus fragment mass is not shown by the high energy extremes of TKE in cold fragmentation. The limiting values of TKE exhibit a rather smooth behaviour. In other words, odd mass fragmentations come closer to their Q-value than even ones by 1 MeV. Thus, odd mass fragments with necessarily one pair broken compete suc-

cessfully with even mass fragments. There is even evidence that even mass fragments are not entirely made up by (even-proton, even-neutron) nuclei. Instead, about 1/4 of them are (odd, odd) nuclei. In the majority of fission events, therefore, nuclear pairs are broken.

To summarize the findings obtained up to now, nuclear matter—even in the violent process of fission — is capable of exploiting energy gains brought about by shell effects and to reach a final state with virtually no internal excitation energy left to the fragments. However, in contrast to the above, in the bulk of cases nuclear pairing is destroyed in fission and, hence, the energy gain connected with pairing is not realized. Does this peculiar behaviour tell us something on the dynamics of fission? It has been put forward that an omnipresent mechanism for pair breaking in fission might be the sudden necking-in of the liquid drop at the scission point. Other models claim that pairs are broken in the descent from the saddle to the scission point by transfer of energy from the collective to the single particle degrees of freedom through viscous forces. For cold fragmentation both pictures would coincide. On the other hand, given a high overall chance to break a nucleon pair, the surprisingly low even-odd effect for neutrons as compared to protons seems to be quite easily understood in terms of the high neutron/proton ratio in heavy nuclei. Finally, statistical arguments should come into place. At given excitation energy the level densities vary rapidly from one nucleus to the other and so do the statistical weight factors from one fragmentation to the other. To answer all those questions, more systematic and more detailed data are needed. Hopefully, the research program underway on Lohengrin and other facilities will provide the data and establish a firm basis for a more thorough understanding of nuclear fission.

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COLLEGE 4 STRUCTURAL AND MAGNETIC EXCITATIONS

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GENERAL SUMMARY

Experiments carried out under the auspices of College 4 extend over a large area of scientific interest. In general these experiments relate to studies of lattice dynamics, magnetic and structural phase transitions, and magnetic excitations. The materials studied, and the reasons for the study itself, are extremely varied and cover almost the entire range of solid state physics. An idea of the degree of diversity can be found by a brief examination of the Experimental Reports and Theory College Activities 1983.

The majority of the experimental work is performed using the five triple-axis spectrometers (TAS), i.e. IN1B, IN2, IN3, IN8, IN12 and D5, although the time-of-flight (TOF) spectrometers, IN4, IN5, IN6 and D7 are also used. The range of available neutron energies and the resultant resolution possible, make it possible to study materials with very different interaction strengths. For example, on IN12, it is possible to measure excitations with frequencies as low as 0.01 THz, while on IN1 excitations with frequencies of the order of 50 THz can be examined.

During 1983, the rebuilding of the "hot source" TAS IN1B was completed and the new instrument is now being regularly scheduled. The IN3 instrument is now controlled by a SOLAR minicomputer and has been equipped with new electronics. For the future, in 1984, IN2 will be replaced by IN20 a thermal beam TAS which uses a polarized neutron beam. The TAS IN14 which is to be situated on a guide from the new cold source will be designed and constructed during 1984-85.

SCIENTIFIC TRENDS AND HIGHLIGHTS IN 1983

Phonons

There exist five different models of the phonon dispersion curves of the semi conductor GaAs which are capable of describing the lattice dynamics of this material ⁽¹⁾. These models are a rigid ion model, two different versions of a shell model, a deformation dipole model and a bond charge model. Each is capable of reproducing the experimentally determined phonon frequencies, however differences are apparent in the calculated mode eigenvectors. The mode eigenvectors determine the matrix elements for the electron-phonon coupling, which are required to understand the first and second order processes in the Raman and Infra-Red spectra, and also influence the band-structure of this material.

An experimental determination of the mode eigenvectors, though of high interest, is rarely performed, since it requires a measurement of the intensity of weak signals using good resolution conditions. Typical count rates may be of the order of five to ten counts per minute. Recent measurements using the IN2 TAS⁽²⁾ have attempted to obtain sufficiently accurate intensity measurements of various phonons that the predicted eigenvectors for the various models may be checked.

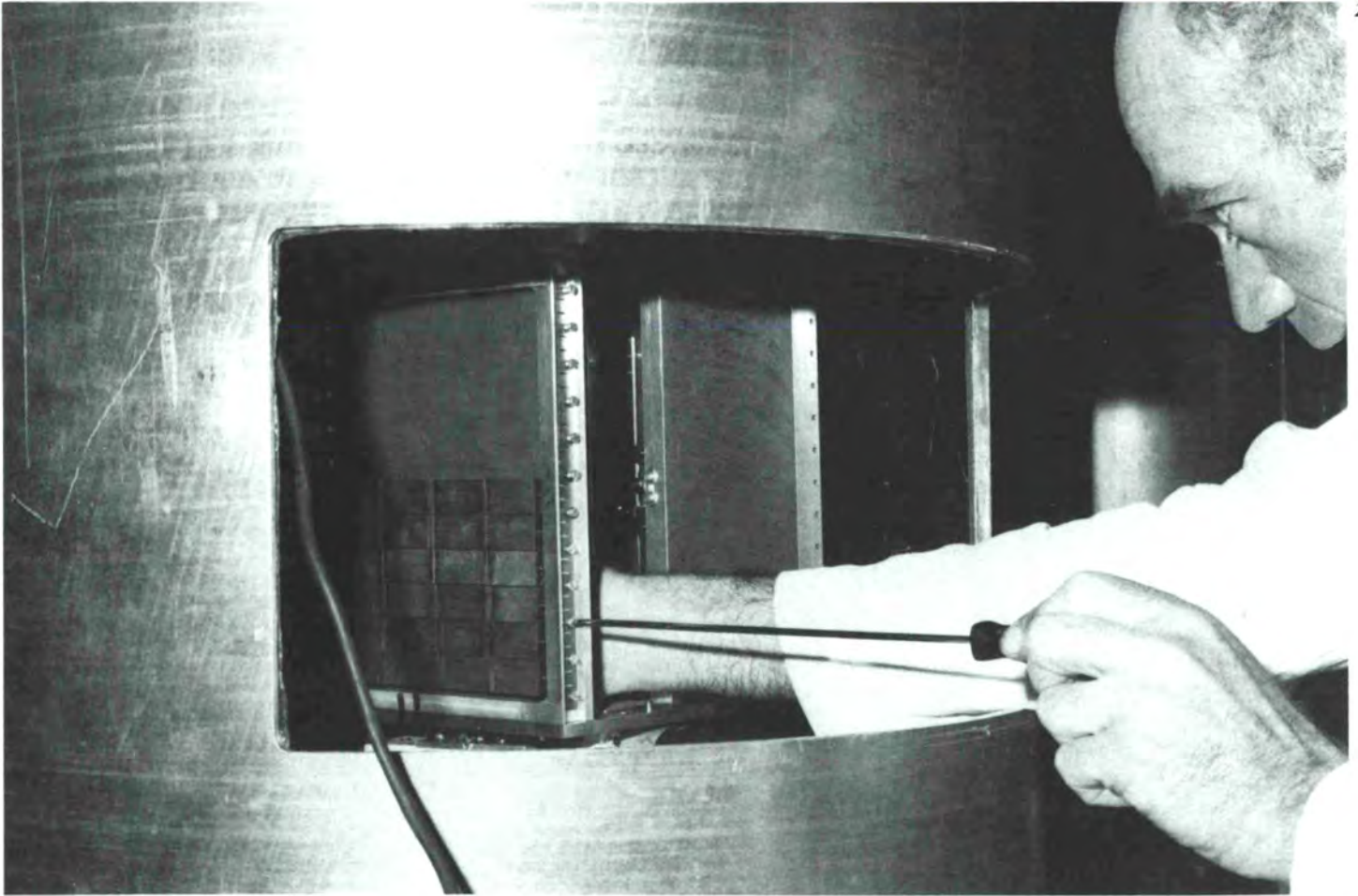
For GaAs the eigenvectors of the two longitudinal modes have been determined at the X- and L- points in reciprocal space. At the X- point, where by symmetry one or other sublattice is at rest for the two modes, it was found that Ga, the lighter ion, oscillates with the higher frequency (7.13 THz) and the As ion with the lower frequency (6.64 THz). At the L-point the two sublattices oscillate against each other in the upper



mode (7.15 THz), but move in phase in the lower mode (6.20 THz). The derivation of the relative amplitudes of Ga and As from the experimentally observed phonon intensities requires precise values for the Debye-Waller factors of the individual atoms, which have to be calculated from a suitable model of the lattice dynamics. It will take some time to select the model which best describes the observed eigenvectors, since each of the proposed models has adjustable parameters which are more sensitive to the eigenvectors than to the frequencies.



1. One of the three IN1 monochromators.
2. The installation of the new composite focussing monochromator IN1.



High Energy Excitations

The return to service of the IN1B TAS will permit further measurements of high energy excitations at the ILL. This machine which takes its beam from the "hot source", and therefore has available large fluxes of short wavelength neutrons, will allow the measurement of excitations with frequencies in the range 5-50 THz. It is expected that IN1 will be in direct competition with many of the new generation of spallation source instruments. For single-crystal measurements of systems where there is appreciable dispersion or anisotropy IN1 has the distinct advantage of being able to carry out scans with constant wavevector transfer or constant energy transfer, in a predetermined crystallographic direction. The new instrument is much simpler to use than the older version, and has greatly increased flux at high energies due to the new design of monochromator mounting.

The first experiment to be carried out on the new spectrometer was a study of the high temperature magnetic dynamical susceptibility of the disordered antiferromagnetic alloy $\text{Mn}_{73}\text{Ni}_{27}$ ⁽³⁾. This material is particularly suited to such studies since the combination of the constituents produces a "null-matrix" alloy thus removing the majority of the nuclear scattering processes. Typical data from this experiment is presented in Fig. 6.

At the present time there is a considerable degree of controversy concerning the high temperature (temperatures greater than the critical temperature), dynamics of magnetic systems. This is particularly true for itinerant transition metal systems, where the magnetic response extends to very large energies. The experimental data for $\text{Mn}_{73}\text{Ni}_{27}$, after the corrections have been made for instrumental resolution, should provide a stringent test of the present theories of high temperature itinerant magnetism. Future experiments include a study of the high energy excitations of nickel in both the ferromagnetic and paramagnetic phases.

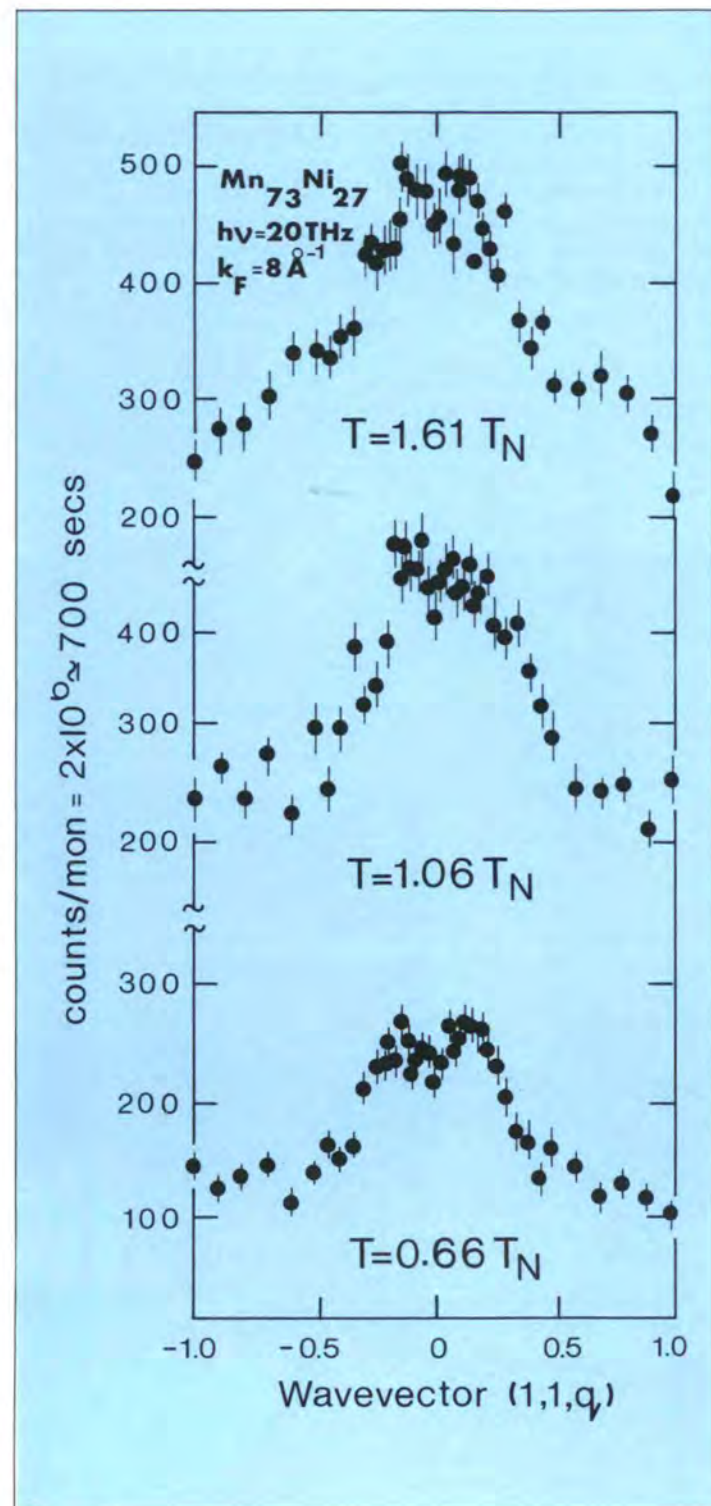


Figure 6: The evolution of the neutron scattering as a function of temperature observed for the antiferromagnetic alloy $\text{Mn}_{73}\text{Ni}_{27}$ ($T_N = 445 \text{ K}$). The data presented is in the form of constant energy transfer scans at 20 THz with a fixed final wavevector of 8.0 \AA^{-1} . The scans were performed around the (110) Bragg position in the (001) direction.



Studies using Polarisation Analysis on IN12

During the year IN12 was equipped for complete neutron polarisation analysis. In addition to the Heusler alloy analyser⁽⁴⁾ described in the 1982 annual report, a Co-Ti bender⁽⁵⁾ was installed between the monochromator and samples to provide a polarised, monochromatic incident beam. A newly designed flat-coil flipper was also tested⁽⁶⁾. At a neutron wavelength of 4 Å the new equipment provided an intensity of polarised neutrons at the detector which was about 15% of that obtained for unpolarised neutrons with an optimised configuration involving pyrolytic graphite monochromator and analyser. A flip ratio of more than 50 was easily obtained.

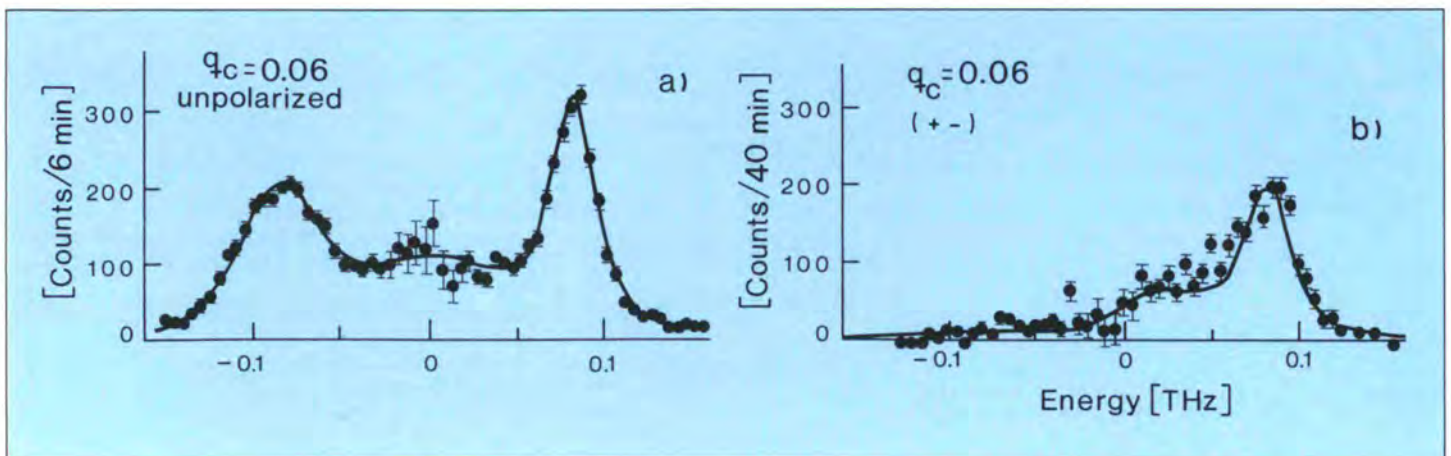
With this equipment an experiment was performed on the quasi-one-dimensional ferromagnet CsNiF_3 ⁽⁷⁾ with a magnetic field applied perpendicular to the chain direction. The aim of the experiment was two-fold; to analyse the neutron polarisation created by magnon scattering and to examine the polarisation dependence of the quasi-elastic scattering which had previously been ascribed to solitons. It is well known that, for an isotropic (Heisenberg) magnet in a saturating magnetic field, magnons observed in neutron energy loss only involve scattering processes in which the neutron spin is flipped from an “up” state to a “down” state, denoted (+ -) scattering.

Conversely, magnons observed in neutron energy gain only involve (- +) scattering. This simple selection rule fails,

however, if the magnetic sample is not isotropic. In particular, for the case of planar anisotropy, which is relevant to CsNiF_3 , Hood⁽⁸⁾ has recently calculated the proportions of (+ -) and (- +) scattering to be expected in the magnon peaks. This calculation, which is valid only at low temperatures is found to be in excellent agreement with the IN12 measurements at a temperature of 2.1 K⁽⁷⁾. As the sample is warmed, the influence of the easy-plane anisotropy diminishes and the behaviour approaches that of an isotropic system. Nevertheless, some planar character remains for the field and temperature region in which solitons have been reported⁽⁹⁾.

A spectrum, measured on IN12 with unpolarised neutrons, which shows both magnon creation and annihilation peaks together with a quasielastic soliton peak is shown in Fig. 7. If the soliton excitation consisted only of a rotation of spins about the chain direction (spins restricted to the easy plane), it is easy to predict the form expected for a (+ -) spectrum. There should be a strong magnon creation peak, a weak (probably unobservable) magnon annihilation peak and a quasielastic soliton peak whose shape ought to be the same as in Fig. 7a. That is, the soliton peak is expected to be symmetric about the zero-energy position. As Fig. 7b shows this is not the case. Rather, the soliton peak seems to obey the same selection rule as the single-magnon peaks; only neutron energy-loss processes are seen in (+ -) scattering. Although a heuristic explanation of this observation has been advanced⁽⁸⁾ no detailed calculation is available and it cannot be claimed that the phenomenon is understood.

Figure 7: (a) Unpolarized and (b) polarized (+ -) neutron scattering from the quasi-one-dimensional ferromagnet CsNiF_3 at $T=2.1$ K.

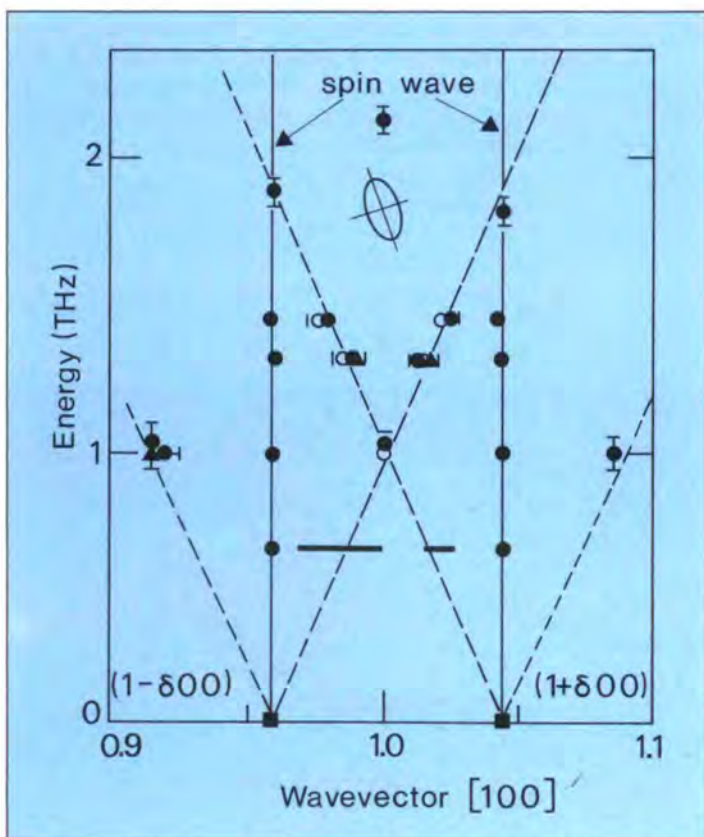




Magnetic Excitations in Chromium

Chromium metal, a sinusoidally modulated antiferromagnet below 311 K, has been extensively studied over the last few years. Interest has centred on the extremely “stiff” spin-wave branches emerging from the magnetic satellite positions, and on the “commensurate excitation” observed at ~ 1 THz at the $(1,0,0)$ position. Recent experiments using IN12 have shown that the spin-wave is *longitudinal* in character at low frequency, changing smoothly to the more-conventional transverse polarisation at higher frequencies. A detailed study of the commensurate excitation, made on IN8⁽¹⁰⁾ has shown that this feature has more structure than previously observed. Indeed, it appears to arise from a crossing of excitation branches from the satellite positions as is seen in Figure 8; since the

Figure 8: Dispersion relations for excitations in the Transverse Spin Density Wave phase of single-Q chromium. The dashed lines show the additional branches of excitations found by Burke et al⁽¹⁰⁾. The full lines are the (vertical) spin-wave branches.



slope of these branches is the same as that of the LA $[1,0,0]$ phonon, it has been suggested that the “1 THz excitation” arises from magnetovibrational scattering, rather than being a true (magnetic) elementary excitation.

Intermediate Valence

The magnetic spectral response of the intermediate valence system CeSn_3 measured using the TOF spectrometer IN4 reveals a broad, well defined magnetic excitation centred on 40 meV in addition to the usual quasi-elastic spectrum centred on zero energy⁽¹¹⁾. With increasing temperature the inelastic hump broadens further and “melts away” such that around the temperature of the maximum in the susceptibility (~ 130 K) no observable trace of its presence remains and the full magnetic response can be described by a single quasi-elastic spectrum. The observed excitation may represent a form of modified crystal field transition, or it could be due to a transition across the hybridisation gap in the f-band or as seems most probable it may represent an excitation of the f-electron to the conduction sea.

Secretary:
D. McKenzie Paul

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Intermediate Valence

Many rare earth alloys and compounds, particularly those of Ce and Yb, the elements at the ends of the rare earth series, but also of Sm, Eu and Tm show anomalous physical properties (e.g. magnetic susceptibility, specific heat, lattice constants etc.) as compared with other rare earth ions in the same series of alloys or compounds. It is generally believed that the peculiar physical properties of the rare earth ion in the so-called intermediate valence state result from temporal fluctuations of the ion between two (or more) well defined valence states. In normal rare earth compounds, 4f electrons are considered as localised. When the 4f level is close to the Fermi energy of a conduction band, hybridisation between the pure 4f configuration and the conduction electron states may occur and the average number of 4f electrons can then assume non-integral values. The fractional change depends on external parameters such as temperature and pressure. In particular, lattice constants are highly correlated to the valence state.

A well defined signature of the intermediate valence state is obtained in the X-ray (L_{III}) absorption edge spectra which show the simultaneous presence of two valence states in many systems. Also Mössbauer effect measurements of some Sm compounds indicate the magnitude of the isomer-shift to be intermediate between that for Sm in the di-valent or tri-valent states.

When one of the two configurations is non-magnetic (in Ce, Sm, Eu and Yb compounds), mixed valent systems do not show magnetic order. However, in the case of Tm ions the two degenerate configurations are magnetic, and then the nature of the ground state is not known.

Neutron scattering experiments are extremely well suited for the study of intermediate valence systems having so far provided a wealth of information regarding magnetic form factor anomalies, characteristic spin fluctuation or valence fluctuation times, magnetic excitations of character peculiar to valence fluctuation systems and about phonon anomalies resulting from the coupling of charge and valence fluctuations.

Neutron Investigation of Modulated Structures*

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1. Introduction

1.1. Modulated Structures

Incommensurably-modulated solids are often described [1] as long-range ordered structures which lack translational symmetry due to the superposition within the same system of several mutually incompatible periodicities. As such IC solids provide an intermediate step between the ordinary crystalline state and the disordered non-periodic amorphous state.

In fact, part of the current work on IC structures is aimed at testing the validity of the above definition. As shown by de Wolff [2] and Janner and Janssen [3], spatial periodicity is hidden rather than absent in the ideal IC solid and may be recovered via a suitable generalization of the concept of symmetry operation. On the other hand, experimental and theoretical evidence indicate that real IC solids close to the C limit [4] or in the presence of frozen defects [5,6] do not qualify as fully long-range ordered structures.

A wide range of physical systems are known to present compositional or displacive modulations and the corresponding physical situations are necessarily very diverse. For instance 2-dimensional systems, such as adsorbed monolayers or intercalates exhibit qualitatively unique features (see Nielsen [7] for an experimental survey). In this review the emphasis will be on displacive modulations i.e. modulations of the equilibrium atomic positions, in ordinary 3-dimensional solids.

Perhaps the single feature common to all IC systems is the occurrence of irrational satellite reflections, in addition to the Bragg reflections associated with the unmodulated reference system. The observation of a continuous shift in the satellite diffraction pattern as a function of temperature or external field has been taken perhaps too readily, as acceptable evidence for the true IC nature of the modulation. As suggested by theoretical models (see Bak [8] for a recent review), an apparent smooth change in modulation wavevector may correspond to an infinite sequence of higher-order C phases separated or not by true IC phases (incomplete or complete devil's staircase). In such models the concept of discommensuration (DC) or domain wall separating locally C regions is of central importance

* Reprinted from "Multicritical Phenomena" Plenum NATO-ASI Series B, Vol. 106 (Physics) (Plenum New York 1984) ed. R. Pynn and A.T. Skjeltorp.



[9]. In particular the value of the modulation wavevector in the IC state is determined by the average DC spacing, the C state corresponding to zero DC density.

Another characteristic feature of IC systems is the presence of global hysteresis affecting the temperature and pressure dependence of the modulation wavevector and of those macroscopic variables (e.g. dielectric constants, optical birefringence coefficients, etc.) which couple to the IC order parameter. As pointed out by Aubry [10], global hysteresis is not compatible with a smooth analytic behaviour. Thus its observation lends support to the (complete) devil's staircase picture where irreversible effects arise as a result of pinning of the DC's by the underlying lattice. Recently, experimental evidence have shown that defects play an important rôle in the observed irreversibilities, giving rise to specimen-dependent behaviour and memory effects [11-14]. Thus in general, both types of pinning mechanisms, intrinsic and defect-induced, are expected to contribute to the observed irreversible behaviour and incomplete ordering.

1.2. Phasons

IC solids are characterized by new types of excitations [15-16], corresponding to fluctuations in the phase and amplitude of the static modulation wave. In the long-wavelength limit the phase mode consists in an overall phase shift of the modulation with respect to the atomic lattice (sliding mode). For a well-behaved IC modulation, for which the atomic displacements can be described in terms of analytic functions of space, such a shift costs no energy and the corresponding phase branch is gapless. For a quasi-C modulation the phase branch becomes identical to the vibrational "phonon" branch of the DC lattice. Its gapless character is preserved as long as the DC's are not pinned.

Recently, it has been shown that phase modes are overdamped, at least at long wavelengths [17]. The damping arises from the fact that the atomic motions involved are inhomogeneous on a microscopic scale and are thus affected by ordinary anharmonic (i.e. dissipative) interactions.

Hence, unlike acoustic modes, phasons do not qualify as true Goldstone modes. In terms of conservation laws, the difference lies in the fact that the total particle-momentum operator commutes with the total crystal Hamiltonian, while the analogous phase-momentum operator commutes with the harmonic part only. The overall phase shift is thus affected by friction.

Practically, the phase mode response is expected to be of the damped harmonic oscillator type:

$$S(q, \omega) = \frac{kT}{\Pi} \frac{\Gamma_0}{(\omega^2 - v^2 q^2)^2 + \omega^2 \Gamma_0^2}$$

where the velocity v and damping coefficient Γ_0 are slowly-varying with q . The response is diffusive at low q :

$$\omega_{ph}(q) = i \frac{v^2 q}{\Gamma_0} \quad (q < \frac{\Gamma_0}{v})$$

becoming progressively underdamped at large q :

$$\omega_{ph}(q) = vq + \frac{i\Gamma_0}{2} \quad (q > \frac{\Gamma_0}{v}).$$

Rough estimates for v and Γ_0 indicate that the two regimes may be probed by Brillouin and neutron scattering, respectively [18]. Underdamped phase modes have been observed by neutron scattering in phase III of biphenyl [19] and in ThBr₄ [20] (see Fig. 9).

1.3. Experimental Techniques

Most of the experimental information on IC solids is based on X-ray, neutron and electron diffraction data. The best q -resolutions ($\approx 10^{-4} \text{ \AA}^{-1}$) are obtained from X-ray sources. In 2H-TaSe₂, minute deviations from commensurability have thus been revealed. In structurally-modulated BaMnF₄, satellite reflections of the type $(h + \xi, k + 1/2, l + 1/2)$, with ξ ranging from 0.39 to 0.40 depending upon temperature (and specimen origin), have been shown to present a finite q -width along ξ , corresponding to a correlation length of a few hundred cells [22]. In view of the absence of any lock-in transition at low temperatures, this result suggests a defect-induced pinning of the modulation.

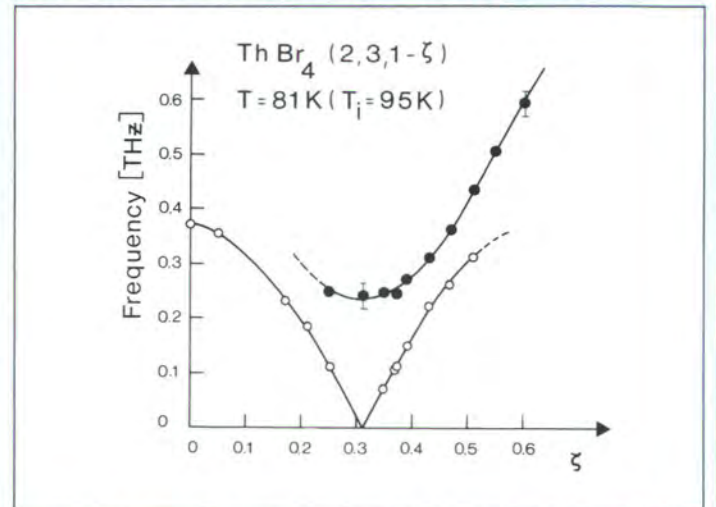


Figure 9: Phase mode (open circles) and amplitude mode (closed circles) in ThBr₄ (from ref. 20).



Real space visualization of DC arrays in 2H-TaSe₂ has been achieved by dark-field electron microscopy [23,24]. In particular, dynamic studies as a function of temperature show that the basic mechanism through which the DC array readjusts its average spacing is “stripple” nucleation (or evaporation) rather than homogeneous expansion.

Local information may be obtained from resonance techniques (see Blinc [25] for a review), or at low temperatures, from optical crystal-field spectroscopy [26]. Resonance lines are broadened inhomogeneously due to the distribution of local environments introduced by the modulation. The line-shape of the resonance spectrum mirrors the distribution of local fields, provided the latter fluctuates slowly on the characteristic timescale of the measurement (inverse linewidth). This condition should be (and appears to be) generally fulfilled except in the immediate vicinity of the IC ordering temperature where motional narrowing should in principle occur due to phase fluctuations. In Rb₂ZnBr₄ a partial crossover to the fast fluctuation regime has been reported [27] at about 10 K below the ordering temperature (T_i = 200 K). The ⁸⁷Rb NMR linewidth at that temperature was ~ 20 KHz.

2. Nowotny phases: an example of uniaxial intergrowth compound

2.1. Structure

The structure of Nowotny phases [28] is based on two interpenetrating tetragonal lattices with identical cell dimensions in the (a, b) plane, but different c parameters. Model systems of this type have been considered by Theodorou and Rice [29] and Axe and Bak [30]. The chemical formula is TX_x where T is a transition metal element and X is an element of group III or IV. The observed variation of the atomic ratio x with the chemical nature of T and X suggests that the stability of the structure is largely determined by the value of the electron concentration per T-atom [31].

For each of the two sublattices one can define an idealized subcell (cf. Fig. 10), of dimensions (a, a, c_T) and (a, a, c_X), with 4 atoms/cell in each case (i.e. c_T = xc_X). The atomic positions on sublattice X are modulated in such a way as to avoid overlap with the surrounding T-atoms. The modulation consists in a rotation of the X-X dumbbells in the (a, b) plane, together with a shift along c. The X-atomic positions along c are expressed as

$$z_X(n) = nc_X + u_X + g_T(nc_X + u_X - u_T) \quad (1)$$

where u_{X,T} are appropriate origins and g_T(z) is a periodic modulation function with period c_T:

$$g_T(z + c_T) = g_T(z) \quad (2)$$

An analogous expression can be written down for the T positions, although the observed distortions are much smaller. In order to calculate the diffracted intensity from such a system let us write the density function of each sublattice as:

$$\bar{\rho}_{X,T}(\vec{r}) = \rho_{X,T}(\vec{r} - \vec{g}_{T,X}(z)) \quad (3)$$

where $\vec{g}(\vec{g}^\perp, g^\parallel)$ is a displacement vector satisfying (2) and $\rho_{X,T}(\vec{r})$ is the unmodulated sublattice density function:

$$\rho_{X,T}(\vec{r}) = \sum_{\vec{G}_\perp, \lambda} \rho_{X,T}(\vec{G}_\perp, \lambda) \exp \left\{ i(\vec{G}_\perp \cdot \vec{r}_\perp + \lambda c_{X,T}^*) \right\} \quad (4)$$

where $\vec{G}_\perp + \lambda \vec{c}_{X,T}^*$ is a reciprocal lattice vector of sublattice X, T.

Combining (3) and (4) one readily shows that Bragg peaks are observed at:

$$\vec{Q} = \vec{G}_\perp + \lambda \vec{c}_X^* + \mu \vec{c}_T^* \quad (\lambda, \mu = \text{integers}) \quad (5)$$

and that in general (i.e. for $\vec{G}_\perp \neq 0$) both sublattices contribute to each reflection.

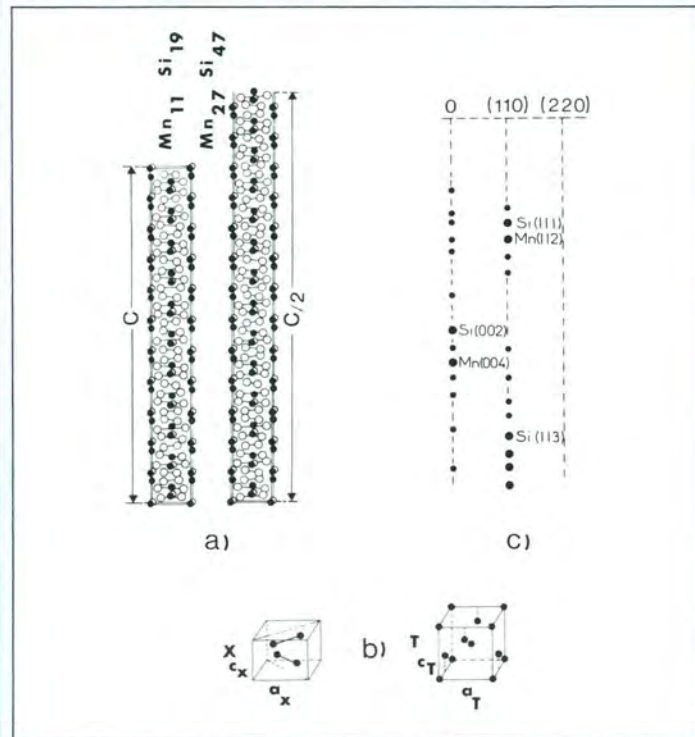


Figure 10: Structure of Nowotny phases TX_x (T = Ti, Zr, V, Mo, Cr, Mn, Rh; X = Si, Ge, Sn). (a) sketch of unit cell for two stoichiometric compounds in the MnSi_x series (x = 1.73 ± 0.02) (from ref. 35); (b) idealized subcells (a_x = a_T; c_x = x c_T); (c) typical diffraction pattern. All spots can be indexed according to eq. (5). Only the main reflections (λ or μ = 0) are labelled in the figure.



For rational values of $x(x = m/n)$, the supercell dimension along c is $\bar{c} = nc_T = mc_X$. The space groups of the corresponding compounds are D_{2d}^6 , D^{12} or D_{2d}^8 , depending upon the parities of m and n . In the $MnSi_x$ system, the following compounds have been reported by X-ray diffraction [32,33]:

Mn_nSi_m	x	$a(\text{\AA})$	$(\bar{c}/n)(\text{\AA})$
$Mn_{11}Si_{19}$	1.727	5.518	4.376
$Mn_{15}Si_{26}$	1.733	5.525	4.370
$Mn_{27}Si_{47}$	1.741	5.530	4.368

Commensurate structures have also been observed by de Ridder et al. [34] by electron diffraction. In addition, these authors observe compositional inhomogeneities across the volume of their specimen, giving rise to an alternance of C and IC diffraction patterns [35].

The observed concentration fluctuations apparently cannot be eliminated by annealing, which would seem to indicate that the equilibrium Si concentration is inhomogeneous even at high temperature. Even though this feature is not understood in detail, it may be tentatively interpreted as resulting from a competition between the band structure energy, which is minimized for some IC value of x , and short-range lock-in terms, which favour simple rational fractions.

2.2. Dynamics

To the extent that the displacement functions $g_{T,x}$ (cf. eq.(1)) are continuous, analytic functions with mutually IC periodicities, excitations polarized along c will propagate independently on each sublattice. Indeed inelastic neutron scattering data taken near a pair of strong Mn(Si) reflections reveal two longitudinal acoustic branches with different slopes [36].

In the long-wavelength limit, however, the microscopic incommensurability of the two sublattices becomes irrelevant and several coupling mechanisms arise [30,37]. As a result, a single combined acoustic mode should emerge. In addition, one expects to observe quasielastic scattering corresponding to the (diffusive) phase mode response. For unscreened ionic crystals, however, the longitudinal phase branch should present a gap, corresponding to the two-sublattice plasmon frequency. All these predictions remain to be tested experimentally.

3. Charge Density Waves

Fermi surface instabilities in low-dimensional metals provide a specific mechanism leading to modulated structures. The modulation in that case, results from the screening of the electronic charge density wave by the nuclei (the "2 k_f " instability). It is essentially through the lattice modulation that the instability is observed in a diffraction experiment.

The IC character of the modulation is connected to that of the Fermi wavevector, the latter arising from non-stoichiometry, as in KCP, charge transfer as in TTF-TCNQ, or just energy band structure as in the transition-metal dichalcogenides. In the latter case the lock-in potential from the lattice is sufficient to eventually drive the CDW periodicity to a commensurate value [38]. This is not so in one-dimensional metals where commensurability can only be achieved by altering the value of the Fermi wavevector, i.e. by changing the conduction electron concentration. The existence within the IC-state of a transition between the analytic, Peierls-conducting regime and the pinned insulating state has been predicted [39,40] and possibly observed in doped polyacetylene [41].

4. Insulators

4.1. General

In insulators the IC-state results either from a soft mode-type of instability (displacive case) or from a collective ordering mode (order-disorder case), both of general wavevector. Within the soft mode picture, the IC ordering transition appears as a mere extension of the conventional ferro- and antiferrodistorsive transitions. While the occurrence of a local minimum around an arbitrary wavevector on a phonon dispersion curve suggests a competition between interactions of different characteristic ranges, it does not in general provide any insight into the nature of these interactions.

It is likely that in ionic crystals the competition involves Coulomb vs short-range forces but this applies equally well to most phase transitions in ionic crystals [42]. Furthermore, microscopic calculations are generally too complex to yield a simple physical picture of the IC instability [43].

In a non-polar molecular crystal such as biphenyl [44] the IC modulation is believed to arise from the competition between the intramolecular potential favouring a finite torsional angle between the two molecular phenyl rings (as in the free molecule) and intermolecular interactions which favour a coplanar conformation.

On a phenomenological level, incommensurability may sometimes be associated with the non-fulfillment of Lifshitz criterion [45]. For example, in non-symmorphic structures, most of the irreducible space-group representations corresponding to special zone-boundary wavevectors are pairwise degenerate and give rise to Lifshitz invariants. In that case a zone boundary phonon softening leads first to a modulated structure with a wavevector close to the high-symmetry zone-boundary point [46].

This type of argument, however, does not apply to IC phases with wavevectors close to the zone-center (and which eventually lock-in at $q=0$), as encountered in $NaNO_2$ [47], quartz [48] and thiourea [49], and alternative models, based on two-mode interactions have been proposed [50-52].

4.2. Thiourea

Thiourea crystallizes in the orthorhombic space group $Pnma$ with four molecules per unit cell (see Fig. 11). Each molecule is planar and possesses a permanent dipole moment oriented in the (a, c) plane. The net dipole moment per cell vanishes due to the (n) and (a) glide planes.

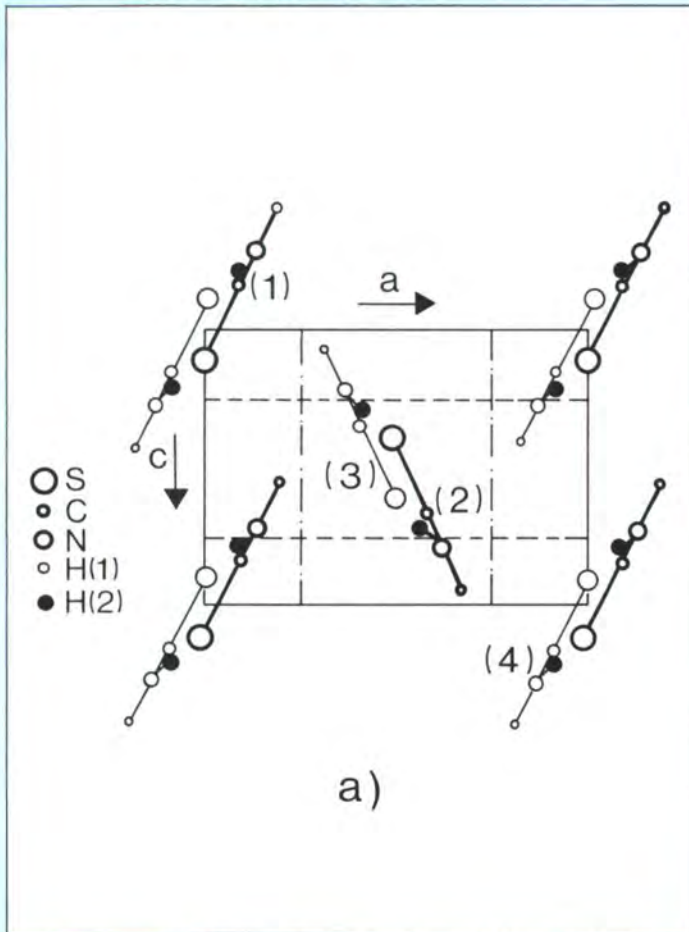


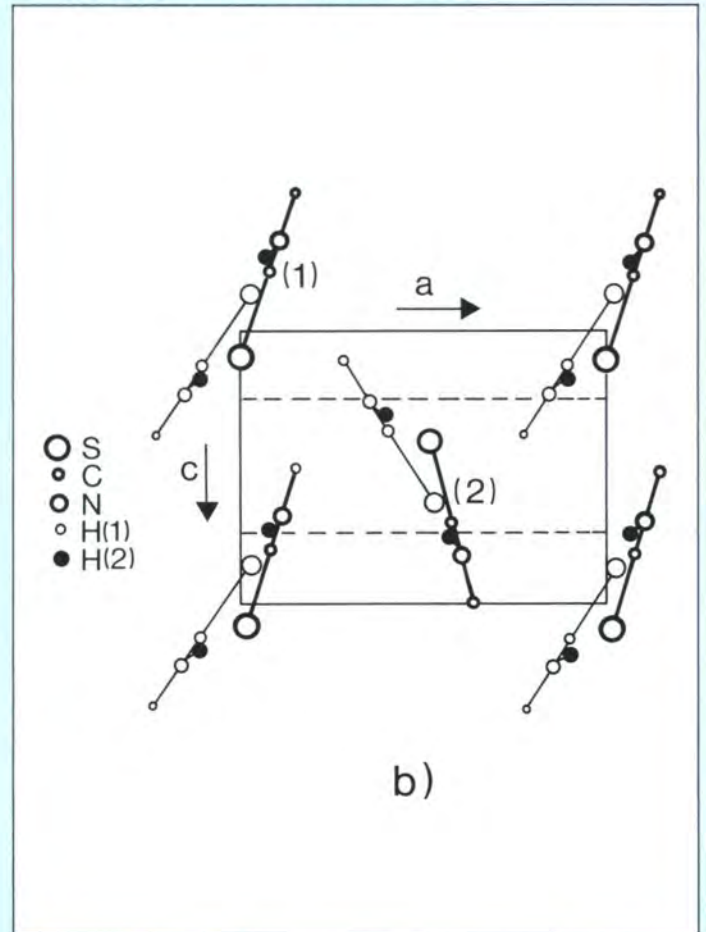
Figure 11: Structure of thiourea in the paraelectric ($Pnma$) phase (a) and ferroelectric ($P2_1ma$) phase (b). Molecules labelled (3) and (4) are displaced by $b/2$ with respect to (1) and (2). (after ref. 57).

Below $T_1 = 218$ K (all transition temperatures refer to the deuterated compound), satellite reflections appear, located at:

$$\vec{q}_\delta(T) = \delta(T)\vec{b}^* \quad (T < T_1)$$

$\delta(T)$ decreases continuously from $\delta(T_1) = 0.141$ to $\delta(T_9) = 0.115$. Between $T_9 = 193$ K and $T_c = 191$ K, δ locks to the commensurate value $1/9$. Below T_c , δ vanishes giving rise to a ferroelectric phase with spontaneous polarization along \vec{a} ($P2_1ma$). Both lock-in transitions are distinctly first-order.

Below room temperature, the softening of a polar optic mode (B_{3u}) is observed by infra-red spectroscopy [53] and neutron inelastic scattering [54]. The soft-mode dispersion minimum lies in the \vec{b}^* -direction where mixing with a TA branch of same symmetry (τ_4) occurs. For $T < 220$ K, a heavily damped coupled mode response is observed.



A moderate (< 1 K) wavevector hysteresis is observed in the IC phase.

On cooling from T_1 , first, second and third order satellites appear successively. Only small intensity discontinuities are observed at T_9 . Critical exponents for the first and second order satellite intensities are found to be in good agreement [55] with the critical behaviour of the $d=3$ XY-model, including a uniaxial perturbation [56].



Fig. 12 shows the isothermal variation of δ with pressure for a few selected temperatures. Pressure hysteresis is within experimental error (± 20 bars). Note the additional step at $\delta = 1/7$ for isotherms below 207 K, and the characteristic shape of the $\delta(P)$ curve just above and below the $1/7$ plateau. Continuous lock-in transitions with logarithmic singularities have been predicted theoretically [10, 8]. Note also the absence of a well-defined plateau on the 157.6 K isotherm. Results are summarized in the (P, T) phase diagram shown in Fig. 13. The values of δ along the $T_i(P)$ and $T_c(P)$ lines are shown as δ_i and δ_c , respectively. The negative sign of dT_i/dP and dT_c/dP is typical of a ferroelectric-type instability [42].

Single crystal diffraction patterns [54] indicate that the high-pressure $\delta = 1/3$ phase belongs to the same class of lock-in phases as the $\delta = 1/7$ and $1/9$ phases. Its persistence to temperatures much above the $T_i(P)$ line is, however, not understood.

As far as the lower part of the diagram is concerned ($P < 2$ kbars), the results may be formulated as follows:

- i) a steady decrease of $\delta(T, P)$ with decreasing T and P is observed across the IC phase.
- ii) When the "natural" value of $\delta(T, P)$ approaches a simple rational value such as $1/7$ or $1/9$, small lock-in free energy terms stabilize the corresponding C-phase over a narrow T or P range. Note the absence of a lock-in phase at $1/8$ and the presence of two distinct $1/7$ phases.

Point i) above may be accounted for in terms of a phenomenological Landau-Ginzburg free-energy of the type [58-59]:

$$F = \int \left\{ \frac{1}{2} A_0 P_x^2 + \frac{1}{4} B P_x^4 + \frac{1}{2} \alpha \left(\frac{dP_x}{dy} \right)^2 + \frac{1}{4} \beta \left(\frac{d^2 P_x}{dy^2} \right)^2 + \gamma \left(P_x \frac{dP_x}{dy} \right)^2 \right\} dy \quad (6)$$

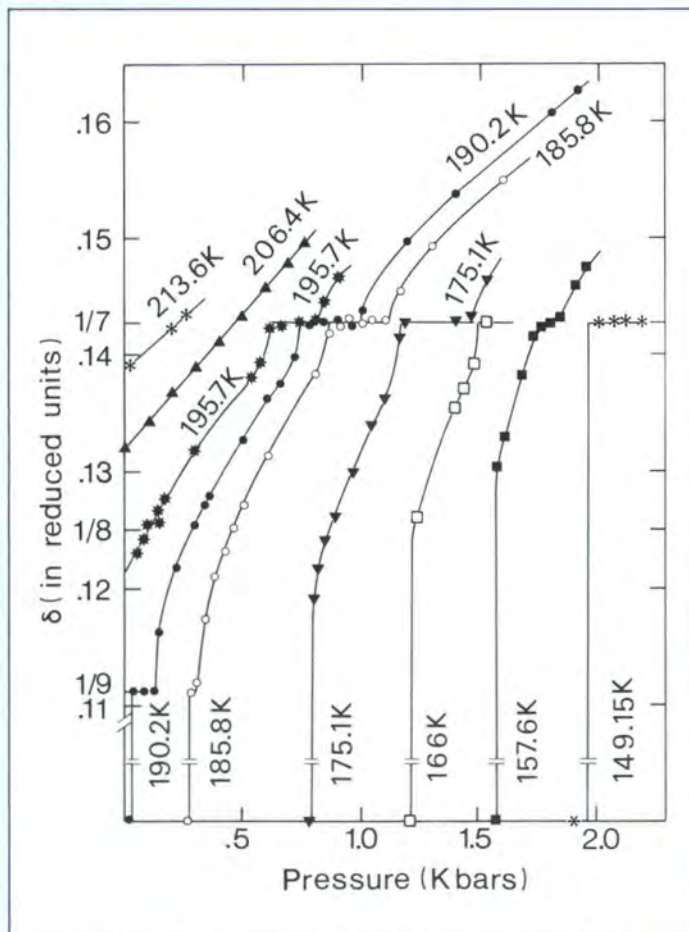


Figure 12: Thiourea: isothermal variation of modulation wavevector δ with pressure (after ref. 49).

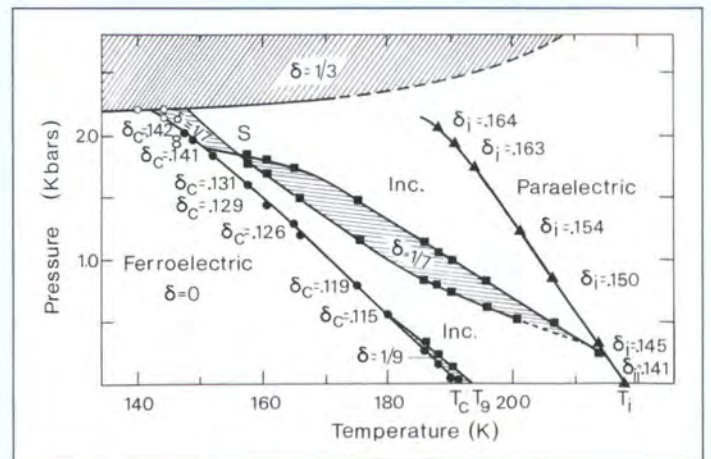


Figure 13: Thiourea: (P, T) phase diagram (after ref. 49).

with: $A_0 = a(T - T_0)$; $B > 0$; $\alpha < 0$; $\beta > 0$; $\gamma > 0$.

Approximating the polarization wave $P_x(y)$ by a sine-wave:

$$P_x(y) = P_0 + 2P_\delta \cos(2\pi \delta y) \quad (7)$$

expression (6) yields:

$$F = \frac{1}{2} A_0 P_0^2 + \frac{1}{4} B P_0^4 + A_\delta P_\delta^2 + \frac{3}{2} B_\delta P_\delta^4 + \frac{3}{2} (B + B_\delta) P_0^2 P_\delta^2 \quad (8)$$

$$\text{where: } A_\delta = A_0 + \alpha \delta^2 + \frac{1}{2} \beta \delta^4 \quad (9)$$

$$\text{and: } B_\delta = B + \frac{4}{3} \gamma \delta^2 \quad (10)$$

Model (8) gives a second-order phase transition (at $T = T_i > T_o$), from the paraelectric state ($P_\delta = P_o = 0$) to the IC-state ($P_o = 0; P_\delta \neq 0$) and a first-order transition (at $T = T_c < T_o$) from the IC-state to the ferroelectric state ($P_o \neq 0; P_\delta = 0$). Minimization of (8) with respect to δ , leads to the required variation of δ across the IC-phase. Presumably the pressure dependence of the various parameters in the model can be adjusted in such a way as to reproduce the observed phase diagram. The inclusion of higher-order harmonics in (7) will simply enhance the T-dependence of δ .

In order to discuss point ii) it is necessary to introduce microscopic order parameters and make use of their symmetry properties. Let $Q(\vec{q}_\delta, \tau_4)$ denote the complex order parameter corresponding to the first Fourier component of the modulation. A commensurate phase with $\delta = 1/n$ is stabilized by an Umklapp free energy term of the form:

$$\Delta F_n = V^{(n)}(\vec{q}_\delta, \tau_4) Q^n(\vec{q}_\delta, \tau_4) + \text{c.c.} \quad (11)$$

$V^{(n)}$ is an appropriate anharmonic coefficient whose symmetry properties are determined by the space group of the paraelectric phase. In particular $V^{(n)}$ vanishes unless:

$$n\vec{q}_\delta = m\vec{b}^* \text{ i.e. } \delta = \frac{m}{n} \text{ (m, n = integers).}$$

Furthermore rotational selection rules require m and n to be of same parity. Hence the 1/7 and 1/9 phases correspond to lock-in terms of order 7 and 9, while the 1/8 phase would require a lock-in term of order 16, which is too weak to be effective. It has been predicted [49], however, and confirmed experimentally [60, 61] that the 1/8-phase could be stabilized by a uniform electric field applied along a. The corresponding lock-in term is of the form:

$$Q^8(\vec{q}_\delta, \tau_4) Q(0, \tau_4)$$

where $Q(0, \tau_4)$ is induced by the applied field. The stability range of the 1/7-phase appears to vanish in the vicinity of the point labelled S in Fig. 13. In fact, satellite intensity patterns recorded on either side of point S suggest two distinct 1/7-phases. This observation can be accounted for if one assumes that the pressure and temperature dependence of the $V^{(7)}$ Umklapp coefficient is such that it vanishes on a curve in the (P, T) plane. Point S would then be at the intersection of the two curves defined by:

$$\begin{aligned} V^{(7)}(P, T) &= 0 \\ \delta(P, T) &= 1/7 \end{aligned}$$

where $\delta(P, T)$ is the natural value of δ , i.e. the value of δ which minimizes the free energy in the absence of Umklapp lock-in terms. Introducing real variables:

$$V^{(7)}(\vec{q}_{1/7}, \tau_4) = iv(T, P); \quad Q(\vec{q}_{1/7}, \tau_4) = \eta e^{i\phi}$$

(11) becomes:

$$\Delta F_7 = v\eta^7 \sin 7\phi$$

Thus the two 1/7 phases are characterized by opposite values of the phase

$$\phi = \pm \frac{\pi}{14} \pmod{\frac{2\pi}{7}}$$

or, equivalently, by opposite signs of the atomic displacements $\vec{u}_{\ell k}$:

$$\vec{u}_{\ell k} = (m_k)^{-1/2} \eta \vec{w}_k(\vec{q}_{1/7}, \tau_4) e^{i(\vec{q}_{1/7} \cdot \vec{r}_{\ell k} + \phi)} + \text{c.c.}$$

The two phases together with the IC phase would then coexist at S.

In fact, in a very narrow T and P range around S the contribution from the next Umklapp term:

$$V^{(14)}(\vec{q}_{1/7}, \tau_4) Q^{14}(\vec{q}_{1/7}, \tau_4) \equiv w \eta^{14} \cos 14\phi \quad (12)$$

should be included into ΔF_7 . Depending upon the sign of w, two different situations may arise, but in either case the isolated character of point S is removed.

Finally we wish to stress that although expressions such as (11) are written in term of the primary Fourier component of the modulation alone, this does not preclude the existence of higher order distortion harmonics, which do contribute additional lock-in free-energy terms. Formally one assumes that the minimization of the free-energy with respect to high-order harmonics has already been performed and that the $V^{(n)}$'s have been renormalized accordingly.

Nevertheless it is of interest to determine the harmonic content of the modulation in both the IC and C phases. In the latter case, the harmonic analysis can be performed using standard crystallographic techniques. Hence a detailed structural study of the 1/9 phase has been initiated and is currently in progress [62]. Preliminary results indicate that the simple ferroelectric-domain model (i.e. a square-wave with 9 planes polarized up and 9 planes polarized down) is not realistic. The harmonic content of the modulation appears to be considerably lower than predicted by the above model. If domain walls are present some degree of disorder must also be present, in such a way as to smooth out the average wave profile. This result is not unexpected since the DC picture is not applicable to the case $\delta = 0$ [63].



4.3. TMATC-Zn

Tetramethylammonium tetrachlorozincate (TMATC-Zn) belongs to a class of compounds of formula $(N(CH_3)_4)_2 XCl_4$ ($X = Zn, Co, Mn, Fe, \text{etc.}$), isomorphous to Rb_2ZnCl_4 and K_2SeO_4 in their undistorted phase (Pnma). Below room temperature these compounds undergo various sequences of phase transitions involving IC, C, and quasi-C modulated structures, with modulation wavevector:

$$\bar{q}_\delta = \delta(T)\bar{a}^*$$

Fig. 14 shows the $\delta(T)$ curve measured on deuterated TMATC-Zn, using neutron diffraction [64]. In addition to pronounced thermal hysteresis, the experimental curve exhibits a quasi-C plateau prior to the onset of the 3/7-phase. A similar effect has been observed in $Ba_2NaNb_5O_{15}$, where the C phase is in fact never reached [65]. It has been ascribed to the stabilization by impurities of phase defects in the C wave [66].

In a later (cooling) run, using the same sample the 1/2 plateau was found to be much reduced (points marked * in fig. 14). In other samples the same plateau appears only under stress [67].

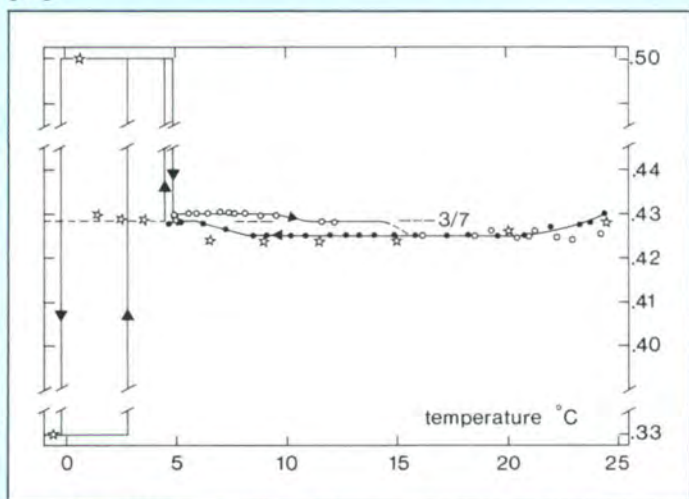


Figure 14: TMATC-Zn: variation of modulation wavevector with decreasing (closed circles) and increasing temperature (open circles). The data points marked as * correspond to a later cooling run. (deuterated compound; from ref. 64).

Different behaviours are observed on deuterated and non-deuterated samples [68]. In particular non-deuterated samples exhibit a plateau at 2/5, which is also observed on the deuterated compound under pressure (a few hundred bars). Clearly the balance of interactions which determines the values of the modulation wavevector, is affected by differences in crystal quality (residual strains, impurities) and by thermal history. The corresponding effects in thiourea are either absent or much attenuated.

Another qualitative difference between the two compounds is the non-monotonic variation of $\delta(T)$ as shown in Fig. 14. Aubry [1] has shown in the context of the discrete Frenkel-Kontorova model, that the average lattice spacing misfit ℓ of the absorbed chain (here the modulation periodicity) needs not vary monotonically with the substrate potential λ (here the temperature). He also points out that very small changes in the chain tension μ , the other parameter in the model, can produce large changes in the $\ell(\lambda)$ curve. Fig. 15 shows two such curves calculated for slightly different values of μ : one shows a monotonous decrease of $\ell/2a$ from 2/5 to zero while the other exhibits a plateau at a maximum value of 1/2. The absence of an IC phase in the low- λ part of the calculated curves is an artefact of the model, related to the particular form of substrate potential used.

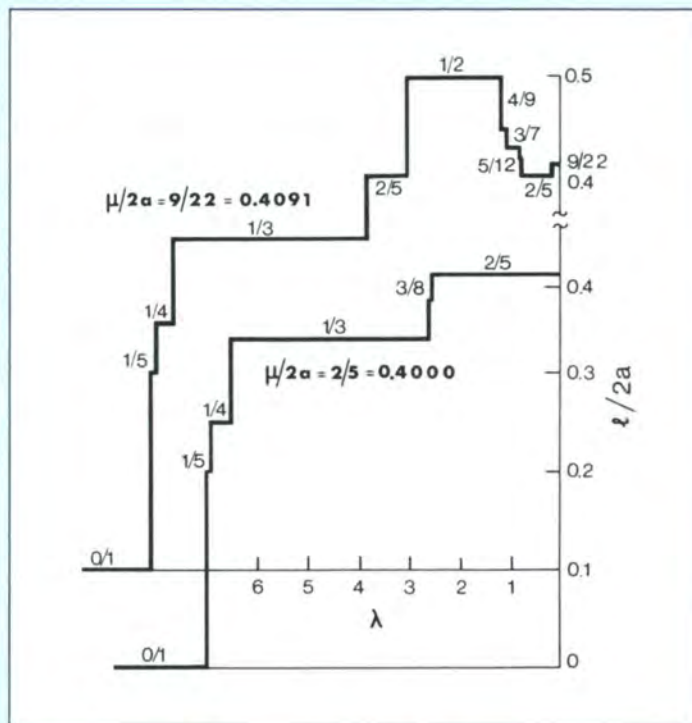


Figure 15: Discrete Frenkel-Kontorova model: Average lattice-spacing misfit versus substrate potential for two values of the chain tension (from ref. 74).

In summary, it seems that the complex behaviour shown by the present compound and by others in the same class, cannot be understood, even qualitatively, without taking explicit account of the discrete nature of the modulated lattice.

5. A Magnetic Example: Cerium Antimonide

Below the magnetic ordering temperature ($T_N = 16.2$ K) CeSb displays a particularly complex behaviour [69] as evidenced by the many specific heat anomalies observed [70] (cf. fig. 16). The complete (H, T) phase diagram is shown in fig. 17 for H along [001]. The magnetic structures of the various phases observed are all based on a periodic stacking sequence of non-magnetic and ferromagnetic (001) planes.

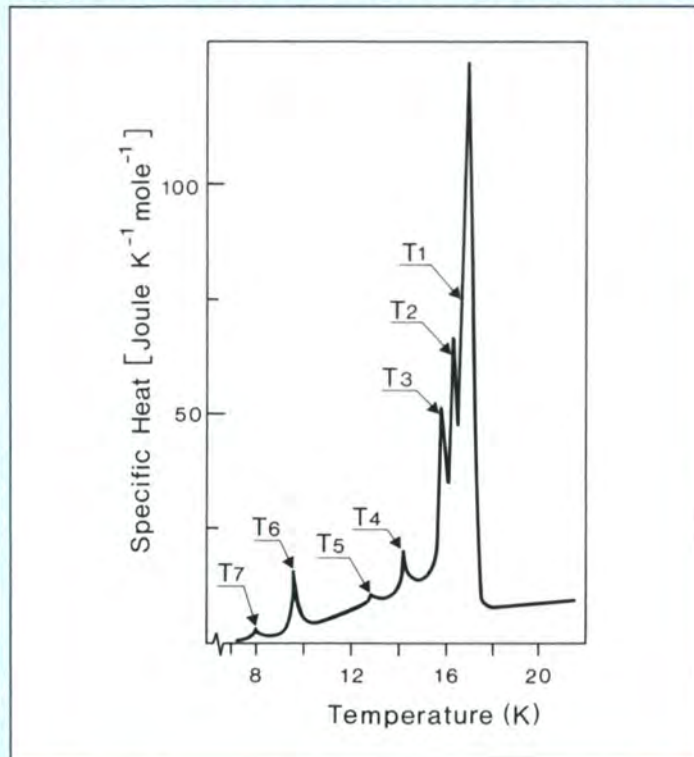


Figure 16: Specific heat of CeSb in zero applied magnetic field (from ref. 70).

The three end-structures are:

- the paramagnetic (P) phase at high T
 - the ferromagnetic (F) phase at high H and low T
 - the antiferromagnetic (AF) phase at low H and low T.
- The other phases can be regarded as intermediate between two of the above three.

The structure of the AF phase consists in a sequence of two pairs of Ce^{3+} layers with opposite magnetization, i.e. (+ + - -). This sequence can be described by a square-wave of wavevector $k = (0, 0, 1/2) \frac{2\pi}{a}$ in the f.c.c. Brillouin zone (interlayer spacing = $a/2$). The structures labelled AFF2 and AFF1 are obtained from AF by removing one down layer (-) every 7th and 3rd layer, respectively, i.e. (+ + - - + + -) and (+ + - -). The corresponding square-wave wavevectors are $k = 4/7$ and $2/3$.

Similarly the AFP phases are generated from the AF phase by introducing one non-magnetic plane every $2n-1$ layer. The resulting wavevector is of the form $k = n/2n-1$ with $n = 2, 4, 5, 6, \dots \infty$ (an exception to the rule is the AFP2 phase of wavevector $k = 8/13$). In all cases no net magnetization is introduced.

Finally between the F and P phases the substitution involves non-magnetic and ferromagnetic up (+) planes. The corresponding structures can be visualized as resulting from the superposition of a ferromagnetic component and of a square-wave of wavevector $n/2n+1$ (FP3, FP4) or $n/2n-1$ (FP1).

The overall shape of the phase diagram is well accounted for in terms of a simple thermodynamic model in which each Ce^{3+} ion is assumed to contribute an entropy of $k \ln 2$ in the non-magnetic state and a moment of $2.1 \mu_B$ in the magnetic state. For example the transitions $AF \rightarrow AFF$ and $AFF \rightarrow F$ involve a change in magnetization and no change in entropy ($\Delta M \neq 0$; $\Delta S = 0$). Hence from Clapeyron's relation:

$$\frac{\partial H}{\partial T} = - \frac{\Delta S}{\Delta M} = 0$$

in agreement with fig. 17. Similarly the $AF \rightarrow AFP \rightarrow P$ transitions correspond to $\Delta S \neq 0$ and $\Delta M = 0$ and thus should be field-independent, while the $P \rightarrow FP \rightarrow F$ ones involve changes in both S and M and thus should have a finite slope in the (H, T) diagram.

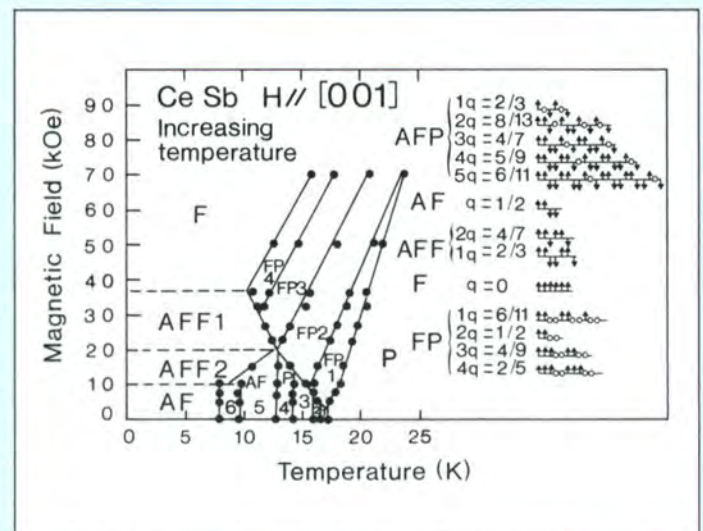


Figure 17: (H, T) phase diagram of CeSb as deduced from specific heat anomalies (from ref. 70).



The physical origin of the non-magnetic planes has not been fully clarified, so far. The possibility of two different electronic groundstates for the magnetic and non-magnetic Ce^{3+} ions has been considered. A related problem is the large anisotropy of the exchange interactions between in-plane (J_0) and out-of-plane (J_1, J_2) Ce^{3+} neighbours. The stability of the AF (+ + - -) structure at $T = H = 0$, suggests $J_1 < 0, J_2 < 0$ and $J_0 > |J_1|, |J_2|$ which is somewhat surprising in view of the cubic symmetry of the structure for $T > T_N$.

On the other hand, the large exchange anisotropy makes CeSb an attractive model system and several attempts have been made at explaining the main features of the experimental phase diagram, particularly the $H = 0$ AF \rightarrow P sequence, within the ANNNI model [71, 72, 73]. Noting that this sequence corresponds to introducing an increasing proportion of non-magnetic defects, Villain and Gordon [73] argue that the true devil's staircase behaviour will only be realized if the effective interaction between defects is repulsive at all distances. This condition imposes constraints on the relative values of J_1 and J_2 which are not met in the case of CeSb. Alternatively [8] one may argue that the missing intermediate phases are suppressed by the metastability of some of the adjacent ones. It has been noted that some samples miss more steps than others which implies that at least in some cases the number of observed phases is limited by (extrinsic) pinning mechanisms.

In any case, it is clear that the experimental limit has not yet been reached, in the sense that finer steps could still be resolved, if present. Until then, the search for the ideal devil's staircase system is likely to continue.

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COLLEGE 5 CRYSTAL AND MAGNETIC STRUCTURES

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GENERAL SUMMARY

The experimental activity of the college was severely curtailed by the long shutdown. The break provided the opportunity to analyse data and a significant increase, over previous years, was recorded in the number of papers published. Scientific con-

tinuity of the college was maintained by an increased number of seminars which reached a fortnightly basis. Many members of the college took the opportunity of continuing neutron measurements at other centres. Some complementary investigations using for example synchrotron radiation were also made. This latter activity was of particular significance since it gave first hand experience in discussions relating to the European Synchrotron Source.

The work carried out during the long shut down involved dismantling several of the diffractometers. In each case the diffractometers were reinstalled according to schedule and the college are particularly grateful to all concerned in the technical services for effecting this work.

At the last scientific council the high level of demand for beam-time was accentuated by the availability of only two reactor cycles. The next sub-committee meeting will have three cycles to schedule which will cover the period up to the long shut-down planned for autumn 1984. To conform with the classification codes listed on the detachable page of the proposal forms, the subcommittee 5a has now become 5b and vice versa.

WORKSHOP

An international workshop on "3d Metallic Magnetism" was organised in collaboration with the Laboratoire Louis Néel of the CNRS Grenoble. The meeting took place over two days and attracted more than 120 participants with groups from Europe, Asia and America being represented. The purpose of the meeting was to bring into discussion both experimentalists and theoreticians. A report comprising the papers presented at the meeting has been published by the I.L.L. The organisers are particularly grateful to the Scientific Coordination and Public Relations Office for their help and efficient organisation of the meeting.

An I.L.L. Workshop on High Resolution Neutron Powder Diffraction will be held on August 1-2, 1984, immediately before the Berlin and Hamburg neutron and crystallographic conferences. Practical sessions on the powder diffractometers D1A, D1B and the new high resolution machine D2B, will be combined with lectures from visiting experts. The complementarity of X-ray and TOF neutron powder diffraction will also be covered, with the emphasis on experimental techniques. For further information, contact A.W. Hewat or J. Pannetier.

NEW INSTRUMENTS

The new shielding of the beam tube H11 will be installed in the experimental reactor hall just before the forthcoming long shut-down of the reactor, in order to test the efficiency of the D19 casemate. As a consequence, the existing diffractometers D2 and D8 should be dismantled in mid-1984 and therefore not scheduled in the February 1984 session of the Scientific Council.

This decision is taken to get the new diffractometers D19, D2B and D20 (with its 128-wires multidetector) operational by the end of 1985.

SCIENTIFIC TRENDS AND HIGHLIGHTS IN 1983

Magnetic Structures

A high demand continued for powder diffraction measurements on new compounds or those for which single crystals are difficult to prepare. In many cases, the profile refinement technique was used to study both the magnetic structure and any associated crystallographic transition. Of particular interest are the measurements made on the natural mineral ilvaite $\text{Ca}(\text{Fe}^{2+}, \text{Fe}^{3+})\text{Fe}^{2+}\text{Si}_2\text{O}_7\text{O}(\text{OH})$ obtained from Seriphos, Greece. Below about 400 K an electronic transition from an itinerant to an ordered state is expected, with the structure changing from orthorhombic to monoclinic. The structure remains monoclinic $P2_1/a$ down to 5 K, with Fe^{2+} almost completely ordered on one of the A-sites and Fe^{3+} on the other: the ordering may increase with decreasing temperature. The B-site contains Fe^{2+} plus a small amount of a Mn^{2+} impurity. There are two magnetic transitions, at 116 K and 40 K: at 80 K the Fe^{2+} and Fe^{3+} spins on the A-sites along one infinite c -axis chain are parallel, and antiparallel to those along the adjoining edge-sharing centrosymmetrically related chain. The spin vectors are all perpendicular to the plane of these chains, i.e. almost parallel to the crystallographic b -axis. At 5 K, this order is maintained, but the Fe^{2+} spins on the B-sites order antiferromagnetically as well, again almost along the b -axis. These results explain the earlier Mössbauer and magnetisation measurements.

The high neutron flux provided by D2 has been used to study the magnetic phase diagram of the Fe-Al system and chromium rich alloys containing non-transition metal impurities. Spin glass behaviour has been found in the concen-

tration range $0.4 < x < 0.8$ of the spinal $\text{ZnCr}_{2x}\text{Ga}_{2-2x}\text{O}_4$. The spin glass phase arises from the frustration inherent in the octahedral sublattice with only antiferromagnetic interactions. The associated magnetic correlations were investigated both as function of composition and temperature.

Many of the single crystal measurements concerned the determination of accurate nuclear structure factors for use with polarised neutron data. However, some magnetic structure studies using single crystals were carried out. These measurements were normally confined to systems having incommensurate structures e.g. Nd-Pr, Gd-Y etc. Scanning of satellite reflections in the spiral-spin antiferromagnetic phase of $\text{Gd}_{0.68}\text{Y}$ on D9 on the hot neutron beam revealed spiral turn angles as small as 5° . These are by far the smallest turn angles observed for a rare earth element or alloy. To resolve the satellites required trading a rapid intensity loss due to absorption for the increased resolution available with increased wavelength (figure 18).

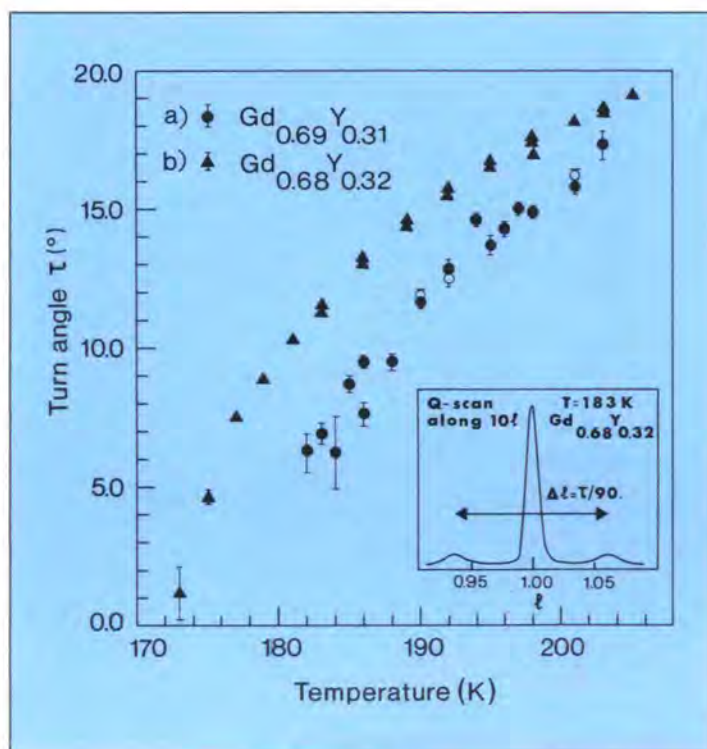


Figure 18: Spiral turn angle versus temperature for
 a) $\text{Gd}_{0.69}\text{Y}_{0.31}$
 b) $\text{Gd}_{0.68}\text{Y}_{0.32}$

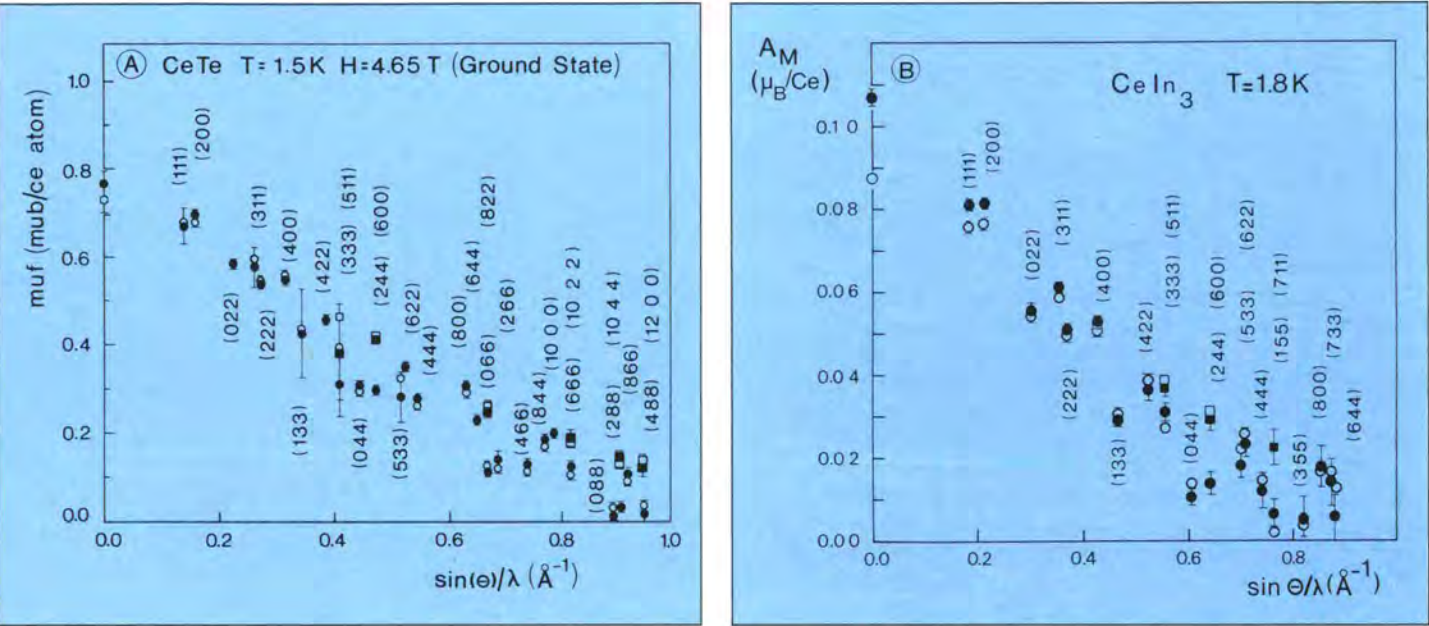


Figure 19: Magnetic amplitudes: observations (full symbols), calculations with fitted ground state wave functions (open symbols). (For more clarity, only the reflections in the horizontal plane have been included).

Magnetisation Density

Extensive polarised neutron measurements have been carried out on anomalous rare earth compounds containing cerium. CeTe orders antiferromagnetically below 2 K with a moment of $0.2 \mu_B/\text{Ce}$ which is much less than that expected for the Γ_7 state. The polarized neutron experiment has clearly shown that the magnetization of CeTe arises from the 4f electrons of the cerium atom. The anisotropy of the magnetization density has the same features as the Γ_7 state but the ground state of Cerium is not pure Γ_7 and contains a large amount of Γ_8 admixture. An attempt to fit a crystal field and exchange hamiltonian with a unique set of parameters Δ and λ , does not fit well the current results and, is not yet in agreement with the crystal field parameter deduced from inelastic neutron measurements. In any case, such a model does not explain the low moment of cerium in the antiferromagnetic ordered state and the other cerium properties in this compound (figure 19a). However, for the antiferromagnet CeIn₃ which has a partially reduced ordered moment of $0.48 \mu_B/\text{Ce}$ atom the agreement between observed and calculated magnetic amplitudes is excellent in the region $\sin\theta/\lambda > 0.30 \text{ \AA}^{-1}$. The main part of

the magnetization density in CeIn₃ is due, as for CeAl₂, to the 4f electrons of the Ce³⁺ ion. The ground state determined in this way is

$$|\varphi\rangle = 0.782(1)|5/2\rangle - 0.445|1/2\rangle - 0.436(5)|-3/2\rangle$$

which corresponds to a Γ_7 state with admixture of Γ_8 , as expected from the form factor anisotropy. Thus, a crystal field scheme is able to account for the form factor experimental results. The crystal field effects were also present in inelastic neutron experiments, but not as well resolved peaks. A simple picture may be that the Γ_7 and Γ_8 levels are broadened by the Kondo like coupling. In such conditions, transition analysis becomes difficult.

In the opposite case the form factor treatment based on spatial distribution rather than on energy is not seriously affected. However, the 4f electrons do not account for the totality of the experimental magnetic amplitudes of the low angle reflections. For $\sin\theta/\lambda < 0.30 \text{ \AA}^{-1}$, there exists a 5d contribution. As for other cerium compounds its sign is positive and opposite to that given by the trivial direct exchange between 4f and 5d spin components. Its relative value is equivalent to that of CeAl₂ but much smaller than that of CeSn₃ at low



temperatures (fig. 19b). Thus CeIn_3 is close to CeAl_2 ; it presents mainly a 4f electron magnetism with crystal field effects, even if, in contrast to CeAl_2 , the corresponding levels are very much broader.

CeInSn_2 is a mixed valent compound as is CeSn_3 but with a susceptibility four times larger. At high temperatures the observed form factor follows that expected for 4f behaviour and is similar to that of CeSn_3 . However, at low temperatures, unlike CeSn_3 , there is no additional large 5d contribution.

Measurements have also been performed on the Pauli paramagnet CeNi in the region (140 K) where a maximum is observed in the static susceptibility. Whereas in the Pauli paramagnet CeNi_5 , the induced magnetisation is localised on the nickel sites only, in CeNi it is localised on the cerium sites. There is no induced moment on the nickel sites. Thus, the magnetism in CeNi arises from the 4f electrons of cerium which is in an intermediate state in agreement with a lattice parameter analysis.

Extensive measurements have also been made on organic free radicals. The stable aromatic free radical α , α -diiphenyl β -picryl hydrazyl (DPPH) was among the first paramagnetic species investigated by electron spin resonance (ESR), and its remarkable chemical stability and narrowness of its resonance line have made it a widespread standard for measuring unpaired spin concentrations and effective gyromagnetic ratios. DPPH crystallizes in several different forms, all non centrosymmetric, with or without the inclusion of solvent molecules. DPPH: C_6H_6 has been chosen as it has at low temperature the highest magnetic susceptibility. The interaction between DPPH molecules, which are negative, are lowered by the intercalation of benzen (fig. 20). As seen in the map, the longest amount of spin density is located on the two central nitrogen atoms. However, and contrary to the case of nitrosade radicals, 30% of the spin density is delocalized on the two phenyl and the picryl rings, with alternatively positive and negative signs.

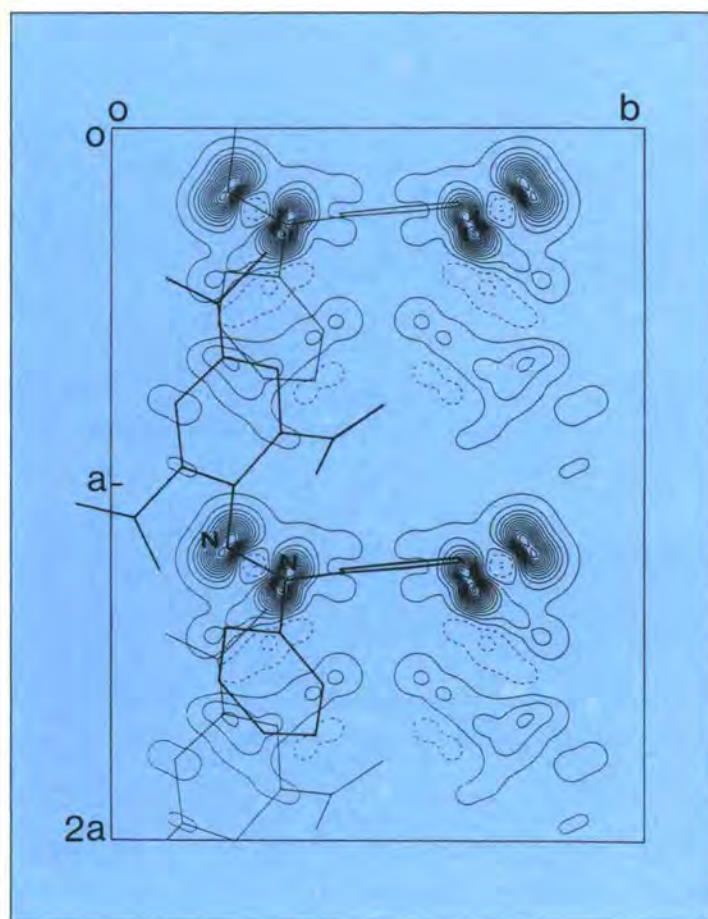


Figure 20: Projection of the spin density distribution along the crystallographic axis \bar{c} . Adjacent contours are separated by $0.03 \mu_B/\text{\AA}^2$.



Measurement of Spin Density Distributions in Non-Centrosymmetrical Crystals - Multipolar Expansion

The neutron intensity of a Bragg reflection for a magnetic material contains both the nuclear structure factor F_N and the magnetic structure factor F_M . Accurate determinations of magnetic structure factors are usually performed with polarized neutrons and the flipping ratio technique. One measures, for each reflection, the ratio R obtained for two neutron spin states up and down

$$R = \frac{I^+}{I^-} = \frac{|F_N + F_M|^2}{|F_N - F_M|^2} \quad (1)$$

If the nuclear crystal structure of the sample under investigation has been determined, then the nuclear structure factor F_N is known and hence F_M may be deduced from measurement of R .

In the case of centro-symmetrical crystals, for which F_N and F_M are real, F_M is obtained by solving equation (1). In the case of non-centrosymmetrical crystals, both F_N and F_M are complex quantities.

$$F_N = F'_N + i F''_N \quad F_M = F'_M + i F''_M$$

and the expression for the flipping ratio becomes:

$$R = \frac{(F'_N + F'_M)^2 + (F''_N + F''_M)^2}{(F'_N - F'_M)^2 + (F''_N - F''_M)^2} \quad (2)$$

The measurements of R alone cannot provide a knowledge of the two unknown quantities F'_M and F''_M . To overcome this difficulty we propose to apply a model which provides an analytical description of the spin density. We have chosen an expansion of the density around the nuclei at rest. Such a model, first used to represent charge densities, has already proved to be very well adapted in the case of spin densities in centro-symmetric crystals. The expansion consists of a superposition of aspherical atomic densities, each described by a series expansion in real spherical harmonic functions:

$$s(\vec{r}) = \sum_{\text{atoms}} \sum_{\ell=0}^{\infty} R_{\ell}(r) \sum_{m=-\ell}^{\ell} P_{\ell m} Y_{\ell m}(\vec{r})$$

The $P_{\ell m}$ are population coefficients. The radial functions $R_{\ell}(r)$ are of Slater type:

$$R_{\ell}(r) = \frac{\zeta^{n+3}}{(n/r)!} r^n e^{-\zeta r}$$

The magnetic structure factors corresponding to eqs. (1) become

$$F_M(\vec{H}) = \sum_{\text{atoms}} e^{2\pi i \vec{H} \cdot \vec{r}} \left[\sum_{\ell=0}^{\infty} \Phi_{\ell}(H) \sum_{m=-\ell}^{\ell} P_{\ell m} Y_{\ell m}(\hat{H}) \right] e^{-w}$$

$$\text{with } \Phi_{\ell}(H) = 4\pi i^{\ell} \int_0^{\infty} R_{\ell}(r) j_{\ell}(2\pi H r) r^2 dr$$

To establish the spin-density map, the set of parameters (ζ , $P_{\ell m}$) which characterize the spin-density and fit the experimental data must be determined. To do this, given a set of parameters, F'_M and F''_M , are calculated and a value R_{cal} for the flipping ratio of each measured reflection is obtained from equations (2). By comparing R_{cal} with the measured flipping ratios R_{obs} it is possible to refine the parameters (ζ , $P_{\ell m}$) which best fit the data.



Polarised neutron measurements have also continued on transition metal magnets e.g. Ni_3Fe , ZrZn_2 etc. The magnetic structure factors of the weak itinerant ferromagnet ZrZn_2 at 5 K and 50 K in an applied field of 4.6 T have been measured using the polarised neutron technique. When normalised by the measured magnetisations, the two sets of structure factors differ little from one another suggesting that the magnetisation in the ferromagnetic and paramagnetic phases is due to essentially the same electron states. Fourier transformation of the magnetic structure factors shows that the magnetisation density is associated mainly with the zirconium atoms, but is drawn out into a tetrahedral framework linking zirconium sites (Fig. 21). The measured structure factors are shown to be in reasonable agreement with a model in which 57% of the magnetisation is associated with electrons in states based on strongly hybridised Zr 4d (T_{2g}): Zr 5p functions and the remaining magnetisation is so delocalised that it does not contribute to the Bragg scattering at finite angles.

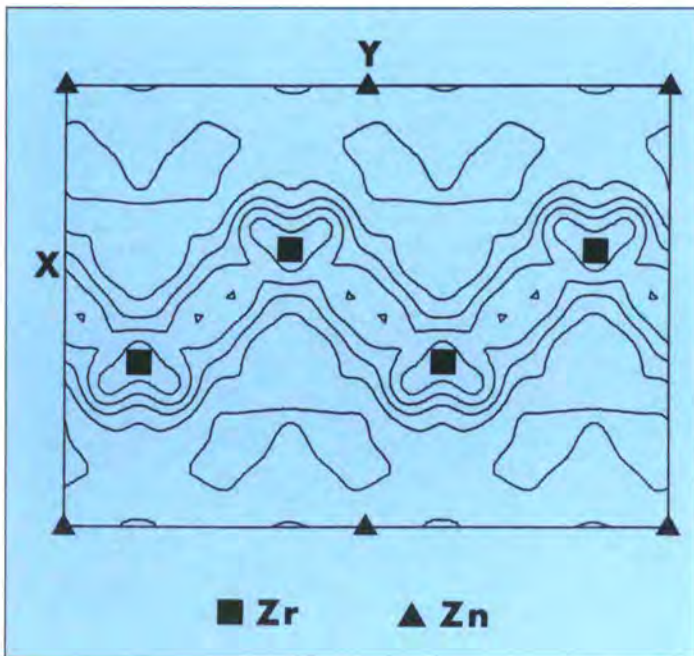


Figure 21: A section of the magnetisation distribution in ZrZn_2 at 5 K perpendicular to $[110]$ and passing through the origin. The X-axis runs from 0,0, -0.5 to 1,1,0.5 and the Y-axis from 0,0, -0.5 to 1,1,0.5. The contour intervals are $0.004 \mu_B \text{\AA}^{-3}$ and the level at the Zr site is $\sim 0.02 \mu_B \text{\AA}^{-2}$. The positions of atoms whose centres lie in the section are marked.

Polarisation Analysis

Paramagnetic neutron scattering measurements on iron and nickel were extended to include energy transfers up to 200 meV. The measurements on iron were confined to large wave vectors, close to the zone boundary, and confirmed the small weight in the scattering within the thermal energy range ($2 K T_c$). These measurements underline the deficiency of the static approximation currently employed in certain model calculations of paramagnetism in metallic system. The purchase of 40 g of Ni^{60} from which a single crystal was grown enabled data of good statistical significance to be obtained at $2 T_c$. These results confirmed the enhancement of the long wavelength fluctuations but also revealed significant scattering at large wave vectors.

Extension of these types of measurements to metallic amorphous systems above the ordering temperature is planned. It is hoped to be able to correlate the magnetic correlations with the atomic structure. Unpolarised neutron measurements on $\text{FePC}(\text{Cr})$ suggest that the magnetic correlation length may be significantly longer than the coordination of the atomic structure. Preliminary measurements on the amorphous metallic magnet $\text{Fe}_{92}\text{Zr}_8$ has revealed significant paramagnetic scattering at $1.3 T_c$.

The technique of polarisation analysis has also been extended to the problem of intermediate valence. Such materials e.g. CePd_3 , CeSn_3 etc. have a Curie-Weiss susceptibility at room temperature but a Pauli like susceptibility at low temperature. Induced form factor measurements indicated a deviation from "4f" behaviour at small wave vectors and low temperatures. These measurements suggested a Kondo like mechanism may be important in these systems. Paramagnetic scattering measurements on CePd_3 at room temperature were consistent with the existence of randomly aligned 4f atomic moments. On cooling, the scattering was found to reduce in accordance with the static susceptibility and consistent with the "disappearance" of the 4f electrons. There was no evidence of a positive contribution from the conduction band. Similar measurements on CeMg , which orders antiferromagnetically at 10 K revealed the persistence of disordered local moments down to below 30 K. The amplitude was found to increase slightly on cooling.

Structural Transitions

In this domain which is still very active in the College, some new interesting results have been obtained. For instance a kinetic study of the sequence of phase transitions of Lithium iodate has been performed on D1B. This investigation has shown that the intermediate phase $\gamma\text{-LiIO}_3$ is always in equilibrium with either $\alpha\text{-}$ or $\beta\text{-LiIO}_3$ (Fig. 22) and that the domain of stability of each phase depends on the particle size.

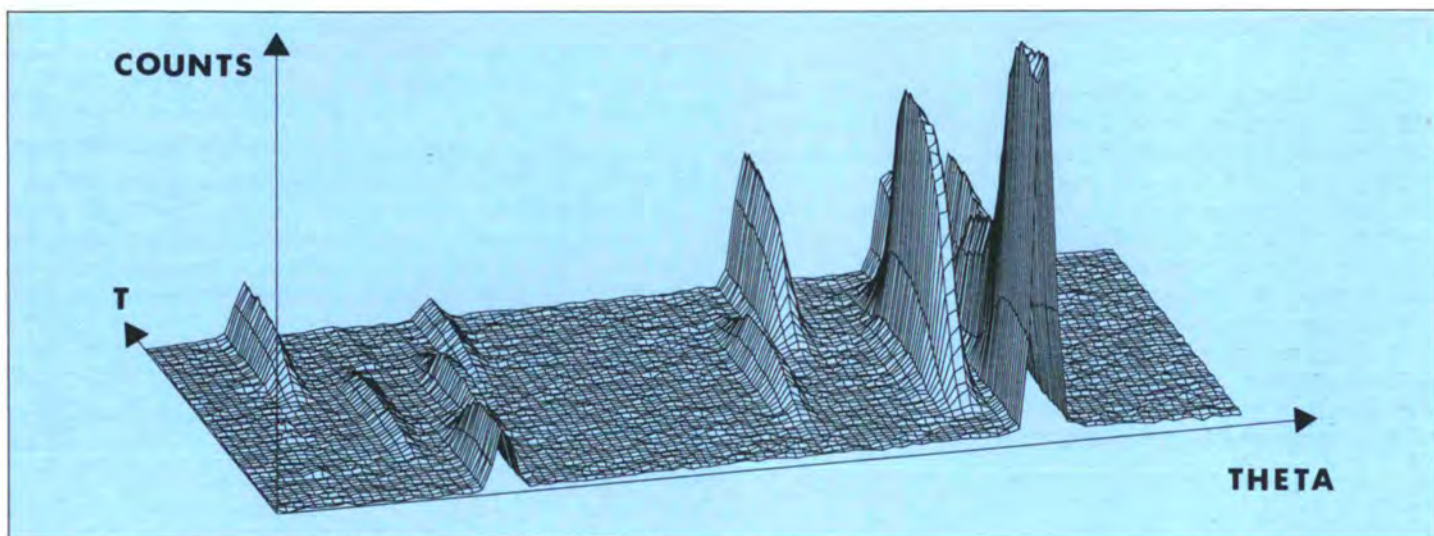
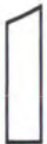


Figure 22: Powder diffractograms showing the α - β - γ sequence of LiIO_3 versus temperature.

Another example is given by the phase diagram of ice which remains a favourite topic. The richness of this diagram is due to the versatility of the tetrahedral coordination geometry, and partly to the possibilities of proton ordering in the different oxygen networks. The differences of free energy between neighbouring phases are small, and theoretical attempts to understand particularly the proton ordering transitions are very sensitive to assumptions of the water-water potential function. The phase diagram of ice therefore provides a critical test for these water models used in simulation calculations on pure water, aqueous solutions and biomolecular systems. However, such tests can only be useful with a good crystallographic knowledge of the orientational order/disorder and there is much uncertainty in the extent and even nature of the proton ordering in several high pressure phases of ice. Most of the crystallographic work was done on recovered samples at ambient pressure. Now, for the first time, the 3 highest pressure phases with two interpenetrating, but not interconnecting sublattices (ice VI, VII and VIII) have been studied under the condition of stability (11-25 Kbar) by neutron powder diffraction on D1A (Exp. no. 5-22-200 and 5-21-166). The crystal structures of these phases have been determined; in contrast to earlier work on recovered samples, ice VI is found to be fully disordered. There is no evidence for any partial ordering in ice VII; thus phase is clearly cubic and exhibits an unusual orientational disorder involving not only the hydrogen but also the oxygen atoms. Ice VIII (Fig. 23) is antiferroelectrically ordered ruling out several proposed models for water-water molecule interactions. Altogether, it seems that the orientational ordering behaviour is much simpler than previously thought. The complicated partial ordering/disordering found in earlier investigations is probably an artefact of the recovery process.

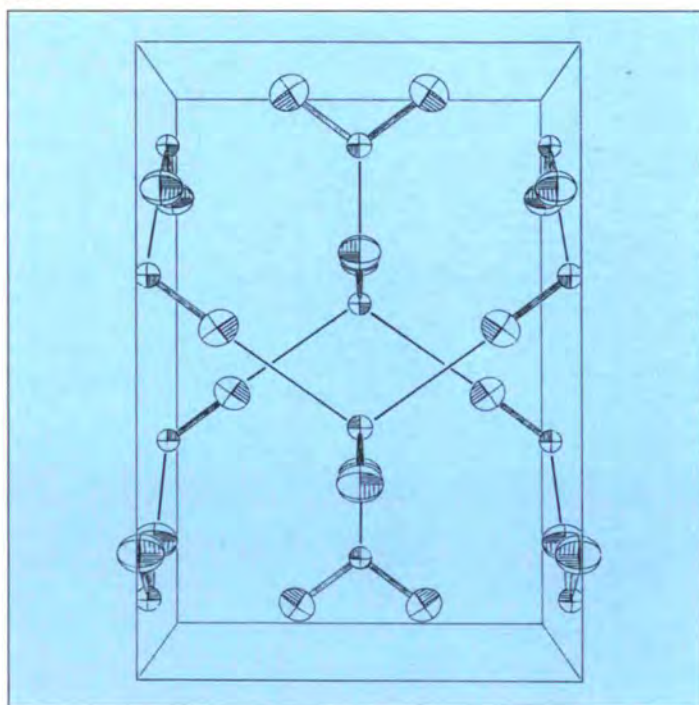


Figure 23: The structure of ice VIII at 10 K viewed along the b -axis (S.G: $I4_1/amd$). The two interpenetrating, but not interconnecting sublattices are closely visible; the H-bonds are indicated as thin sticks. Thermal motion probability ellipsoids are drawn on the 50% level.



Incommensurate Phases

Thanks to the especially well adapted diffractometer D10, the ILL continues its role of excellence in this domain. For example, the intermediate phase of quartz existing in a 1.3 K range between the α and β phases is in fact incommensurate. Six satellites are observed around most Bragg peaks along the three [100] directions of reciprocal space (Fig. 24). Modulation corresponds to the superposition of sinusoidal plane waves as no higher order harmonics are observed. With decreasing temperature the modulation vector decreases from 0.033 to 0.029 reciprocal units. Premonitory diffuse scattering is observed in the β phase a few degrees above $T_i = 847.2$ K (the incommensurate transition temperature). The results are in many respects analogous to the situation of NaNO_2 .

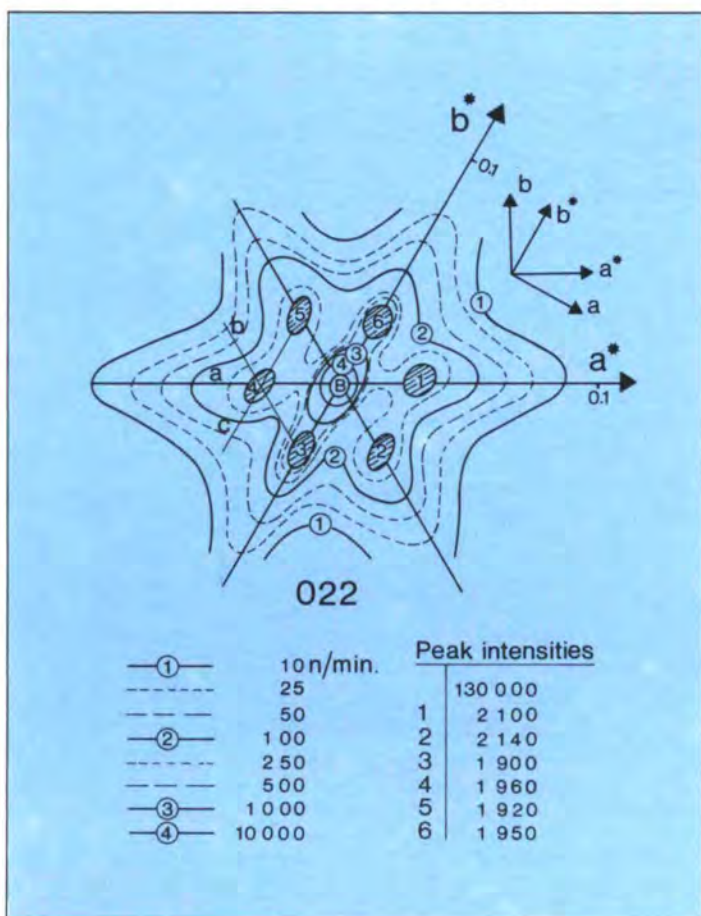


Figure 24: Intensity map in the (00l) plane from Q-scans around the (022) reciprocal point at $T_i = 0.8$ K. The hatched ellipsoids (labelled 1-6) correspond to the section of the satellite peaks at half their intensity; the central one (B), corresponding to the Bragg peak, roughly gives the experimental resolution. The lines a, b, c show the scan directions used to check for higher order components.

Another good example is given by the Kondo compound TmS. Single crystal neutron diffraction experiments have revealed a modulated antiferromagnetic structure below the Néel temperature $T_N = 5.2$ K. At 1.5 K the propagation vector \vec{q} is $(\frac{1}{2} - \eta, \frac{1}{2} + \eta, \frac{1}{2})$, with $\eta = 0.075$ (fig. 25). In the simplest assumption, where no coupling does exist between the different Fourier components, the magnetic structure can be described as an amplitude modulation of the magnetization propagating along the [110] direction. The magnetic moments are aligned along [112] directions and (111) planes are antiferromagnetically coupled.

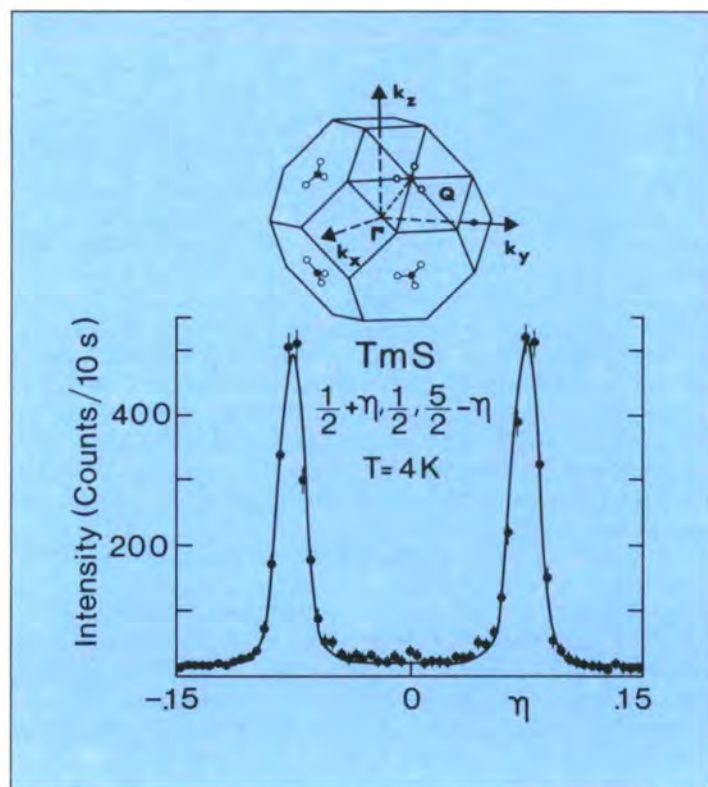


Figure 25: Single crystal neutron diffraction by the Kondo compound TmS. A modulated antiferromagnetic structure below the Néel temperature $T_N = 5.2$ K was observed.

Measurements under pressure provided useful information about the valence state of Tm ions, the incommensurate wavevector η and the Néel temperature increasing with pressure. Recently neutron diffraction experiments on D10 have been performed on another Thulium compound: TmTe. At very low temperature, below $T_N = .5$ K it exhibits a type II antiferromagnetic structure.

Temperature Factors

Structural studies carried out by neutron or X-ray diffraction are based on the co-ordinates and temperature factors of the atoms in the unit cell. The temperature factors describe the way in which the mean scattering density associated with the atoms is smeared out by thermally excited atomic vibrations. In the analysis of diffraction data the atomic motions are commonly modeled as harmonic oscillations about an equilibrium position, in which case the atomic scattering factor of each atom is reduced by a temperature factor $\exp^{-\left(\sum_{ij} \beta_{ij} K_i K_j\right)}$ where β_{ij} is a temperature dependent tensor, defined for each set of equivalent atoms, which describes the harmonic oscillation and \mathbf{K} is the scattering vector. The β_{ij} are constrained to have the point symmetry of the sites to which they refer. Because the neutron nuclear atomic scattering factor is independent of scattering angle, neutron diffraction is a powerful tool for obtaining precise values of the temperature factors, even for light atoms.

The anisotropy of the temperature factors is often illustrated by a drawing of the structure in which the atoms are represented by ellipsoids whose axes are proportional to the principal components of the thermal vibration tensor (figure 26). In some cases, precise neutron diffraction studies carried out to high q values can demonstrate anharmonicity in the thermal motions. Such anharmonicity can be used to obtain information about the shape of the potential wells in which the atoms vibrate. A contour map of an asymmetric double potential well whose shape was deduced by analysis of the anharmonic temperature factors is shown in figure 27.

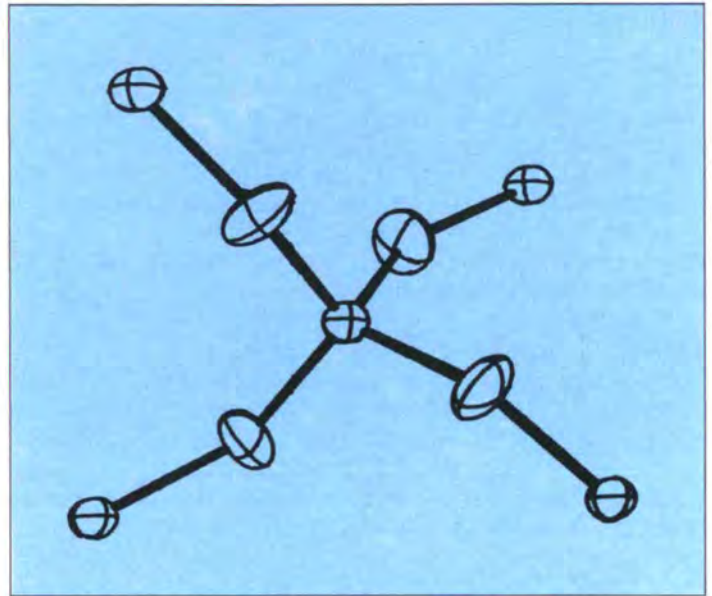


Figure 26: α -quartz. Thermal motion just below the α - β transition.

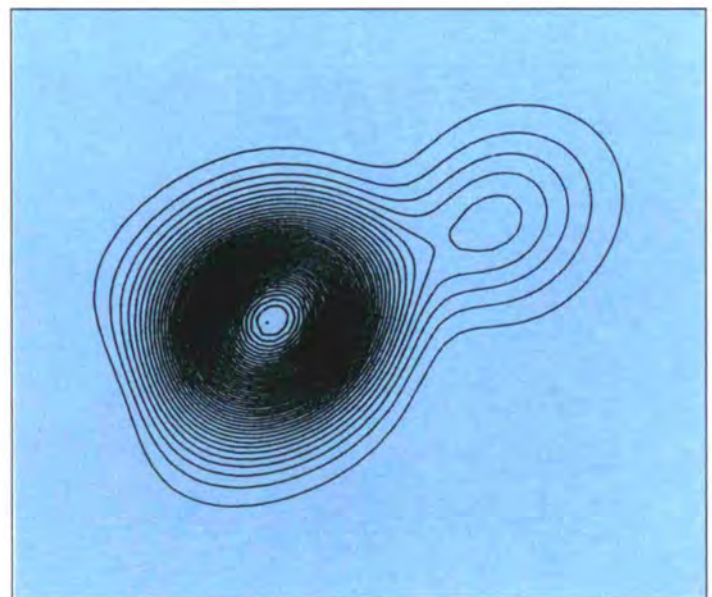


Figure 27: Asymmetric double potential well in DKDP 0.5° below the ferroelectric transition temperature.



Intercalates

The interest for such compounds is still very high, and a question of current importance is whether a magnetic order can occur between layers or not. The first experiment performed on D2 with FeCl_3 intercalated graphite is very promising. In the first and second state, strong 2-D magnetic correlations develop below 30 K. In the first stage, at 3.8 K, a transition from the 2-D phase to a 3-D order is observed. The in-phase order remains the same and corresponds to an incommensurate magnetic modulation of propagation vector 0.394 \AA^{-1} .

Organic Compounds

The recent discovery of the so-called Bechgaard salts $(\text{TMTSeF})_2\text{X}$ (with TMTSeF: Tetramethyltetraselenofluovaline and X: small anions such as ClO_4^- , PF_6^- , ReO_4^- , FSO_3^- , AsF_6^-) have attracted great interest as the first organic material exhibiting superconductivity. The transition occurs at about 1 K under a pressure of several Kbars or even at ambient pressure (ClO_4^- salt). One of the relevant parameters in the study of these compounds is the inter and intra-chain coupling via Se...Se interactions, this being emphasized by this absence of superconducting phase of the isostructural homologous salts $(\text{TMTTF})_2\text{X}$ which contain sulphur. Due to the excellent resolution, low background and the special cyostat, the 4-circle diffractometer D10 enabled the 7 K structure of $(\text{TMTSeF})_2\text{ClO}_4$ ($R=0.09$) to be determined using a single crystal of $<1 \text{ mm}^3$. Very recently the structures of $(\text{TMTSeF})_2\text{PF}_6$ have been determined at 3.9 K ($R=0.06$) and at 20 K. Similar measurements on TMTTF PF_6 are in progress.

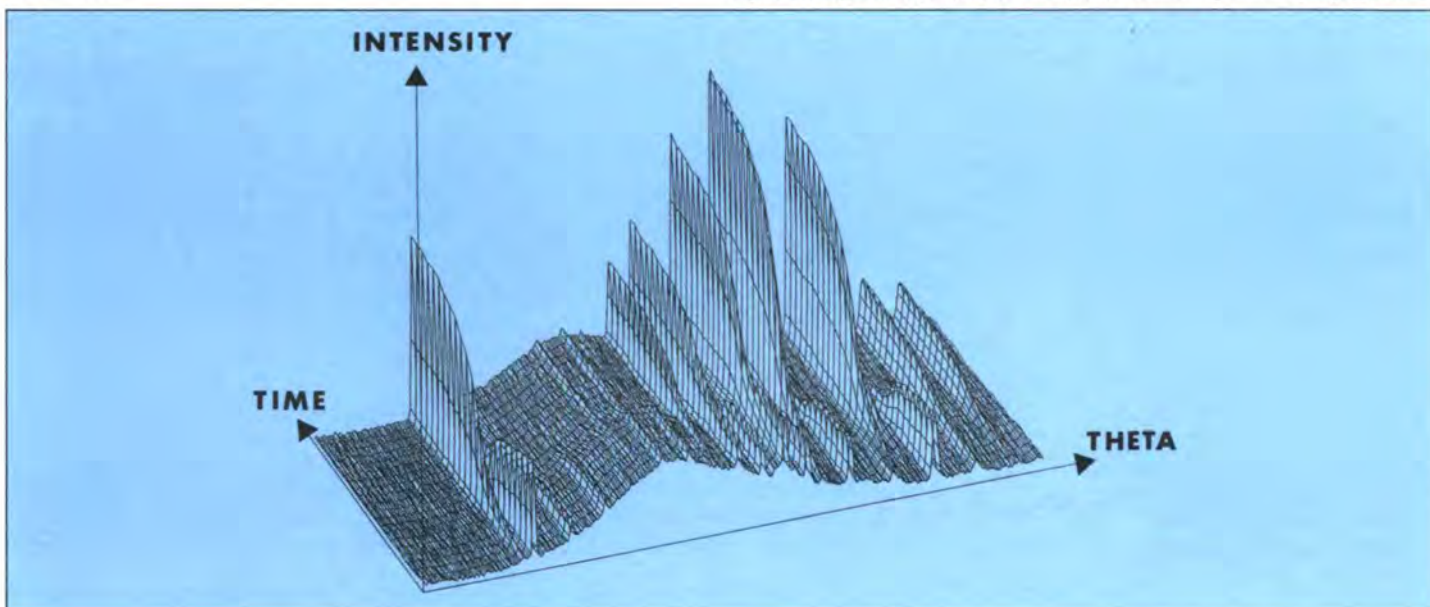
Material Research

The mixed metal oxides of calcium and aluminium and of calcium and silicon are made in solid state sintering reactions from calcium oxide, aluminium oxide, and silicon dioxide, and are technologically important materials. They are the main constituents in cement, and they react easily with water to produce amorphous as well as crystalline products. High alumina cement, a special product for refractory use, contains mainly mixed calcium aluminium oxides. The rate of the reaction between D_2O and the mixed metal oxides $\text{Ca}_3\text{Al}_2\text{O}_6$, $\text{Ca}_3\text{Al}_6\text{O}_{14}$, CaAl_2O_4 , and CaAl_4O_7 was investigated by on-line neutron diffraction powder methods at temperatures from room temperature to 100°C , using the spectrometer D1B. The reaction rate of the hydration increases with increasing calcium content of the mixed oxides, and with increasing temperature for each of the mixed oxides. Fig. 28 shows the diffraction patterns from the reaction between D_2O and $\text{Ca}_5\text{Al}_6\text{O}_{14}$ at 49°C . The crystallographic stable hydrate $\text{Ca}_3\text{Al}_2(\text{OD})_{12}$ is the end product of the reaction that goes over an amorphous intermediate phase.

The college would like to accord their thanks to the former secretary S.K. Burke who returned to Australia in March and wishes him success in his new post.

Secretaries:
J. Bouillot
K.R.A. Ziebeck

Figure 28: Diffraction pattern from the reaction between D_2O and $\text{Ca}_5\text{Al}_6\text{O}_{14}$ at 49°C .



COLLEGE 6 LIQUIDS, DISORDER AND DEFECTS IN MATERIALS

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GENERAL SUMMARY

The scientific field covered by College 6 is now quite broad, reaching from fundamental physics of quantum liquids to the applied field of irradiation damage in solids. This is reflected by the very wide range of use of instruments; all types of spectrometers have been used for College 6 experiments, except four circle diffractometers.

The new diffractometer on the hot source D4B, came into scheduled operation in October. It will permit a reactivation of the research on the structure of disordered materials: liquids, solutions, glasses.

SCIENTIFIC TRENDS AND HIGHLIGHTS IN 1983

Quantum Liquids

Recent work on bulk liquid ^4He has focussed on high-precision determination of phonon frequencies and lifetimes (Expt. No. 6-01-72). The anomalous (positive) dispersion of the phonons in superfluid helium was first observed directly some years ago using IN5. Since a detailed knowledge of the dispersion curve is an important prerequisite for an understanding of the properties of liquid helium, these measurements have now been improved, particularly in the wavevector definition at very small wavevectors ($<0.3 \text{ \AA}^{-1}$) using IN12. The measured phase velocity, which demonstrates directly the anomalous dispersion, is shown in figure 29.

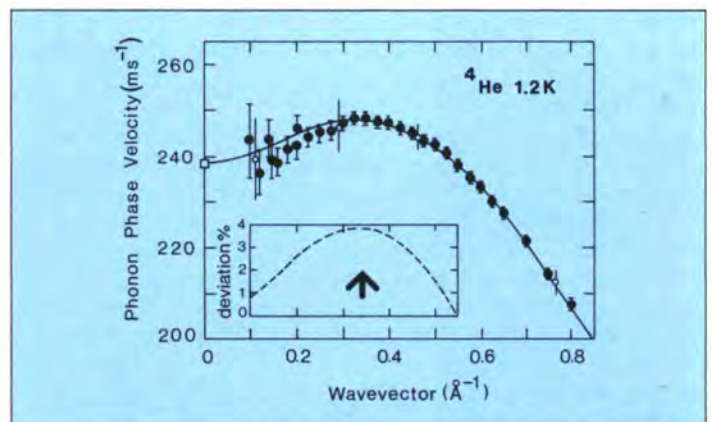


Figure 29: Phonon phase velocity as a function of wavevector. Closed circles are data obtained by present work. The line is a fit to theory. The insert demonstrates the deviation from linear dispersion with the maximum deviation marked.

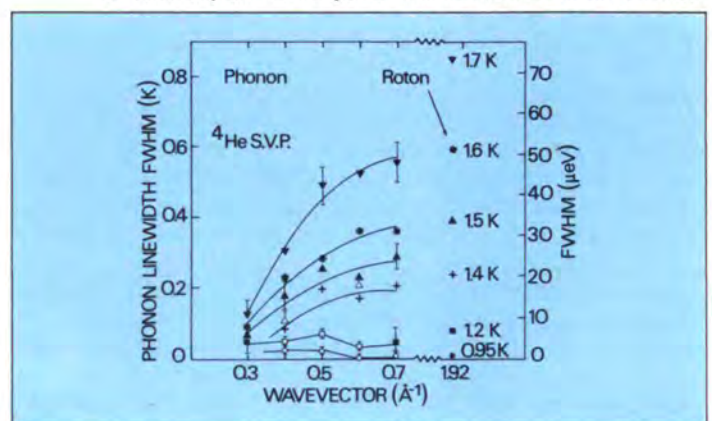


Figure 30: Phonon linewidths in liquid ^4He . Open symbols are NSE data, closed symbols are TAS data. For comparison, the relevant roton linewidths are also shown. The lines are guides for the eye.



The wavevector and temperature dependence of the lifetimes of phonons has been measured on IN11, using the spin-echo focussing technique (resolution $\sim 1 \mu\text{eV}$) and IN12 (resolution $\sim 40 \mu\text{eV}$) for wavevectors between 0.3 and 0.7 \AA^{-1} and the temperature range between 0.95 and 1.7° K . These results are shown in figure 30.

For the first time direct existence is provided of the cross-over from the 3-phonon decay regime ($\sim <0.5 \text{ \AA}^{-1}$) to the 4-phonon regime at low temperature. Further the lifetimes are seen to depend strongly on wavevector at higher temperatures.

Liquid Alloys

Theoretical work performed at the ILL shows that for monoatomic liquid alkali metals $S(q)$ and its density derivatives may be calculated in good agreement with existing experimental data using the mean spherical approximation (MSA) and a simple repulsive Yukawa potential $W_v(r)$ to describe the interaction between the particles. On the other hand, the authors demonstrate that at the present state it is impossible to extract reliable pair potentials from measured structure factors. This might be different from extracting the ordering potential $W_0(r) = W_{11}(r) + W_{22}(r) - 2W_{12}(r)$ from the $S_{CC}(q)$ partial structure factor of a binary alloy. Diffraction data of liquid Li_4Pb measured at the ILL yield a $W_0(r)$ curve and a RCF curve which were combined to calculate an "ordering enthalpy" ΔH_0 . The result agrees well with theoretical predictions. $d\Delta H_0/dT$ agrees with values to be expected for the excess specific heat. $W_0(r)$ looks similar to a Yukawa potential indicating charge transfer for which the same value has independently been obtained from thermodynamic data using appropriate recent theories. Also the screening length and its temperature variation seems reasonable. $W_v(r)$ guessed from $W_0(r)$ was inserted into the MSA and yields $S_{CC}(q)$ curves very similar to the experimental ones. This altogether shows that in favourable cases very detailed quantitative information may be obtained from diffraction data on the interaction between the particles in binary systems.

Progress has also been made in the interpretation of the structure of liquid semiconductors of which liquid tellurides are of special interest because pure liquid Te is on the metallic semiconducting border and the addition of an electro-positive element M can enhance either the semiconducting character ($M \equiv \text{Cu(I), Ag, Tl or Mn}$) or the metallic character ($M \equiv \text{Cu(II), Ni, Fe or Co}$).

Neutron studies of isotopically enriched samples have proved decisive in understanding the structure and the electrical properties of these alloys. It has been shown that charge transfer occurs as M is added to Te so that at stoichiometry the alloy can be thought of in first approximation, as Te^{2-} and M^+ or M^{2+} . For s-p cations, this change in bonding type will lead to a reduction in conductivity. For transition metals structural studies have shown that there is sufficient M-M overlap

to produce a *delocalised* d-band for Cu(II), Ni, Fe and Co, thus explaining the high conductivity of liquid NiTe, FeTe etc. On the other hand liquid MnTe, though of similar structure, is non-metallic because the d-bands formed by Mn-Mn overlap are on the *localised* side of the Mott transition.

Molecular Liquids

The molecular structure and hydrogen bond geometry in liquid formamide have been obtained by a combination of electron, neutron and X-ray diffraction studies. The molecular parameters are in good agreement with those obtained from gas electron diffraction for the free molecule. The mean O...N and O...H bond distances are 2.9 \AA and 1.9 \AA respectively. Four H-bonds per molecule are found on average. Their deviation from linearity is estimated.

The technique of isotopic substitution in the case of liquid chloroform (Exp. No. 6-05-48) has made it possible to obtain the complete set of atom pair correlation functions (figure 31). The most probable orientation between two molecules is the one in which the molecular dipoles are inclined with respect to each other and the hydrogen atoms is tilted towards the hollow between two chlorine atoms.

Several attempts have been made to obtain the water structure at temperatures below the melting point, either in bulk sample or in confined geometries such as high surface area silica samples (ex. no. 6-05-45 and 61). A difference method has been used to follow the changes as compared to the structure above the melting point. There is an enhanced local order through the effects of hydrogen bonding: the system progressively evolves towards the continuous random hydrogen bonded network similar to that exhibited by amorphous ice.

Molten Salts

The inelastic neutron scattering spectra of molten RbCl , CsCl and NaI have been measured by time-of-flight technique (expt. no. 6-06-15). A first order isotopic substitution experiment performed on RbCl has permitted a substantial separation of the contributions from the acoustic-type and optic-type collective modes. Single ion motion has been shown to be consistent with simple diffusion up to the first peak in $S_{+-}(Q)$ after which it becomes more gas-like. De Gennes narrowing of the quasi-elastic peak due to collective motions is observed. The collective motions are represented by mass ("acoustic" type mode) and charge ("optic" type mode) current correlations. Quantitative comparison has been made with the results of computer simulation for both the solid and molten states.

A further experiment has been performed using IN6 on three samples of molten SrCl_2 with isotopically substituted Cl, in order to achieve a more complete separation of the collective modes (Expt. no. 6-06-24). This represents the first use of the technique of second order isotopic substitution for in-

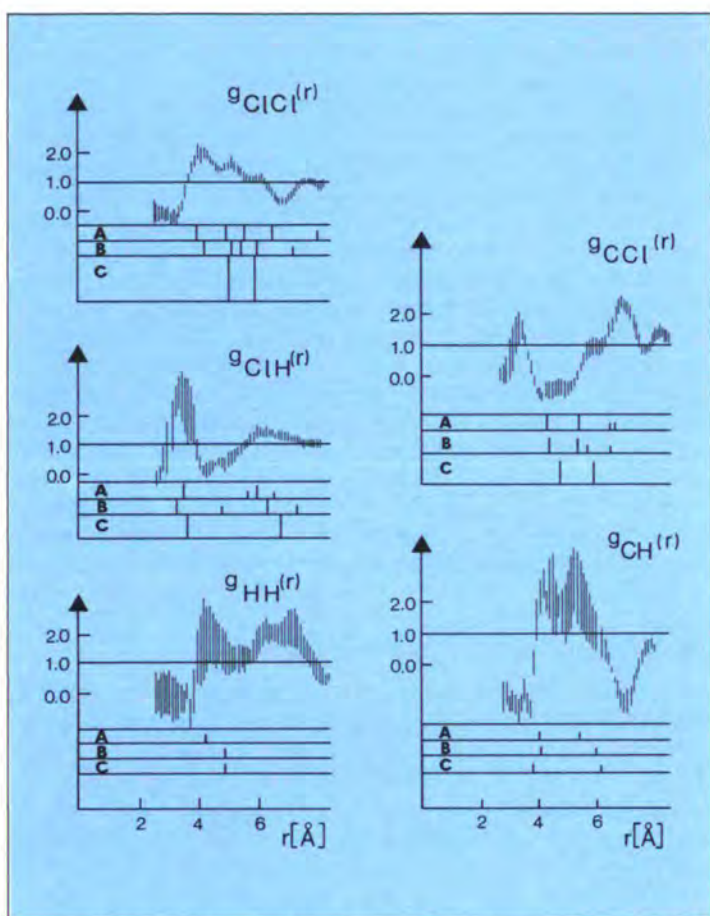


Figure 31: Partial atom pair correlation function of liquid chloroform. The spread arises from experimental errors. The histograms displayed in A, B and C show the distances calculated for different orientations between two molecules.

vestigating the dynamics of liquids of binary mixtures. This success has shown that the technique can be used to give information on collective motions in liquids that would otherwise not be measurable.

Ionic Solutions

The hydration of complex ions in solution has been studied by diffraction with the first order difference technique. In the case of sodium perchlorate some unexpected results have been obtained which provide the first clear evidence of a molecule undergoing a significant change in shape on entering aqueous solution (exp. no. 6-07-57). For example the Cl-O bond length is found to be 1.65 Å compared to 1.45 Å in the sodium perchlorate monohydrate crystal. These results have to be checked by measuring over a wider Q-range.

It is now well established that quasielastic neutron scattering gives interesting and unique information on the dynamics of

protons about an ion in aqueous electrolyte systems. In particular the existence of a second-zone of hydration at intermediate concentration (~ 1 molal) has been confirmed and characterized in a quantitative way by a proton diffusion coefficient D_2 . New experiments have investigated the effect of the counter-ion (exp. no. 6-07-58). Consecutive runs on $NiCl_2$ and $Ni(ClO_4)_2$ solutions at the same temperature and concentration confirmed that the water molecules associated with Ni^{2+} in both solutions are in the slow exchange limit. However, detailed analysis has shown, that with respect to the chloride ion, the perchlorate ion acts as a "structure breaker" in that D_2 (perchlorate) > D_2 (chloride). In highly concentrated (15.5 molal) aqueous solution of HCl, it has not been possible to detect any fast H^+ -ion motion (exp. no. 6-07-44). This seems to indicate that the high electric conductance of HCl solution is due to a motion of all the protons in the solution, including the water protons and not only of those protons in the H^+ -ion state.

Glasses and amorphous materials

The investigation of the local order in various binary metallic glasses (MgZn, TbCu, NiY, CuY...) has been pursued. (Expt. 6-08-85). The sample characterization, however, is still a problem. A method has been developed to evaluate and correct for the hydrogen contribution to scattering, especially important in sample prepared by sputtering.

A series of experiments on D17 has revealed that the small angle scattering in metallic glasses is anisotropic, and depends on the orientation of the ribbons and on their method of elaboration (Expt. No. 6-08-82). Ribbons of a melt spun $Pd_{80}Si_{12}Ge_8$ alloy contain scattering centres of the order of 400 Å wide, slightly elongated in the direction of the ribbon length (fig. 32a) and very thin along the direction perpendicular to the substrate of the meltspinner. Plates of an electrochemically deposited $Ni_{80}P_{20}$ glass exhibit a column on structure with long defects along the direction perpendicular to the electrode (fig. 32b, c). The nature of these defects (concentration or density fluctuations, impurities) is not yet known. The medium range order of amorphous hydrogenated silicium has been studied by small angle neutron scattering (Expt. No. 6-08-80). From an investigation on sputtered samples, it seems possible to point out:

- i) the evidence of structural heterogeneities with a mean radius of gyration of a about 125 Å in pure or hydrogenated a-Si,
- ii) the very strong enhancement of small angle scattered intensities versus hydrogen concentration. These results seem to indicate the presence of low density regions in a-Si and the location of hydrogen in these regions in a-Si: H.

The study of the reversible thermal behaviour of the structure factor of amorphous $Fe_{81}P_8C_{11}$ alloy on D1B and D2 has shown the validity of the Debye model (Expt. No. 6-08-91). This has permitted the proposal of a method for deducing the

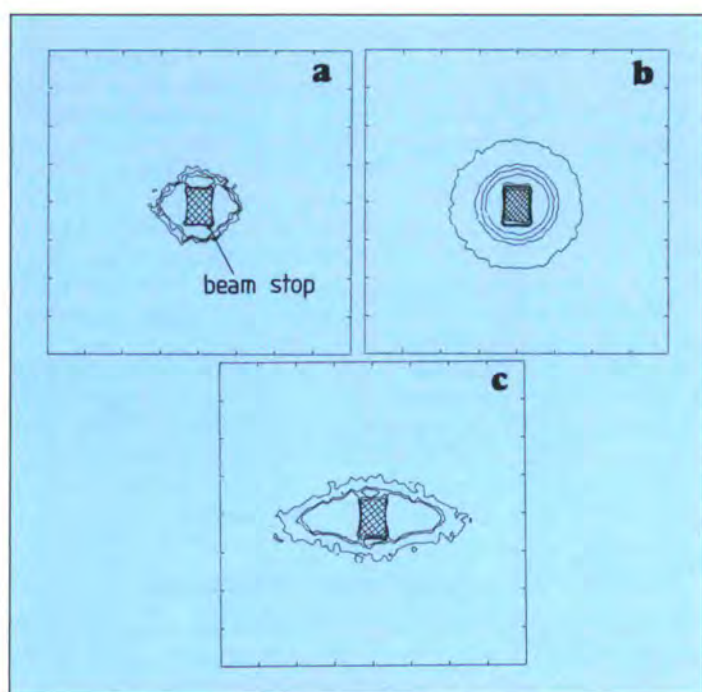


Figure 32: Small angle isointensity contour maps (a) melt-spun Pd-based glass with the ribbons placed parallel to the detector of D17 with their length in the vertical direction. Electrochemically deposited Ni-based glass with plate surface (b) parallel and (c) tilted by an angle of 20° to the detector plane.

static or 0-phonon structure factor $a(k)$ providing information on the true positional disorder.

The influence of structural relaxation on the atomic dynamics of the metallic glass $Mg_{70}Zn_{30}$ has been studied on IN6 (Expt. No 6-08-78). The dynamic structure factor and the generalized vibrational density of states were determined before and after isochronal and isothermal annealing at about 50 K below the crystallization temperature. The results are interpreted in the framework of recent computer simulations, which permit the identification, on a microscopic scale, of the possible origin of the low frequency "disorder characteristic" modes.

Defects and disorder in solids

Comparative studies of the crystal nucleation in a silicate glass using complementary techniques is giving excellent results. Small angle neutron scattering, line narrowing laser spectroscopy, electron paramagnetic resonance and electron microscopy are being used to study crystallization of Cr^{3+} ions. This combination of techniques can be very powerful for observation of the transformation between ordered and disordered states, in which intermediate phases and clusters occur. Results so far indicate that Cr^{3+} clustering occurs up to ~150 Å diameter; above this size, transformation to a

Cr^{3+} doped spinel occurs. In the same base glass containing TiO_2 as nucleating agent, nucleation centres as small as 10-15 Å diameter have been identified by SANS, and then developed continuously up to 100 Å diameter.

Defects in insulators created by heavy ion bombardment are investigated using SANS. Samples of mica and Hostaphan have been irradiated with uranium ions at a dose of 3×10^9 ions/cm² (Expt. No. 7-03-262). Results of computer fitting of the scattered intensity distribution in SANS yielded the possibility of discriminating between different three-dimensional models of the scattering defects.

The photo-induced changes in the structure of the chalcogenides glass As_2S_3 have been investigated by neutron diffraction (Expt. No. 7-03-254). The glass was first examined in its irradiated state, then annealed in situ on the diffractometer and finally measured again. The results confirm that changes extend to the highest values obtained on the spectrometer D2 ($Q_{max} = 10.4 \text{ \AA}^{-1}$), indicating that photo-induced changes in the local structure are produced: there is an obvious change in the bond-length and also the bond-angle.

In-beam NMR spectroscopy

In the superionic conductor Li_3N spin-lattice relaxation (SLR) measurements on the β -emitter 8Li have been performed at temperatures $T = 8 \dots 300$ K and magnetic fields $B = 35 \dots 600$ mT. Li_3N has a hexagonal layer structure consisting of alternating Li_2N and Li planes with Li ions labelled Li(2) and Li(1), respectively. In the T range 200...300 K intralayer diffusion involving only Li(2) ions dominates the 8Li SLR. Nevertheless, by applying a special radiofrequency

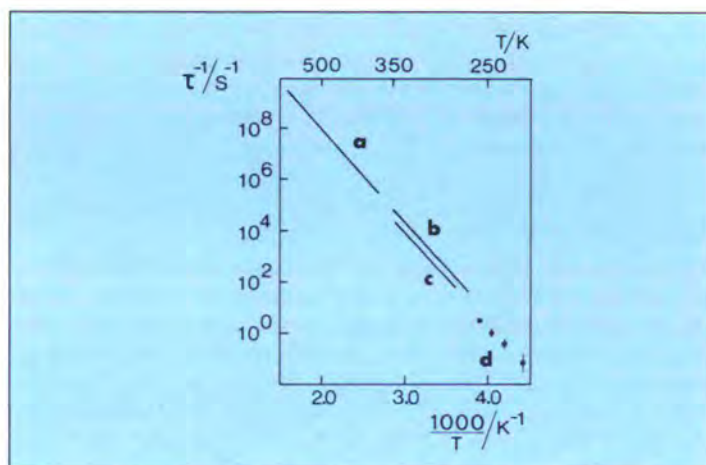


Figure 33: Temperature dependence of the Li jump rate for interlayer diffusion in Li_3N (a) conventional NMR (b/c) conductivity (d) in-beam NMR.



irradiation scheme, the relatively slow interlayer diffusion along the crystal c-axis in which both Li(1) and Li(2) take part were studied. Jump rates as small as 0.1 s^{-1} were measured (Fig. 33). The activation energy found for interlayer diffusion agrees well with that obtained from conductivity and conventional NMR measurements at $T > 300 \text{ K}$.

Diffusion in bulk material

In a number of investigations it has been shown that O or N dissolved in Nb can trap H atoms. At low temperatures the H becomes delocalised over (two) sites in the neighbourhood of the heavy defects. The low temperature dynamics of NbO_xH_x ($x = 0.002$) has been investigated by both specific heat and neutron spectroscopic measurements. The specific heat data suggest an excitation energy of $0.19 \pm 0.02 \text{ meV}$. Neutron scattering allows a direct spectroscopic measurement of the matrix element. The spectrum shown in Fig. 34 was taken at the instrument IN2 with the temperature set to 0.1 K (dilution insert). Inelastic scattering has been found at $0.21 \pm 0.03 \text{ meV}$ in agreement with the specific heat data. Note that at 0.1 K all H are in the ground state and no neutron energy gain process is possible. The small inelastic intensity as compared to the elastic scattering is due to interactions between the defects. This makes the potentials slightly asymmetric and the H wave functions become partly localised. The random distribution of the defects in the Nb host leads to an energy width of the excitation. There are, however, two significant differences in comparison with the well known low temperature anomalies of glasses: i) the matrix element has a well defined low energy cut-off and ii) the tunnelling entity is known.

Quasielastic neutron scattering experiments have been carried out to study the microscopic mechanisms of anomalous fast diffusion in metals. For example the diffusion of Co in β -Zr (rather high solubility of Co in Zr), is at least two orders of magnitude faster than the self diffusion of Zr. (Expt. No. 7-06-144). Measurements of the temperature and Q-dependence of the quasi-elastic broadening on polycrystalline samples yielded the surprising result that *all* Co atoms ($\geq 2 \text{ at.}\%$) are on sites where they can participate in the fast diffusion process. The appearance of *two* broadened components, having widths different by an order of magnitude, indicates that the diffusion process itself involves two jump frequencies. Comparison of the relative intensities showed that about $1/4$ of the Co atoms contribute to the very fast diffusion jumps. Further measurements on *single* crystals (very difficult to grow due to the phase transition from α to β -Zr) are planned in order to get detailed information about the jump vectors. The anion diffusion in a single crystal of SrCl_2 has been studied at temperatures of 1001 K and 1087 K using IN12

(Expt. No. 7-07-52). The quasielastic linewidth has been measured in the [100], [110] and [111] crystallographic directions and the results analysed in terms of both the Chudley-Elliott model of jump diffusion and the more physically realistic encounter model of Wolf, which takes into account both spatial and temporal correlations of hops.

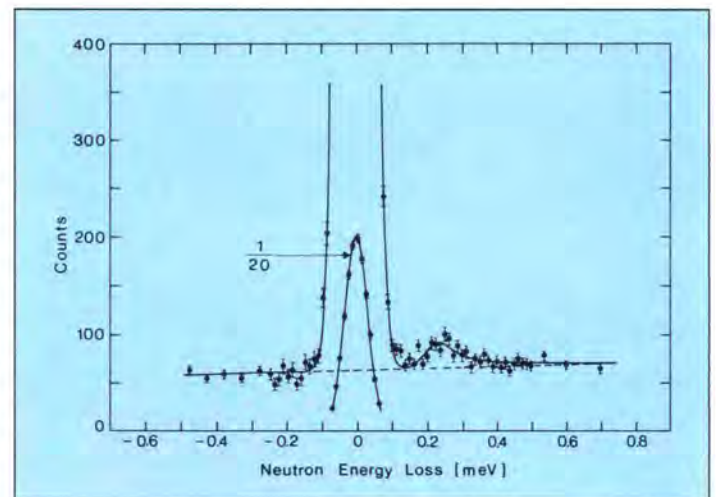


Figure 34: Neutron spectra of NbO_xH_x ($x = 0.002$) measured at 0.1 K . The energy resolution of the instruments is 0.07 meV .

Another series of experiments has been performed on the hydrides of various LaNi_5 based alloys (Expt. Nos 7-06-139, 157, 166) to clarify the hydrogen diffusion mechanism. The use of widely different resolutions (1 and $130 \mu\text{eV}$) revealed motions with different time scales. The dynamical behaviour of hydrogen in all these hydrides is well described in the framework of the structural model, by grouping the available interstices into two sets of sites.

Secretary:
A.J. Dianoux

COLLEGE 8 AND EMBL GRENoble: BIOCHEMISTRY

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M. Zulauf

GENERAL SUMMARY

Since the biology college and the outstation of the European Molecular Biology Laboratory (EMBL) moved into the same building 2 years ago, there has been a noticeable increase in scientific exchange. Visitors are also benefiting due to the easy on site access to a range of physical and biochemical techniques. Biological samples are usually friable so the time spent between preparation and subjection to the desired suite of experiments needs to be as brief as possible. In order to best characterize samples and glean the maximum reliable information about them it is usually essential to use a number of techniques in addition to the neutron experiments. Consequently, the ILL/EMBL staff are often involved in sample preparation and the application or development of other techniques. The physical techniques currently available include X-ray diffraction, light scattering and electron microscopy. Also there is an analytical centrifuge and equipment for the determination of parameters such as density and viscosity.

SCIENTIFIC TRENDS AND HIGHLIGHTS IN 1983

Two areas of growth can be identified: low-resolution crystallography and inelastic neutron scattering. The increasing interest in low-resolution crystallography has resulted in a joint ILL/EMBL project to design and build the dedicated diffractometer DB21. This instrument will have a 2-dimensional position sensitive detector (resolution 1.0-1.5 mm) which can be positioned from 20 to 50 cm from the sample and will be capable of horizontal displacement as on D17. The wavelength will be fixed at 8 Å. The first tests are planned for the summer of 84.

The potential use of inelastic neutron scattering as a tool with which to study some aspects of protein dynamics has come to the fore in recent years. There have nevertheless been relatively few experiments as instrument time is difficult to obtain. Hence it will probably be some years before the scope of this technique can be confidently assessed.

In addition two techniques that have been exploited relatively rarely in the past are beginning to attract interest. Firstly as mechanically strong cells can be used with neutrons, without a significant loss in flux, pressure has been employed in a few instances as a thermodynamic variable with which to study biological processes. Secondly, it has been demonstrated that a variety of samples are sufficiently magnetically anisotropic to enable a high degree of orientation in a magnetic field. For example, near complete alignment of a number of biopolymers has been achieved by allowing them to polymerise slowly in a strong field. As the orientation is usually due to diamagnetic anisotropy, which is common to most molecules, this technique appears to have a lot of potential, which is not restricted to biology.

A suit of programs written by O. Glatter (Graz) have been installed for general use on the ILL computer. They perform (a) indirect Fourier transformation of scattering curves from particles of limited size, (b) real space deconvolution of scattering data from particles with spherical symmetry (shell models) and (c) calculate scattering curves from models built of large numbers of small spheres.

Low-Resolution Crystallography

The crystal structure analysis of the nucleosome core particle has now been completed to a resolution of 16 Å. The DNA is best described as an ideal superhelix of 1.8 turns with a radius of 42 Å and a pitch of 25.5 Å. The protein core, consisting of 8 histones, appears to be broken up into four hetero-dimers of two kinds: (H2A-H2B) and (H3-H4). The four dimers are arranged in an approximate helical structure following the DNA from the inside and having the linear sequence: (H2A-H2B) (H4-H3) (H3-H4) (H2B-H2A). The analysis suggests that the monomers associate at a hydrophobic interface to form each kind of dimer while association of the dimers within the protein core is more hydrophilic in character (ILL, EMBL, MRC Cambridge). The RNA structure of satellite Tobacco Necrosis Virus has been refined to resolution of 25 Å using the icosahedral symmetry of



the particle. The RNA does not uniformly fill the inside of the virus but occupies specific regions, one being a shell of radius 30 Å and another being along each of the 12,5-fold icosahedral axes at a distance of 55 Å from the centre. Because hydrophilic amino acids have a similar scattering density to RNA, the details at the protein/RNA interface require careful analysis which is now in progress (ILL, EMBL, Uppsala). Diffraction data from crystals of complex t-RNA^{ASP}-tRNA synthetase have been collected at 5 contrasts. The match-point contrasts of the enzyme and tRNA have been determined and a detailed analysis is in progress (ILL, Strasbourg). Measurements have begun on single crystals of the membrane protein matrix porin-detergent complex. Three dimensional data at 100% D₂O and projection data from 2 other contrasts have been collected (Bâle, EMBL, ILL).

Protein Crystallography

The 1.4 Å analysis of deuterated triclinic crystals of hen egg-white lysozyme is near convergence. Several features of the molecular structure are shown in the accompanying figures 35 and 36. In order to account for the anisotropy of thermal motion, and the conformational disorder of certain residues, and to exploit fully the relatively-high ordering of the inter-molecular water, we are undertaking joint least-squares refinement and Fourier analysis using neutron diffraction data from both deuterated and undeuterated crystals. X-ray data might also be used (ILL).

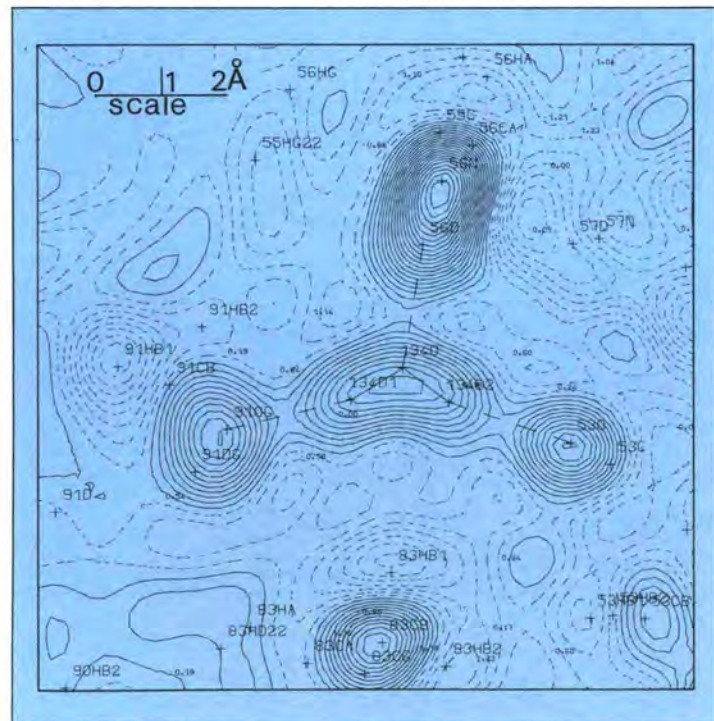


Figure 35: A strongly hydrogen-bonded water molecule linked to the residues Tyr53, Leu56 and Ser91, near a buried β-turn in deuterated triclinic crystals of hen lysozyme.

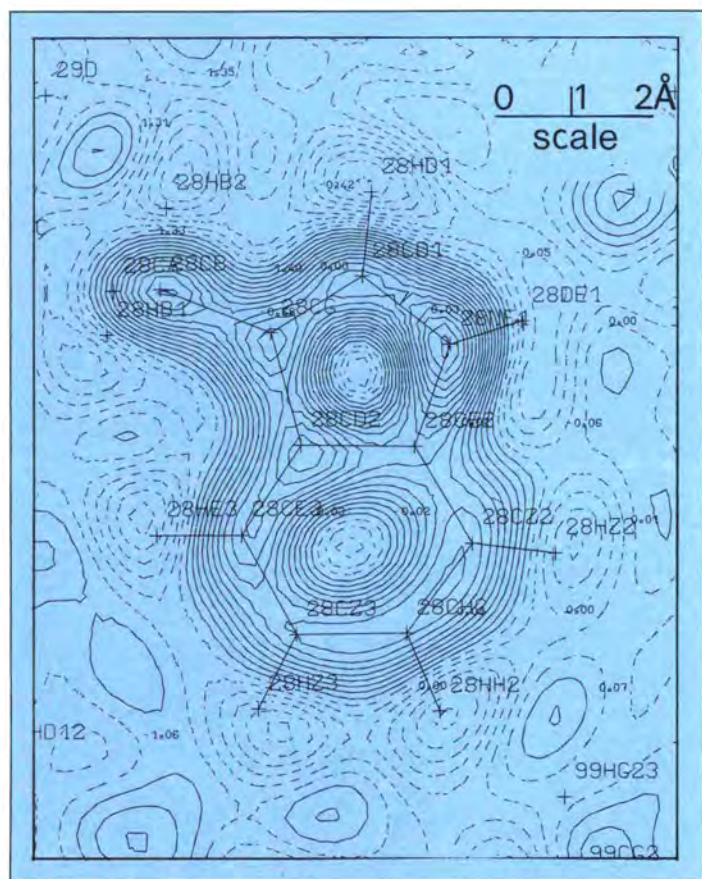


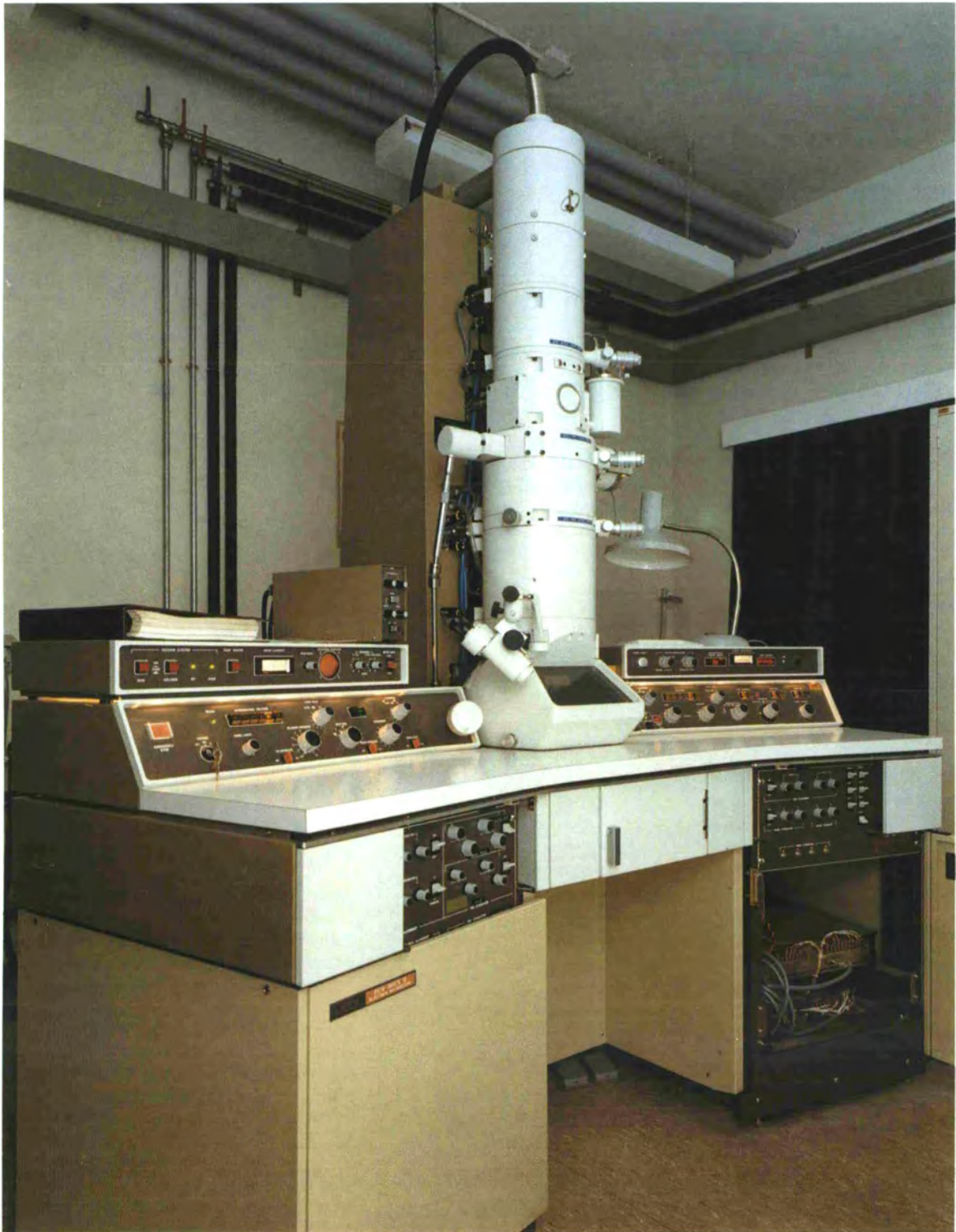
Figure 36: A buried tryptophan side-chain (Trp 28) in which the exchangeable hydrogen atom on Ne1 is highly protected and hence does not exchange. There, as in Fig. 35, the atoms shown were excluded from the phases on which the difference map was based.

Chromatin

Neutron diffraction is being used to study the long range ultra-structural organisation in chromosomes at different stages in the cell cycle. At this level electron microscopy is often unreliable because of the harsh treatment delicate samples must undergo. In interphase the structure loosens and isolated buffer-filled spaces (35-45 nm) develop as the ion concentration is decreased. At even lower ionic strength the distance distribution functions derived from the diffraction patterns by Fourier transformation indicate the formation of supranucleosomal particles with an overall diameter of 40-50 nm. These are considered to be the fundamental units of higher order structure (ILL, Hamburg, München). Nucleosome core particles have been dissociated and reconstituted into particles that are indistinguishable from the native. Future studies can therefore make use of core particles reconstituted with selected histone H2A or H2B or (H3, H4)₂ deuterated (Portsmouth, ILL, EMBL).



The high-performing electron microscope of the EMBL.





E. Coli 50 s Ribosomal Subunit

The progress in the determination of the spatial arrangement of the proteins in the 50 s subunit of E. Coli ribosomes is now mainly determined by the amount of measuring time allocated as the conditions required for specific deuteration are now well established. In the past year the radii of gyration *in situ* of nine proteins and six protein-protein distances were determined.

Viruses in solution

A first series of experiments have been carried out on the temperature sensitive mutant ts 112 of human adenovirus. This mutant has only 20% of the normal DNA content and lacks the two DNA associated proteins. From a comparison of the radial scattering density with that of the native virus the position of the absent proteins can be radially located (ILL, EMBL, Lille). In a test experiment measurements were made for the first time on a Reovirus, rice dwarf virus which is icosahedral and has a genome consisting of 9-12 pieces of double stranded RNA. The data indicate that the virus molecular weight is around 80×10^6 and that the nucleoprotein core is compact (ILL, Japan). Capsids of bromegrass mosaic virus can be dissociated by pressure if the pH of the buffer has low sensitivity to pressure and the pH is near the value which produces the associated-dissociated transition. The results suggest that the capsid protein which is ionized by increasing pH, is also ionized by increasing hydrostatic pressure. Pressure can therefore be a useful additional variable with which to study polymerisation and depolymerisation of protein assemblies.

Membranes

Purple membrane is the highly crystalline light activated proton pump of "Halobacterium halobium". The chromophore retinal is bound with a stoichiometry of one to the only species of protein present, bacteriorhodopsin. Neutron diffraction was recorded from membranes containing either protonated or deuterated retinal and by Fourier difference synthesis the position of the retinal has been located (ILL, MRC Cambridge, Argonne). (Fig. 37). Myelin is the spiral double membrane sheath which surrounds certain nerve axons. Studies of myelin membrane adhesion have been extended using temperature and pressure as thermodynamic variables in addition to biochemical treatments. It has been shown that the adhesion of myelin at the extracellular interface is much weaker in developing peripheral nervous system of embryonic chicks than in mature birds. The results correlate well with the reduced amount of the major glyco-protein in immature myelin thus implicating this protein in extracellular adhesion. Modifications of specific groups of the membrane surfaces were also undertaken to further establish what functional groups are involved (ILL Grenoble). (Fig. 38)

Retinal rods are the site of the primary events leading to visual excitation. It has been established that light induced changes in

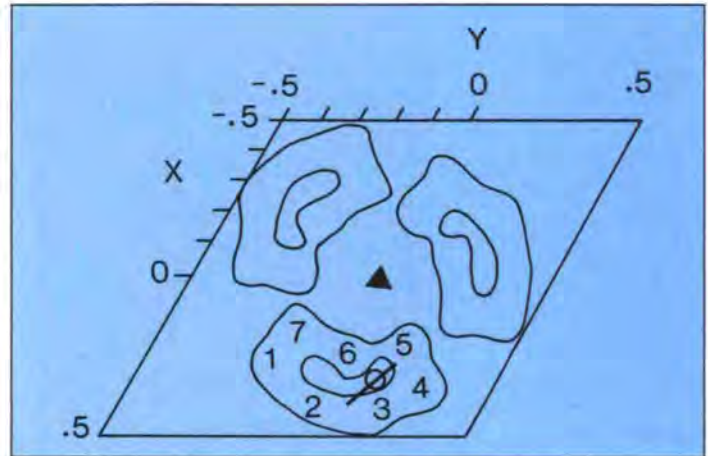


Figure 37: Contour map showing bacterio-rhodopsin molecules in the membrane plane around the 3-fold axis. On one molecule the seven α -helices are numbered conventionally and the location found for the retinal by neutron diffraction is shown (Jubb et al., EMBO J. in press).

the diffraction patterns from magnetically oriented retinal rods are not related to the structural changes of rhodopsin but rather reflect the triggering of a cascade of amplifying reactions by photoexcited rhodopsin (R^*). These reactions are carried out by GTP-dependent peripheral proteins (G proteins) which bind selectively to R^* . Kinetic neutron diffraction measurements down to 1 second resolution is providing, by Fourier synthesis, a structural description of the successive events (CEN Grenoble, Stanford, ILL).

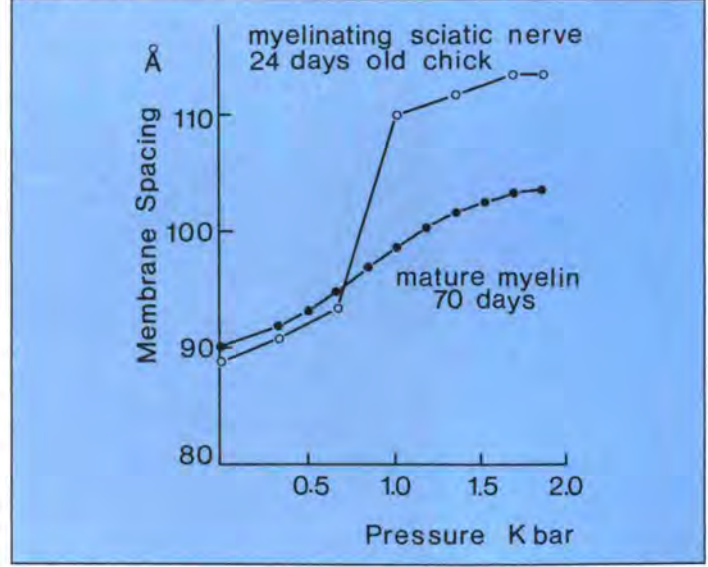


Figure 38: The mature myelin repeat unit is 180 Å and consists of a pair of membranes. The figure shows this half repeat unit plotted as a function of hydrostatic pressure.



Laboratory equipment of EMBL: Recovery of $^2\text{H}_2\text{O}$ from fermentation process by vacuum distillation.



Water Structure in Macromolecules

Biological macromolecules in solution have preferential interactions with solvent components which are important in determining their behaviour. These interactions can be studied with small angle neutron scattering. In a first group of experiments the amount and localization of electrostriction around tRNA was found to depend on the concentration and species of counter-ion. For example, in 0.1 M NaCl, tRNA has an excess mass of 85 water molecules which could be accounted for by a 10% increase in water density over that of bulk (ILL, Strasbourg). In a second series of experiments the hydration of ribonuclease in mixed solvents was examined. In alcohol/water there is no preferential association of water whereas with glycerol/water a glycerol excluding water layer is observed (ILL).

Inelastic Neutron Scattering

The inelastic scattering spectra have been predicted from theoretical models which simulate the dynamics of bovine pancreatic trypsin inhibitor and these are being compared with measured spectra. It is hoped that this combination of experiment and theory will lead to a better appreciation of the usefulness of inelastic scattering (EMBL, ILL, London, Harvard).

Coherent quasi-elastic scattering from hydration-induced inter-subunit motions in fully deuterated phycocyanin from blue-green algae was measured using the spin-echo spectrometer IN11. The corresponding activation of rotational side-chain motions at the protein surface give rise to substantial Lorentzian-like wings, observed in high-Q backscattering on IN13 (London, Edinburgh, Argonne, ILL). Quasi-elastic scattering from lamellar stacks of purple membrane fragments has been measured. Small lineshape changes and a possible discontinuity in the broadening between 1.6 and 300 K were observed on IN13; these effects need to be examined at higher resolution. An IN5 test run confirmed the existence of a feature near 5 cm^{-1} already discovered in earlier work at Harwell. Equipment is being made that will allow "stroboscopic" illumination-dependent difference experiments to be performed so that sample heating effects are eliminated (London, San Francisco, ILL).

The investigation of the modification in internal dynamics which accompany ligand binding to the enzymes hexokinase (EMBL, ILL, Yale) and lysozyme (Edinburgh, London, ILL) are continuing.

Secretary: J. Torbet
Head of EMBL Outstation: B. Jacrot

Protein Dynamics

High resolution X-ray crystallography resulted in a picture of proteins as well-defined more or less static structures. As a result it was believed that proteins moved abruptly from one rigid state to another on binding a substrate or during enzymatic activity. Indeed this picture has been successful in accounting for a number of important protein properties. However, it is now realised that proteins are dynamic structures and that the crystallographic image is a representation of the average atomic positions. The temperature factors needed to fit protein electron-density maps give an indication of the amplitude of internal motion but impart no information about the variety of the time scales involved which only became apparent with the introduction of computer simulations of protein dynamics. The simulations show that the atomic fluctuations can be separated into local oscillations superposed on motions with a more collective character. The latter might involve displacements of chain segments or even the bending of whole domains about molecular hinges. There are now a number of clues indicating that these movements are crucial to biological function. The binding of a ligand to an enzyme can have a marked effect on internal mobility even though, as with lysozyme, the mean atomic positions are relatively unchanged. The diffusion of oxygen into myoglobin and hemoglobin requires dynamic packing defects to open up a passage in what is apparently a closely packed region.

The picture given by simulated protein dynamics needs testing against experimental data some of which is potentially accessible to inelastic neutron scattering and ILL is unique in having suitable instruments.

COLLEGE 9 CHEMISTRY

Members of the College

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R. Ghosh

M. Lehmann
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9a: Molecular Spectroscopy, Surfaces and Mesophases

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9b: Colloids and Polymers

S. Bantle
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GENERAL SUMMARY

Amongst the experiments of College 9 many, in particular the tunneling experiments, require low temperatures. To meet this requirement a $^3\text{He}/^4\text{He}$ dilution refrigerator insert has been developed by K. Neumaier (Garching) and fits into standard ILL Helium (orange) cryostats. Temperatures of about 20 mK can be attained and it is easy to handle.

Subcollege 9a is satisfied about the reinstallation of the Be-filter (INFB) on the hot source and although it disposes only of 20% of the total beam time available, due to the time sharing mode of operation (together with IN1 and D4), the new instrument has shown considerable improvement: The frequency range (6.5-130 THz) covered by the Cu(220) monochromator plane is larger than that previously obtained by the Cu(200), (220) and (331) planes together and avoids discontinuity in intensity arising from the change of planes. This is advantageous for precise experiments, such as surface work etc. In addition, background and resolution have been improved and the comparison, using the same Cu(220) plane as for the old version, shows an intensity gain of factor 5. For higher energies this gain is even larger.

First tests with a graphite filter between Be-filter and detector yielded the expected resolution of 0.5 THz up to an incident energy of about 25 THz.

D7 is of increasing importance for experiments requiring separation of coherent and incoherent scattering.

SCIENTIFIC HIGHLIGHTS AND TRENDS IN 1983

Physisorption

The number of substrates of which the best known are graphite and lamellar halides, has been extended by a new one, MgO (Marseille). By using these substances the influence of the different surface potential symmetry (square compared to hexagonal) on the adsorbed layer is investigated through the changes in the phase diagram, different behaviour of commensurate-incommensurate transitions or melting transitions.

Neutron diffraction is particularly competitive in the investigation of adsorbed light atoms. An exception is ^{36}Ar due to its very high scattering cross section. Studies of ^{36}Ar on graphite were carried out to understand the phase transition from the solid gas phase to the fluid phase, which is probably not of the first order. These experiments included diffraction studies, inelastic scattering (2-dimensional phonons) and quasielastic scattering. The latter also demonstrated the de Gennes narrowing in a two-dimensional system (ILL).

A growing interest is observed in the study of simple molecules on graphite as C_2N_2 or Neopentane (Saclay).

Graphite Intercalate Compounds (GIC)

The study of the two-dimensional diffusion on graphite based compounds has been continued successfully (ILL, Urbana, Washington). E.g. for the stage compounds the Q-dependence of the quasi-elastic linewidth for the coherent scattering alkali shows a de Gennes narrowing at the peak of the structure factor at $Q \approx 1.2 \text{ \AA}^{-1}$ - a signature for a liquid. A further decrease of the linewidth is found at larger $Q \geq 1.5 \text{ \AA}^{-1}$, indicating well defined jump vectors. These measurements have been extended to include the stage 1 compound LiC_6 . It is both of scientific and technical interest, because of the incoherent cross section of Li and due to its potential for technical applications. Results shown in Fig. 39 indicate that the jump vector is determined by the Li inplane structure. Also in-beam NMR on S6 supported this study.

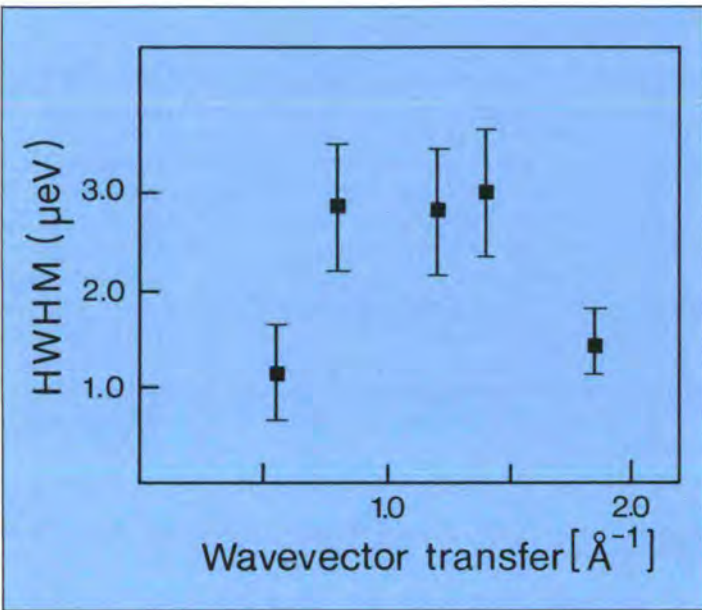


Figure 39: LiC_6 - stage 1 - Q -dependence of the quasielastic linewidth.

Magnetic properties of graphite intercalated by FeCl_3 (Paris; ILL) are treated by College 5. Very interesting is the change from 2- to 3-dimensional behaviour between stage 2 and 1 respectively. Attention is also focussed on acids in graphite (Paris; ILL) which are supposed to show hexatic phases probably connected to Halperin-Nelson phase transitions.

The study of the tunneling of H_2 in graphite intercalates (e.g. in C_{24}Cs) is progressing (Oxford; ILL). The fine structure observed is related to domain structures caused by static distortion waves.

Tunneling Spectroscopy

This research field continues to be very active. The studies can now be extended easily to very low temperatures of the order of 20 mK using the He^3/He^4 dilution refrigerator insert for the standard ILL Helium cryostats, as previously mentioned in the summary. Two exciting experiments were performed, one on solid methane in phase II (Jülich, McMaster, Garching, ILL), the other on tunneling of methyl groups in Manganese Acetate (Nottingham, Garching, ILL). In both cases the study of the temperature dependence of the spectral shape at temperatures below 1 K yielded detailed information about coupling effects between the tunneling groups.

More experiments have been performed to investigate the transition from the quantum to the classical regime with special emphasis on the isotope effect. Example: Temperature

dependence of the spectral shape of protonated and deuterated methyl groups in Toluene and Nitromethane (Bordeaux, Nottingham, ILL).

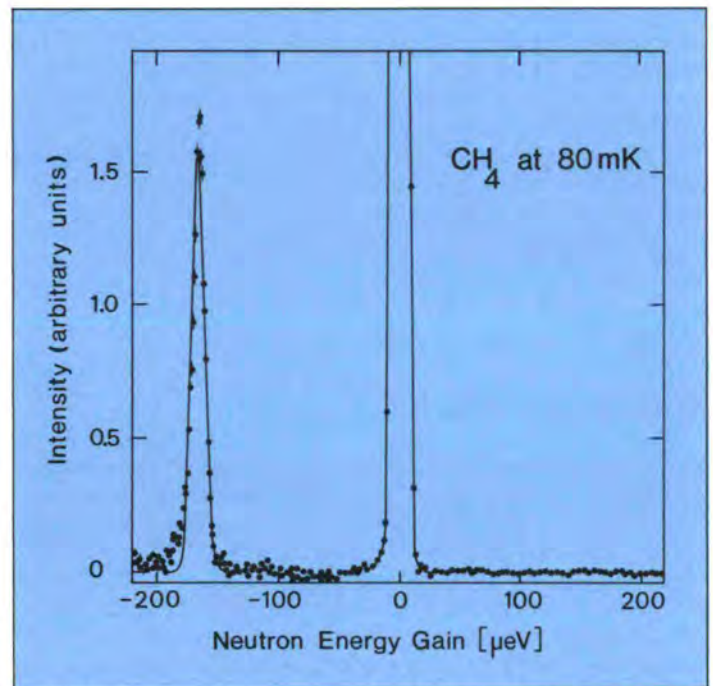


Figure 40: Tunneling spectrum of solid CH_4 at 80 mK (instrument IN5, wavelength 13 Å, energy resolution 9 μeV FWHM).

Vibrational Spectroscopy

As mentioned above the most important feature in the field of vibrational spectroscopy is the installation under improved conditions, of the Be-filter INFB on the hot source.

During the period of disconnection of the instrument from the beam the following results obtained with the previous facility have been published:

- The vibrational modes of neopentane were recorded on IN4 and IN1. A reassignment of the normal modes, based on a coupled calculation of the vibrational frequencies and of the neutron scattering intensities was proposed (ILL, Montpellier, Lyon).

- Neutron Inelastic Spectroscopy (NIS) has been used, in conjunction with volumetric methods, to study the chemisorption of cyclohexane on nickel. At high coverage hydrogen, benzene and cyclohexane are detected on the surface and at low coverage only hydrogen and benzene are present on the nickel (Lyon, ILL).



— The NIS spectra of norbornane obtained on IN1 and IN4 have also been used to determine a valence force field which accounts for the observed optical frequencies and the neutron intensities. This force field will be used to interpret the optical and NIS spectra of the mono and dimethyl derivatives. The NIS spectra are particularly useful to characterize the low frequency vibrations which have a predominant role for the thermodynamic properties (St. Martin d'Hères, ILL).

— Finally, the observation of high frequency molecular modes is still stimulating experimental and theoretical work. There is now a general agreement on a major result: the Debye-Waller factor due to lattice motion appears to be ineffective on the intensities of the high frequency molecular modes.

Molecular Crystals

Rotational motions in plastic molecular crystals have been investigated by incoherent quasielastic neutron scattering. Measurements were carried out with three similar molecules, norbornane, norbornylene and norbornadiene, in their different phases. Reorientation about molecular axes or about lattice axes were analysed in all the successive phases. The existence at the same temperature, of two possible crystalline phases was unambiguously proved, and the motions analysed in each of them.

Pivalic acid (CH_3)₃CCOOH is an especially complicated case of four simultaneous motions. Partial deuteration was used to analyse each motion individually (IN6). Correlation times related to methyl, t-butyl and carboxylic group rotations were obtained. A high resolution measurement (IN10) enabled the analysis of the overall tumbling of the molecule.

Other experiments were performed with trimethylsulfoxonium halides. The two similar compounds, hexamethylethane and hexamethyldisilane were investigated with IN5.

The rôle of the tetramethylammonium ion (TMA) in the successive phase transitions of TMAZnCl₄ was also analysed.

The problem of the dynamics of H₂O adsorbed in the synthetic NaA zeolite was studied with IN5. The variation of activation energy for the dynamics of Na⁺ reactions, obtained from dielectric relaxation measurements, was related to the dynamical behaviour of H₂O molecules.

In the study of organometallic complexes composed of alkyl chains bonded to Fe or Cu ions, the successive phase transitions can be interpreted by the increase in the number of degrees of freedom of the chains. At low temperatures, the chains are rigid and the stacking is not very compact. At higher temperature, the chains become mobile, fold and thus the stacking is more compact.

Protonic Conductors

Dynamics of protons in several protonic conductors exhibiting H₃O⁺, H₅O₂⁺, H₃O⁺ · 3H₂O species have been studied in order to elucidate the proton transfer mechanism (Montpellier; ILL). In H₃O⁺ClO₄⁻ protons jump in a three-fold potential. In H₅O₂⁺ protons are dynamically disordered in a double well potential between adjacent oxygen atoms. With increasing temperature (above 300 K) the water molecule starts rotating. In H₂UO₂PO₄ · 4H₂O, the two motions seem to occur as a long range proton motion which apparently follows a Grotthus mechanism. In CsH₃O₂ (Berlin) dynamics of protons in hydrogen bond indicate a dynamical disorder occurring too in a symmetric well potential between adjacent oxygen atoms. No information on the proton diffusion process is presently available.

Zeolites

The work on hydrocarbons in zeolites (Lyon, ILL) was continued using the wide variety of ILL methods: localization of hydrocarbon molecules at low coverage was measured with diffraction. Distribution (clustering) in the network at higher coverage was investigated by small angle scattering. With quasielastic scattering the dynamics of the molecules not located on well defined crystallographic sites were determined.

Colloids and Polymers

The spin-echo spectrometer (IN11) continues to provide unique information on polymer and colloidal dynamics, but the polarisation analysis capabilities of IN11 are also increasingly in demand to measure static incoherent background levels for the many experiments in which the background is produced by the sample rather than the solvent or support matrix. Among the dynamic studies of polymers, contrast variation using marked molecules has been a major feature, and has enabled experimental demonstration that the chain dynamics are effectively the same at the centre of a long molecule as they are towards the ends (Strasbourg, ILL).

A highlight of the spin-echo experiments has been the collaboration between light scattering and neutron groups to study microemulsions (Malvern, Bristol, ILL) and critical dynamics in both micellar (Pavia, Milano, EMBL, ILL) and microemulsion systems (Saclay, MIT, ILL). Small angle scattering studies of micelles have concentrated on looking at absorbates in the micelles, using alcohols (Saclay, ILL) and aromatic/aliphatic hydrocarbons (RAL, ILL). Contrast variation plays an important role in these studies, which have been extended up to high absorbate-to-monomer ratios as high micellar concentrations.



Experiments in the field of polymers covered a broad spectrum of sample environments. Measurements in solution used contrast matching in the case of block copolymers in order to study the dimension and the shape of the "visible" block. Varying the contrast while keeping the thermodynamic properties as close as possible gave information on both parts of the copolymer (Strathclyde), which in this case was a styrene-methyl methacrylate block copolymer. In the chosen solvent the methyl methacrylate blocks have a compact structure and form the core for the spherical micell which is stabilized by solvated styrene blocks.

Other experiments with polymers in solution are devoted to the study of local conformations of partially labelled polystyrene chains (ILL, Strasbourg). The design of a pressure cell means that experiments can be carried out under pressure in the range up to 2000 bars. A first experiment with a solution of a polyelectrolyte was carried out showing a remarkable effect (Osnabrück, ILL).

The large difference in scattering lengths of hydrogen and deuterium and the good transparency of many materials for neutrons is successfully used in determining dimensions of polymer chains in solids, melts and networks. Part of the material is labelled and gives rise to coherent scattering from which form and structure factors can be deduced. To quote some examples, the research on amorphous and crystalline polymers is continuing (Mainz, Bristol) and of special interest are the dimensions of the crystalline phase and the order of different crystalline regions. Also the segregation of multiblock copolymers is studied (Mainz, Freiburg).

The fruitful experiments studying phase separation in polymer blends are continuing (London). Diffraction and scattering studies from doped polyacetylene gave additional information to investigations with x-rays, because different reflections are seen with the two techniques. In addition, contrast variation elucidated certain parts of the crystalline or amorphous phases (Basel, Hamburg).

Polymeric networks are studied under different conditions: in the dry state, swollen in various solvents, unstretched or stretched to certain elongations. Of main interest is the behaviour of single (marked) chains in the network (Strasbourg, Mainz, Saclay, Strathclyde).

A first successful experiment was carried out with the stretching apparatus designed for use in the neutron beam (Mainz, ILL, Strasbourg). The sample, a strip of PSMS-rubber, is macroscopically deformed by applying a periodic stress. Scattering is recorded in different channels during the stretching and releasing process. At low frequencies the periodic stress is followed by a periodic change of the mean square radius of gyration whereas at higher frequencies the relaxation process is too slow to follow. In another time-resolved experiment (Bayreuth, ILL) the relaxation process of structures which were aligned by an electric field is recorded. From this the scatter-

ing curves at different stages of the order-disorder process can be studied.

The successful experiments with the shear gradient apparatus were extended to other polymeric systems. In addition polymer solutions micellar systems and amphiphilic aggregates in micellar systems were studied (ILL, Mainz).

Workshops

Two workshops were organized in 1983 by College 9 at the ILL. The first was held in March with the title "SANS data treatment for concentrated polymer and colloid solutions", organized by R. Ghosh, J.B. Hayter and R. Oberthür. The meeting was attended by 46 participants from many external laboratories as well as the ILL. Problems of data reduction, data treatment and interpretation of scattering results were discussed.

The second workshop took place in October and was devoted to "Use of neutrons in technologically important problems in powders, gels and colloids", organized by J.P. Beaufils and J.B. Hayter. Limited to 16 industrial and 8 ILL scientists, this first meeting of its type allowed a fruitful interchange of ideas and the identification of several areas of industrial science which posed interesting fundamental problems amenable to study with cold neutrons.

Seminars

The scientific life at the ILL was enriched by lectures given by outside scientists: S. Edwards (Cambridge), H. Hoffmann (Bayreuth), W. Burchard (Freiburg), H. Hässlin (Basel), W. van Megen (Bristol), D. Fink (HMI Berlin), G. Velasco (Thomson-csf), P. Knözinger (Siegen), J. Suzanne (Marseille) and D. Scherson (Berlin).

Secretaries:

H.J. Lauter / S. Bantle



**SURVEY ON NEW INSTRUMENTS
OR INSTRUMENT MODIFICATIONS**

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AND NUCLEAR PHYSICS**

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THREE-AXIS SPECTROMETERS**

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**INSTRUMENT GROUP
TIME-OF-FLIGHT
HIGH RESOLUTION
AND DIFFUSE SCATTERING**

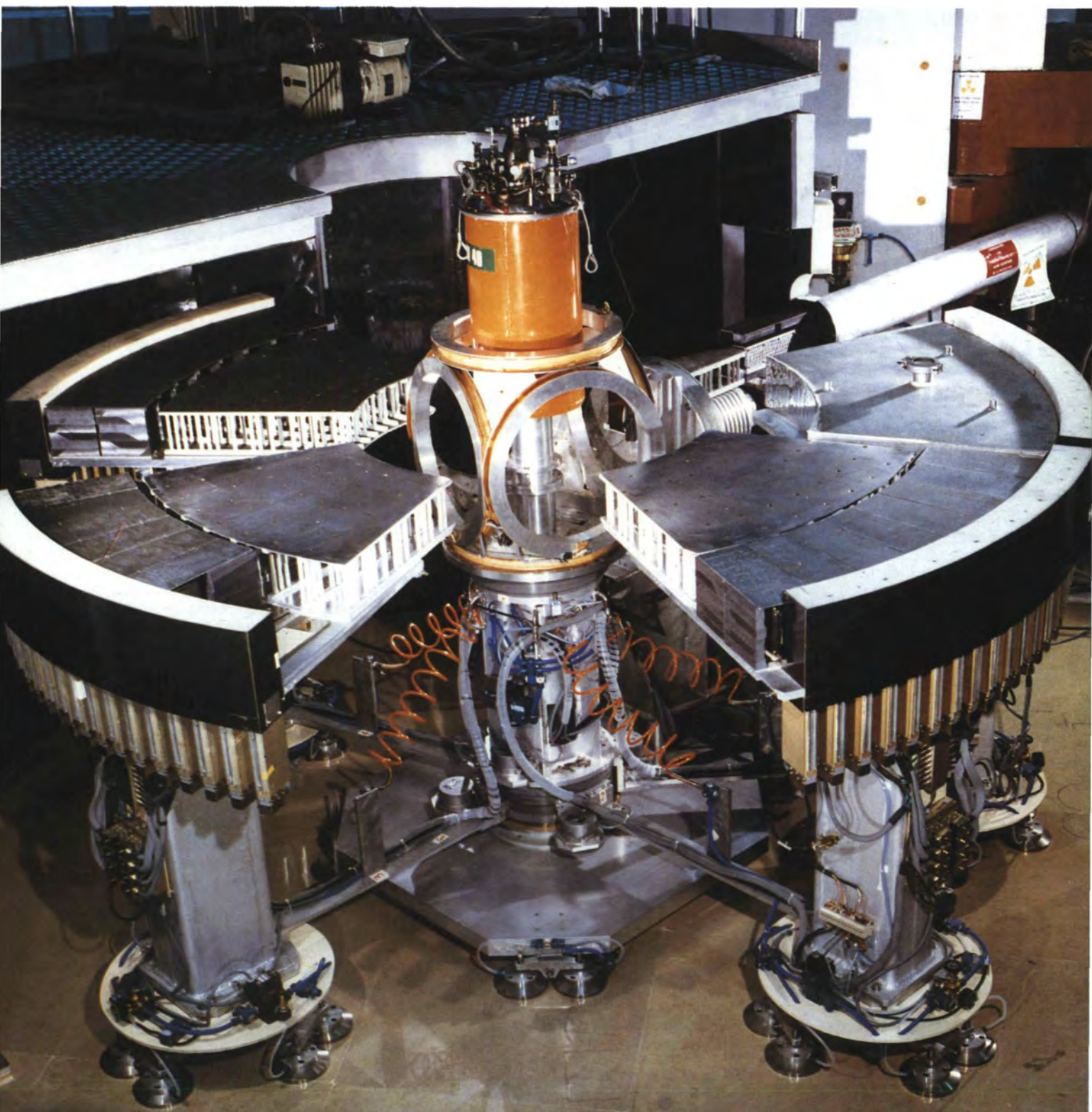
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**INSTRUMENT GROUP
DIFFRACTION INSTRUMENTS**

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INSTRUMENT OPERATION DEPARTMENT

D7 in its version for polarisation analysis (in the 3.1 Å position). Behind the collimator, the picture shows subsequently the polariser, guide field, chopper, Mezei flipper and spin turning coils (3 orthogonal coil pairs) with a cryostat on the rotatable sample table in the centre. Four detector tables on air cushions can be moved automatically and are controlled by electronic decoders. The detector bank on the extreme right is only equipped with a collimator box whereas the three others are associated with super-mirror analysers in a strong magnetic field in front of each detector. Between the spin turning coils and the analysers are permanent guide fields.



Introduction

The instrument operation department has overall responsibility for the operation and improvement of the instruments. It also provides necessary technical assistance to enable the visitors to prepare and carry out their experiments. The instruments are divided amongst five instrument groups which ensure their operation and development. The other groups and services of the department provide facilities and expertise needed by the instruments and visitors.

The internal structure of the department was slightly reorganised in 1983 in order to increase the efficiency of the groups. The monochromator group was transferred into the section "Instruments and Methods" of the technical department. The sample environment group was split up into two sections:

1) the cryogenics service is responsible for developing and operating special cryostats working below 1 K and the cryomagnets.

Einleitung

Die Abteilung Instrumentenbetrieb ist verantwortlich für den Betrieb und die Verbesserung der Instrumente. Ausserdem stellt sie die nötige technische Hilfe, um den Gastforschern die Vorbereitung und die Durchführung ihrer Experimente zu ermöglichen. Die Instrumente sind auf 5 Instrumentengruppen aufgeteilt, die den Betrieb und die Weiterentwicklung der Instrumente sicherstellen. Die anderen Dienstleistungsgruppen der Abteilung stellen die Einrichtungen und die Erfahrung, die Instrumente und Besucher benötigen, zur Verfügung. Die interne Struktur der Abteilung Instrumentenbetrieb wurde 1983 geringfügig umorganisiert, um ein effektiveres Arbeiten der Gruppen zu ermöglichen. Die Monochromatorgruppe wurde in die Abteilung "Instrumente und Methoden" der technischen Abteilung transferiert. Die Gruppe "Probenumgebung" wurde in zwei Sektionen aufgeteilt:

1. In den "Kryogenie-Dienst", der für die Entwicklung und die Bedienung von Kryomagneten und speziellen Kryostaten, die bei Temperaturen unter 1 K Messungen durchführen können, verantwortlich ist.

Introduction

Le Département Exploitation des Instruments a la responsabilité globale de l'exploitation et de l'amélioration des instruments. Il fournit en plus le soutien technique nécessaire pour permettre aux chercheurs invités de préparer et exécuter leurs expériences. Les instruments sont répartis en cinq groupes pour assurer leur fonctionnement et leur développement. Les autres groupes et services du département fournissent les moyens et les connaissances nécessaires pour les instruments et aux visiteurs.

La structure interne du département a été légèrement modifiée en 1983 afin d'augmenter l'efficacité des groupes. Le groupe monochromateurs a été transféré au service Instruments et Méthodes du Département Technique. Le groupe "Environnement des échantillons" a été divisé en deux parties :

1. Le service cryogénie, responsable du développement et de l'exploitation des cryostats spéciaux qui fonctionnent au-dessous de 1 K ainsi que des cryo-aimants.

2) the "sample environment group" is responsible for the development and maintenance of vacuum systems, high pressure cells, furnaces and normal cryostats. It also organises the supply of cryogenic liquids (He, N₂) and of gases.

The central group which serves as a link between the requirements and the demands of the scientists and the general services had to plan and execute in close cooperation with the reactor department the work connected with the beam tube exchange programme during the extended reactor shutdown. Instruments like PN1, IN8, D15, D2, D8 and D3 were dismantled completely and reinstalled on or before the estimated dates. The long reactor shutdown was also used to modify and improve most of the other instruments. Apart from some exceptional cases the instruments became fully operational again once the reactor started up.

2. In die Gruppe "Probenumgebung", die für Entwicklung und die Wartung von Vakuumsystemen, Hochdruckzellen, Öfen und normalen Kryostaten verantwortlich ist. Ausserdem organisiert sie die Versorgung mit kryogenischen Flüssigkeiten (He, N₂) und mit Gasen. Die Zentralgruppe, die als Bindeglied zwischen den Wissenschaftlern und deren Erfordernissen und den allgemeinen Dienstgruppen dient, musste in enger Zusammenarbeit mit der Reaktorabteilung die Arbeiten, die mit dem Strahlrohraustauschprogramm während des langen Reaktorstillstands zusammenhängen, planen und durchführen. Instrumente wie PN1, IN8, D15, D2, D8 und D3 wurden völlig demontiert und zu oder sogar vor den geplanten Terminen wieder installiert. Der lange Reaktorstillstand wurde ausserdem dazu benutzt, die meisten anderen Instrumente zu verbessern. Abgesehen von wenigen Ausnahmen waren alle Instrumente wieder voll funktionsfähig beim Reaktorstart.

2. Le groupe environnement des échantillons, responsable du développement et de l'entretien des systèmes à vide, des cellules à haute pression, des fours et des cryostats normaux. Il s'occupe également de l'alimentation en liquides (He, N₂) et en gaz cryogéniques.

Le groupe central, qui sert de liaison entre les besoins et les demandes des physiciens et les services généraux, devrait projeter et exécuter en étroite collaboration avec le Département Réacteur les travaux liés au programme d'échange des canaux pendant l'arrêt prolongé du réacteur. Des instruments tels que PN1, IN8, D15, D2, D8 et D3 ont été complètement démantelés et réinstallés aux, ou avant les, dates envisagées. L'arrêt prolongé du réacteur a également été utilisé afin de modifier et améliorer la plupart des autres instruments. Outre quelques cas particuliers les instruments sont redevenus opérationnels dès le démarrage du réacteur.

SURVEY ON NEW INSTRUMENTS OR INSTRUMENT MODIFICATIONS

The following four tables give an overall view of the new instruments built in the framework of the modernization programme, and instrument modifications which have led to improvements in efficiency.

TABLE I

New instruments with no present day equivalent

		<i>available</i>
IN14	triple axis spectrometer	1986
IN15	ultra high resolution spin echo	1986/87
DB21	biological diffractometer	1984/85
D22	low Q spectrometer	1986
PN8	coincidence fission spectrometer	now

TABLE II

Instruments rebuilt to give gains in flux/detection of 5-10

<i>Present instrument</i>	<i>New instruments</i>	<i>available</i>
D1A	D2B powder diffraction	1984/85
D2	D20 powder diffraction	1985/86
D4	D4B liquids and amorphous solids diffraction	now
D8	D19 large unit cell diffraction	1985
D9	D9B small unit cell diffractometer	1985
D7	D7B* diffuse scattering quasielastic scattering with full polarisation analysis	now
IN1 (+ Be filter)	IN1B hot source triple axis	now
IN2	IN20* triple axis with full polarisation analysis	1984
IN4	IN4B time of flight spectrometer	1984/85
IN11	IN11B spin echo	1984
D17	D17B small angle scattering; gain at 6-10 Å	1985

* effectively new types of instrument.

TABLE III

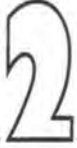
Instruments with gain in flux/detection ~2

<i>Present instrument</i>	<i>New instruments</i>	<i>available</i>
D11	D11C small angle scattering	1985
D16	D16 4 Å diffractometer	1985
IN5	IN5B cold source, time of flight, variable resolution	1985
IN6	IN6 cold source, time of flight, high intensity	1985
IN10	IN10B high resolution backscattering	1985/86

TABLE IV

Instruments with more modest improvements

PN1	fission spectrometer	numerous minor improvements
PN2	conversion electron spectrometer	new detector
PN3/PN4	γ spectrometer	new ultra high resolution spectrometer - late 1983
D3	polarised beam diffractometer	transfer to hot source 1986
D10	4 circle diffractometer	spin echo developments
D15	single crystal diffractometer	new computing system 1982
IN8	triple axis spectrometer	modernised 1982
IN13	high Q backscattering spectrometer	completed 1981



CENTRAL GROUP

With the reactor shutdown for 6 months a major part of the Groups workload was associated with the planning and preparation, for the dismantling of the instruments, the radiation shielding, and the infra-structure, to permit access to the reactor face for changing of the thimbles (PN1, IN8, D15, D2, D8, D3). All of this depended upon close coordinated collaboration between the different ILL Departments and Services. This was achieved by daily meetings.

Whilst in general an instrument site can be completely cleared in about 2 weeks, the reinstallation, reequipment, and realignment takes from a minimum of 5 weeks for a straightforward site to 1 year in the case of a site like D15 which is dependent on adjacent installations. The detailed planning for the dismantling not only needed to take into account the access to the reactor building for heavy mobile cranes, but also the fact that the limited floor loading and available space obliged practically all shielding to be removed outside. In addition, to allow even minimum access, in certain cases adjacent protections had to be dismantled. For the reinstallation phase, coordination was even more important, because of the large number of different groups obliged to work in the same, often confined space, and each with interdependent needs. Despite the problems, all instruments were reinstalled on or before the estimated dates.

In all about 1000 tons of shielding and equipment were transported; opportunity was taken during the shutdown to modernize, maintain, and modify equipment and installations, including:

- replacing the rotating secondary beam shutters by a translating model.
- modification of primary shielding to simplify future dismantling.
- maintenance on the nitrogen reservoirs.
- pressure testing of the He cylinders.
- inspection of the internal state of the effluent and gas recovery lines.
- studies on the clean computer electrical distribution.
- assessment of the hazardous materials in long time storage for visitors.

In preparation for the installation of the H11 complex (D19, D2B, D20) in 1984:

- two new elevated platforms were constructed, which permitted the transfer of material which in turn allowed the dismantling transfer, and reconstruction of the low activity laboratory.
- the secondary shielding around Gams 3 was altered.
- the floor in the D19 zone dug up and prepared for the laying of the marble.
- a complete new experimental position was constructed on

H22 to allow partial testing of the D2B and D20 instruments. New experimental positions were also created on H142 for T16, on H18 following the dismantling of the n- \bar{n} experiment and an off-line position for the new thin film evaporator. The creation of the T16 position involved major work on the adjacent H22 beam-line including:

- the complete dismantling and remodelling of the S51 shielded zone.
 - partial modification to S10 and S34.
 - the entire rewiring of the electrical distribution and the replacement of water, gas and alarm services.
- Before the start-up of the reactor, as a result of the intense work program, all instrument safety interlocks, alarms and beam-line controls were tested, involving about 1500 verifications:
- extensive repainting was required (800 hours),
 - and a major cleaning campaign carried out (1300 hours).

Planning for the 1984/1985 shutdown is now well in hand.

During the year the normal rhythm of the experimental program has required, apart from the supplying and maintaining of general services required by the ILL scientists and visitors:

- the study of the use of explosive gases for experiments (hydrogen, methane, isobutane), which has led to the development and installation of programmable microprocessor units to control the various parameters (pressure, presence of gas, electrical power, etc) on PN8, PN7 and S51.
- the examination and coordination of 20 hazardous experiments, generally connected to the control room via the SADI microprocessor alarm network.
- background measurements to define protection modifications for T16, PN8, PN1, D2, IN8, D9, Gams 4.
- definition of the safety control systems procedures for IN20, and participation in the examination of the shielding for D19, D20 and IN20.
- development of special materials (lithium in glass, and graphite guide windows).

The special scientific exhibition posters which were prepared last year have been displayed on several occasions in England and France.

The plan of the entire experimental layout has been completed, and a large scale panel is in preparation for the entrance hall. Among other projects completed, are included the design and construction of an elevating X, Y table for D15 and D3, whilst development continues on the new instrument T12.

D.A. Wheeler

SAMPLE ENVIRONMENT GROUP

A. STANDARD CRYOGENICS

1. Cryogenic fluids

Consumption of:

- a) Liquid nitrogen: 320 850 litres at 0.49 F/l
- b) Liquid helium: 35 490 litres at 29.1 F/l.

This consumption continues to be very high. The long shut-down permitted the optimisation of certain systems with a high consumption of helium. A more frequent use of superconducting magnets is noted.

2. Cryogenics

The neutron experiments necessitating the use of standard cryostats amounted to 148, or 1090 cryostat days. Some new cryostats were commissioned:
 one standard cryostat for high pressures
 one standard cryostat for conventional electro-magnets
 two top-loading cryogenic machines with a 12 K closed helium circuit
 one horizontal operation cryogenic machine with a 12 K helium closed circuit.

3. Vacuum

Maintenance of 550 pumps on the site
 600 routine interventions
 180 special interventions

Acquisition of new pumps:
 35 primary pumps
 3 ROOTS pumps
 4 turbo molecular pumps.

Assembly of 15 complete helium pumping systems
 Approximately 600 leak tests were carried out with helium spectrometers.

B. HIGH TEMPERATURES

Level of Activity

The number of approved experiments requiring furnaces is rapidly increasing. 37 requests were received for the 2 reactor cycles of 1983. This is a factor of 3 over the level of activity in 1980. Furthermore, 7 of these requests were for special set-ups requiring detailed or extensive intervention.

The third version of the very high temperature (2500°C) powder furnace is now operational close to its design temperature, but given the existing supply difficulties for refractory metal components, no more than 2 experiments per year above 2000°C can be envisaged at the present time. Temperatures above 2000°C are not yet routinely available.

Development

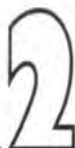
New furnaces are now being equipped with the secondary vacuum pump mounted directly on the top plate. This design gives a much improved vacuum by elimination of the secondary pump line. The design has been tested with the very high temperature furnace mentioned above using a small diffusion pump, and with the IN13 furnace using a turbo-molecular pump. A newly designed furnace for the 3-axis group instruments also adopts this feature. This latter furnace designed jointly by the high temperature group and the 3-axis scientists and technicians, employs a new sample mount with access from below. It will be delivered in February 1984.

Tests on heating elements for particular neutron experiments have been carried out and appear promising. These are:

- (i) an aluminium element (50 μ) giving a low incoherent background, suitable for IN5 at temperatures up to 400°C
- (ii) a flat double spiral heater giving a very weak magnetic field, probably suitable for IN11.

Projects started or planned:

- 1) Non-magnetic furnace for IN11.
- 2) Horizontal tube furnace for small angle scattering. The mechanical support incorporating precision translation and rotation adjustments is already under construction.
- 3) Single crystal furnace operating up to 2000°C for D15. This will be an adaptation of the 2500°C powder furnace with newly designed sample loading and support.
- 4) Reconstruction of the metallurgical heat treatment furnace for D11.



C. HIGH PRESSURES

Most of the experiments under hydrostatic pressure have required the use of a helium gas pressure generator ($P = 5$ kbar). This set-up is fully operational and allows for pressure control. Accurate pressure calibration is under way.

New clamped pressure cells have been built. Pressures up to 10 kbar can be achieved by using C_8F_{18} as pressure medium. These cells are made of maraging steel and copper beryllium alloy, and can be used down to very low temperature below 1 K in dilution refrigerators. Higher pressure values can be reached with clamped Al_2O_3 cells.

Furthermore, some experiments have been performed on crystals subjected to uniaxial stress.

C. Vettier

SPECIAL CRYOGENICS

ELECTRONICS

Six of the ILL designed precision temperature controllers are being tested on instruments under normal experimental conditions. This allows us to determine that their functions correspond to users needs before making a final decision on their design. When this is done, it is intended to equip every ILL instrument with one of these controllers, thus allowing completely automatic precision temperature programming.

The tests so far carried out, show that the instruments perform to their design specifications. During 1984 it is intended to extend their capabilities in order to automatically control the cold valve of the cryostats.

SUPERCONDUCTING MAGNETS

The D2 5 Tesla horizontal field magnet has been installed and is fully operational. It has successfully completed approximately 60 days of experiment time on the instruments D2, IN2, and IN12.

The 7 Tesla vertical field magnet has been repaired and is now entering into scheduled operation. An experiment scheduled in early 1984 requires the mounting of this magnet to a cast iron goniometer bed. The very large forces produced by the interaction with the stray fields (4×10^4 N) will be balanced out by a magnetic counter mass, depending on a measurement of the residual forces.

— This system is being developed mainly by the team of physicists who will do the experiment.

— The triple axis, 6 Tesla, vertical field system has still not been delivered. Severe "training" problems have appeared on this magnet, thus several scheduled experiments had to be cancelled, or postponed.

Due to impurities in liquid Helium, severe problems have appeared owing to the blocking-up impedance of the cold valve controlling the flow in the variable temperature insert of the D3 magnet. Several modifications of that part of the system have improved the reliability. However, the results are not satisfactory. Filtering very dirty liquid helium appears to be a more serious problem than previously thought.

In an attempt to overcome these difficulties we are studying, in close cooperation with the instrument responsible, an automatically controlled cold valve.

VERY LOW TEMPERATURES

— U.C.N.

The pumping system of the U.C.N. cryostat has shown several faults. It has been repaired and, until now, seems to work correctly.

— S.E.R.C. Dilution cryostat (25 mK)

This cryostat has been successfully used in various arrangements:

- magnetic field up to 0.2 Tesla
- sapphire windows (low angle scattering)
- N M R associated measurements.

— Dilution inserts for standard cryostats

The first dilution insert at the ILL which had been developed by K. Neumaier of the Meissner-Institut in Garching has been used with great success on IN5, IN13 and on IN6. Temperatures down to 40 mK could be obtained. The time necessary for a complete sample change is of the order of only 4 hours!

The second dilution insert, with improved performance, has been developed again by the Garching group. It reaches temperatures down to 20 mK.

— Sample gas handling systems

Two gas handling systems have been built, for pressures up to 30 bar. One is mainly for He^3 handling.

FAST BOTTOM LOADING DILUTION CRYOSTATS

The system, developed in collaboration with the C.R.T.B.T., allows fast sample change and cooling (few hours), keeping the main parts of the cryostat cold. The first cryostat, with a simple tubular heat exchanger, has been working for 7 months, and gives temperatures down to 55 mK in 3 hours.

An improved model, with better heat exchangers is under construction, and is nearly finished, as well as the fully automatic pumping system. Temperatures below 10 mK reached in less than 5 hours are expected.

D. Brochier

Part of the ILL cryogenics workshop.



INSTRUMENT GROUP FUNDAMENTAL AND NUCLEAR PHYSICS

- PN1: Fission product separator (LOHENGRIN) on beam tube H9.
- PN2: Beta spectrometer (BILL) on the vertical beam tube V3.
- PN3: Three curved crystal gamma spectrometers (GAMS 1, 2, 3), one flat crystal spectrometer (GAMS 4) on the through-going beam tube H6/H7.
- PN4: Ge(Li) pair spectrometer on the through-going beam tube H7.
- SN5: Ultra-cold neutron (UCN) source on the inclined beam tube IH3.
- PN6: On-line mass separator for thermally ionized fission products (OSTIS) on neutron guide H23 L.
- SN7: Cold polarized neutron beam on neutron guide H142.
- PN8: Fission product coincidence spectrometer (COSI FAN TUTTE) on beam tube IH1.
- H17: Cold neutron guide: liquid helium UCN-source.
- H18: Cold neutron guide.
- H22: Thermal neutron guide: neutron induced particle emission (H22 D); γ - γ angular correlations (H22 F); neutron induced fission (H22 E).

PN1 FISSION PRODUCT SPECTROMETER "LOHENGRIN"

(H.R. Faust, R. Brissot, I. Gartshore, M. Taylor).

In 1983 the beam tube exchange was performed on LOHENGRIN. The reassembly of the instrument was completed in July and with the resumption of the normal reactor operation the spectrometer has been available again for scheduled experiments.

The shutdown period was used to considerably improve the apparatus. New turbomolecular pumps in both the condenser and magnet section ensure a vacuum better than 10^{-6} torr. The modification of the high voltage system was completed and the stability of both polarities is now approaching the 10^{-6} level.

The new ionization chamber which covers 30 cm of the focal plane was tested. The energy resolution is better than 600 keV and the space resolution along the parabola is better than 5 mm. This detector will be used for measuring fission events with very low cross sections e.g. cold fragmentation in ^{239}Pu fission and yield measurements for fission following double neutron capture.

PN2 BETA SPECTROMETER "BILL"

(K. Schreckenbach, G. Colvin, G. Blanc).

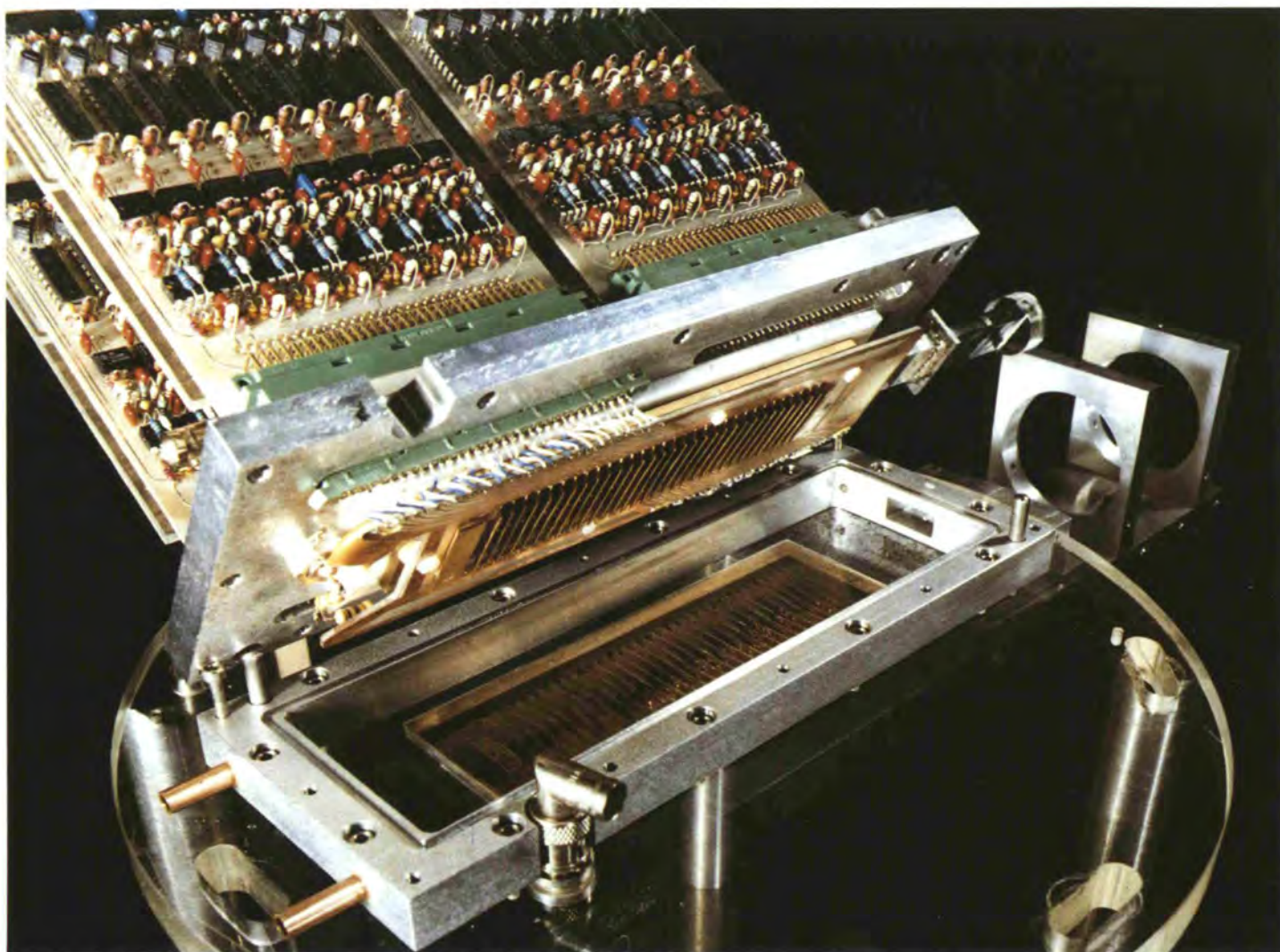
In 1983 the beta spectrometer BILL operated without any major breakdown during the available reactor cycles. Several of the reactor shut-downs were used to study radioactive decays after neutron activation of the sample. In the ^{152}Eu decay intensity standards for electron spectroscopy in the range $300 \text{ keV} \leq E_e \leq 1400 \text{ keV}$ have been established. The intensity response function of the spectrometer, including the electron multidetector, was found to be constant within 5% in this range of energy.

A new 32-wire, position sensitive proportional counter was constructed where the back of the gas cells has been kept open, thus permitting the electrons to enter a common rear-mounted plastic scintillator. The energy dependent signal from the scintillator is used to gate the events in the proportional counter. In this way it was possible to reduce the hall background by an order of magnitude whereas the efficiency was kept at a level of 80% (for $E_e > 300 \text{ keV}$) relative to the ungated mode. The PDP 11 computer at BILL is now linked to the concentrator (PPN) of PN3 and to the central PDP10 computer.

PN3 CURVED CRYSTAL GAMMA RAY SPECTROMETERS "GAMS 1" AND "GAMS 2/3" AND DOUBLE FLAT CRYSTAL SPECTROMETER "GAMS 4"

(H.G. Börner, S.A. Kerr, F. Hoyler, G. Greene, M. Taylor).

The bent crystal spectrometers were operational for most of the reactor time. One cycle was lost due to a mechanical fault in the source changing device. The shut-down period of the reactor was used for an entire recabling of the GAMS 1-spectrometer and for further extension of both the data acquisition and the data treatment systems.



Multi-wire gas counter for detecting electrons in the 45° declined focal plane of the BILL spectrometer. For better illustration the detector box is dismounted from the beam tube and opened. The electrons enter through a slit system and a foil into the detector's 32 chambers (64 chambers have also been tried) where the wires detect the electrons as proportional counters. The rear mounted scintillator (exit visible on the right hand side) gates, with energy sensitivity, the events in the wires.

A new gamma-ray spectrometer (GAMS 4) was installed on the GAMS 2/3 side of the H6/H7 channel. The geometry consists of two flat crystals used in transmission and installed at a distance of ~ 15 metres from the source position. This instrument was developed and used at the National Bureau of Standards (NBS) Washington and was installed as a cooperative effort between ILL and NBS. The spectrometer rests on a 1×2 metre cast iron surface plate which is supported on air cushions for vibrational isolation. The actual crystal spectrometer is a $75 \text{ cm} \times 25 \text{ cm} \times 20 \text{ cm}$ hollow cast iron block

with two precision vertical spindles separated by 50 cm. Gamma radiation is collimated by an entrance collimator, diffracted by the first crystal, passes through an inter crystal collimator, is diffracted by the second crystal, passes through a third collimator and is finally detected. Each crystal axis is equipped with a polarization sensitive angle measuring interferometer which allows angular measurements with a precision of ~ 0.05 milliarc sec. These interferometers are calibrated by summing to closure the external interfacial angles of a 24-side optical polygon.

Precision flat (GAMS 4) and curved crystal spectrometers (GAMS 1, 2, 3) are complementary. They differ considerably in resolution, efficiency and procedures of calibration. The bent crystal spectrometers have lower resolution ($\Delta E/E = 5 \times 10^{-4}$ at 1 MeV in 2nd order of reflection) higher efficiency ($\sim 10^{-7}$), and require *standard* wavelengths in order to establish an absolute wavelength scale. The flat crystal spectrometer is expected to have a resolution of $\Delta E/E \approx 5 \times 10^{-5}$ at 1 MeV in second order, an efficiency of 10^{-11} , and obtains an absolute wavelength scale by use of crystals whose lattice spacing has been determined by very precise combined X-ray and optical interferometry.

PN4 GE PAIR SPECTROMETER

(S.A. Kerr, F. Hoyler)

The spectrometer was operational for 100% of the 1983 reactor time. In order to suppress disturbing background radiation (both from neutrons and gamma rays) in the reactor hall, the spectrometer was enclosed in a concrete housing lined with boron carbide.

A new coaxial intrinsic Ge-detector has been purchased for the single measurements (30% relative efficiency, 1.8 keV resolution at 1.3 MeV). Collimation of the γ -beam has also been improved by adding a lead collimator of continuously variable aperture which allows the reproducible selection of optimum counting rates in the spectrometer. Finally digital gain and zero stabilizers have been included in the data acquisition system.

SN5 ULTRA COLD NEUTRON SOURCE

(P. Ageron, W. Mampe, A. Beynet)

The ultra cold neutron source has been used for the measurement of the electric dipole moment of the neutron (EDM). Improvements in the EDM experiment gave a sensitivity increase of a factor of 2 compared to the earlier version of the apparatus. The total sensitivity of the detection limit is at the old level due to radiation damage of the curved borated glass guide, reducing the UCN-flux. The damaged section of the guide was replaced during the shut-down at the end of 1983. The adjustment of the neutron microscope has been successfully continued and studies for the development of the vertical UCN source have been carried out.

PN6 ON-LINE MASS SEPARATOR FOR THERMALLY IONISED FISSION PRODUCTS "OSTIS"

(B. Pfeiffer, U. Stoehlker)

Considerable effort was put into on-line tests of new ion sources. A source for negative ions had been developed at the University of Giessen. In first tests even the very neutron-rich 0.64 sec. ^{91}Br was extracted. Additionally a heat shield implemented on the surface-ionisation source allowed the extraction of indium isotopes up to mass number 130 as well as samples of ^{80}Ga . For future experiments it is expected that the range of elements directly ionisable at OSTIS can be extended to Ga, Br, Rb, Sr, In, I, Cs, Ba and some rare earth elements.

The modernisation of the separator was continued: A new tape transport system controlled by micro-processors was constructed, and a new correlation table with three detectors developed. The PDP8 based data acquisition system will be replaced by one using a PDP11 and CAMAC interface. The technique used for measurement of coincidences between β -delayed neutrons and γ -rays has been improved.

SN7 POLARIZED NEUTRON BEAM

(B. Heckel, O. Schärpf)

The investigation of the γ -ray asymmetry (A_γ) following neutron capture by protons (ISN, Harvard collaboration) was continued. The year 1983 was devoted to tests of the apparatus with respect to an isotropic γ -source, empty target tests, and calibration. An unoriented radioactive source (^{60}Co) was used to examine the set-up to a level of accuracy of $< 1.1 \times 10^{-8}$. The asymmetry signal due to the empty target was determined as $< 15 \times 10^{-8}$ which, assuming a signal/noise ratio of 10, gives a contribution $< 1.5 \times 10^{-8}$ for A_σ . The calibration was carried out, using ^{35}Cl and yielding $A_\gamma = (-21 \pm 3) \times 10^{-5}$ in agreement with previous measurements. The 32ltr parahydrogen target was filled during November 1983.



The test set-up for the He-4 source on H17 for the production of super-thermal ultra-cold neutrons.



The double flat-crystal γ -ray spectrometer (GAMS 4) installed at the H6-H7 beam-tube by a team from the NBS Washington.

PN8 FISSION FRAGMENT COINCIDENCE SPECTROMETER “COSI FAN TUTTE”

(A. Oed, P.E.J. Perrin, R. Brissot, F. Gönnerwein, E. Aker, P. Geltenbort, T. Manning).

The commissioning of PN8 was delayed by the reactor shut-down and is approximately 2 cycles behind schedule. The spectrometer is now fully assembled and being tested for long term stability. Further improvements on detector performance were achieved, the data acquisition system was made operational and the background problem for neighbouring instruments was largely overcome. The front cover of this report shows a time-of-flight vs. energy correlation matrix for fission fragments from $^{235}\text{U}(n, f)$. The lines coming from top left to bottom right correspond to discrete masses of fission fragments and demonstrate the mass resolving power of the instrument. First experiments on PN8 are just about to start.

SPECIAL BEAM EXPERIMENTS

(P. Ageron, R. Brissot, B. Heckel, F. Hoyler, C. Jewell, S.A. Kerr, W. Mampe, O. Schärpf)

The neutron guides H141, H17, H18 and H22 were used for nuclear spectroscopy, fission and fundamental physics experiments.

At H17 further tests have been carried out using the superthermal ultra cold neutron source installed in 82 (He-4 source). During the reactor shutdown improvements in the cryogenic systems have been effected. Studies of UCN transmission of $(\text{CH}_2)_n$ foils at low temperatures were carried out for the development of high transmission windows in the UCN extraction system.

At H18 the $n\bar{n}$ experiment has been dismantled and shipped to CERN. Currently an irradiation facility for study of biological material is installed.

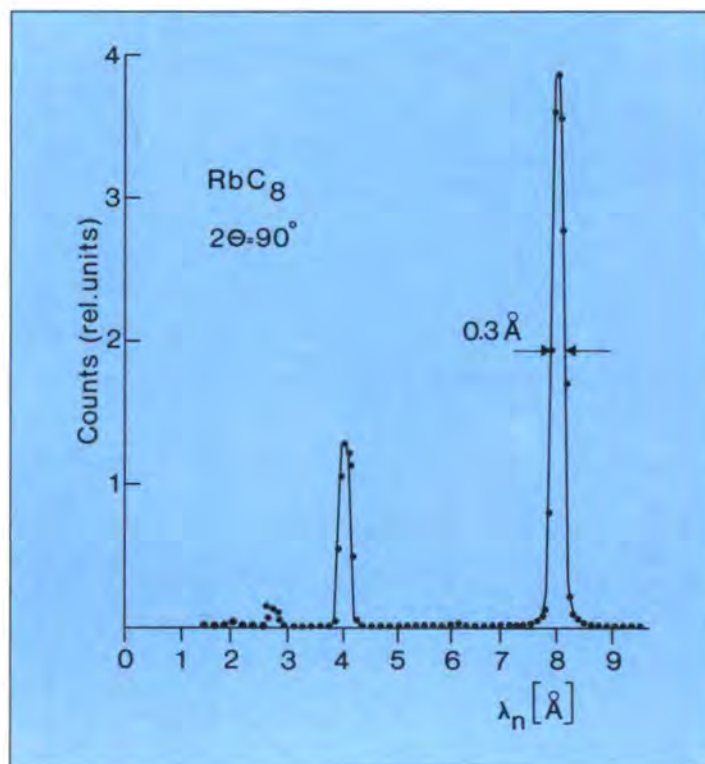
H22D and E were used for (n, α) cross section measurements and fission experiments, respectively. Considerable effort had to be put into the equipment of the H22E site before fissile targets such as Pu were accepted for study in the ternary fission spectrometer “DIOGENES”. On H22F measurements of angular correlations of λ -rays after thermal neutron capture have been continued.

A new secondary monochromatic beam of $\lambda_n = 8 \text{ \AA}$ neutrons was created at the cold neutron guide H141. An intercalated crystal of RbC_8 , 1 cm^2 in size, is used at a Bragg angle of $2\theta = 90^\circ$. Neutrons are guided by a Pyrex tube of 150 cm

length and 1 cm diameter. At the exit of this guide a neutron flux of $10^7 \text{ n cm}^{-2} \text{ s}^{-1}$ is obtained with a beam divergence of $\sim 0.5^\circ$. The energy spectrum was determined by time of flight, showing an intensity ratio of 5: 1 for the 1st to 2nd order of reflection in the RbC_8 crystal (at the exit of the Pyrex guide) (Fig. 41). Impurity peaks contributed to these main peaks by less than 10^{-3} . As soon as it is available a larger monochromator of $3 \times 5 \text{ cm}^2$ will be installed. Amongst the experiments to be carried out at this beam-port will be a neutron lifetime measurement (Annecy, ILL collaboration).

Co-ordinator: H. Börner

Figure 41: TOF spectrum of the monochromatic neutron beam at S52, recorded at the exit of the 10 mm Pyrex guide.



INSTRUMENT GROUP THREE-AXIS SPECTROMETERS

- IN1: 3-axis and beryllium-filter spectrometer on the hot beam-tube H8.
- IN2: 3-axis spectrometer with a double monochromator on the thermal beam-tube H13.
- IN3: 3-axis spectrometer on the thermal guide-tube H24.
- IN8: 3-axis spectrometer on the thermal beam-tube H10.
- IN12: 3-axis spectrometer on the cold guide-tube H142.
- IN14: 3-axis spectrometer on cold guide-tube on second cold source.
- IN20: 3-axis spectrometer with polarised neutron option on thermal beam-tube H13.

INTRODUCTION

In common with the other instrument groups, the three-axis group instrument schedules were disrupted by the problems with the reactor during 1983. There have also been some important changes in the instruments themselves. IN1 is now essentially ready for final tests and routine operation, IN3 has been equipped with a dedicated computer, new electronics and step-motors, IN8 was dismantled to permit the replacement of the H10 beam-tube, and then re-installed, and IN20 is under construction on the test platform in the Hall d'Essais. Only IN2 and IN12 operated normally from the reactor start in August.

The personnel of the group has remained relatively stable with several internal changes. U. Steigenberger became First Responsible of IN1 after the departure of A. Kollmar and

H. Jobic. M. Hagen has joined IN8 as (temporary) Second Responsible; B. Renker has returned to Karlsruhe. During the year, R. Currat took over responsibility for arranging the weekly triple-axis group seminars.

IN1 HOT SOURCE 3-AXIS AND Be FILTER SPECTROMETER

(U. Steigenberger, B. Dorner, H.J. Lauter and P. Cross)

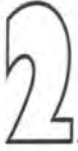
The mechanical installation of the triple-axis instrument on the hot source beam-tube H8 was completed in the summer of 1983. This instrument is equipped with three copper monochromators, (002), (220) and (331), each of which can be individually curved. The first "test" experiment showed that, compared with the "old" IN1, the flux has increased considerably, due mainly to the vertical curvature. There has also been a dramatic improvement in the background. Extensive, detailed tests of the monochromator system, and also of the secondary spectrometer, remain to be carried out.

A comparison has been made between the ILL Beryllium filter and the one on loan from A.E.R.E., Harwell, using the Cu(220) monochromator. Both filters have similar signal to noise ratios but the larger solid angle of the ILL filter produces a higher (absolute) signal. Tests are underway with the A.E.R.E. graphite filter with the aim of producing a new design.

IN2 THERMAL BEAM 3-AXIS SPECTROMETER (DOUBLE MONOCHROMATOR)

(R. Pynn, J. Lynn, P. Flores)

During the last full calendar year before replacement by IN20, IN2 and the venerable CARINE computer functioned reliably. There were no major modifications to this instrument which has operated faithfully since 1972.



IN3 3-AXIS SPECTROMETER ON THERMAL GUIDE

(D. Paul, H.J. Lauter, R. Arthaud)

During the past year there have been considerable changes to the instrument. A dedicated SOLAR 16-40 computer and new motor control electronics have been connected to the spectrometer; the existing d.c. motors have been replaced by step-motors. At the present time the new control program and the positioning of the machine are being tested. It is hoped that the instrument will be available for scheduled experiments early in 1984.

The design of the new monochromator system has been completed and will be constructed in the coming year. This system incorporates P.G. (002) and Cu(111) monochromators, both with variable vertical curvature. It is intended to install this system during the long shut-down in 1984. IN3 now has the option of either a single detector (5 cm diameter) or the multidetector unit (24.1 cm diameter detectors).

IN8 THERMAL BEAM 3-AXIS SPECTROMETER

(R. Currat, B. Renker, C. Vettier, A. Brochier)

IN8 operated for a few weeks during January 1983 prior to the long reactor shut-down. During that period, a new software package was installed and tested, permitting the automatic exchange and alignment of the four vertically focussing monochromators.

The instrument was then dismantled to allow the replacement of the H10 and IH4 beam-tubes. Reassembly work started shortly after the H10 beam-tube was installed in mid-July and continued till mid-October. The first neutron tests of the rebuilt spectrometer took place during the last few days of Cycle 2 and the instrument returned to its normal mode of operation as scheduled, at the start of Cycle 3 (Nov. 8).

During the shut-down, several modifications were carried out:

- (1) Part of the tanzboden floor was replaced.
- (2) New lead shielding elements were installed in the casemate drum. This greatly facilitates the exchange of the drum collimation while not affecting the γ -activity level in the sample area.
- (3) A new motorised sample goniometer with PRECILEC coders was installed; automatic sample alignment will eventually be possible.

No further major changes are planned at present and users may expect uninterrupted operation until Autumn 1984.

INI2 3-AXIS SPECTROMETER ON COLD GUIDE

(W.G. Stirling, K.A. McEwen, D. Puschner)

The detailed design of the new automatic analyser-detector system has been completed and delivery is expected early in 1984. This unit will extend the range of the detector scattering angle and should improve the shielding of the analyser. Tests of an ILL temperature controller, connected to the SOLAR Computer, were carried out during December 1983. The regulation temperature of an ILL "Orange" cryostat can now be changed automatically by the computer, resulting in a more flexible control of the experiment by the user. During 1983, the instrument operated normally with little time lost due to instrument malfunction.

INI4 3-AXIS SPECTROMETER ON COLD GUIDE (SECOND COLD SOURCE)

(W.G. Stirling, W. Kaiser)

Progress has been made with the detailed specifications and preliminary design of this new instrument. A decision has been made to limit the choice of monochromators to two, pyrolytic graphite and either silicon or beryllium. During 1984, the detailed design of the instrument will be carried out and fabrication of the mechanical and electronic elements will be initiated.

IN20 THERMAL BEAM 3-AXIS SPECTROMETER WITH POLARISED NEUTRON OPTION

(R. Pynn, W. Kaiser)

The construction of IN20 on the test platform in the Hall d'Essais continued on schedule. The completed monochromator drum and the support structure of the secondary

spectrometer were installed, cabled and moved under the control of electronic modules similar to those designed originally for IN8B. Tests of the mechanical parts of the spectrometer and of the control of its movements by a PDP 11/24 computer began in November 1983, to be completed early in 1984. The removal of IN2 and its replacement by IN20 is scheduled to begin in February 1984 and should be well advanced before the reactor shut-down foreseen for September 1984. It is hoped to perform the first tests of IN20 with neutrons during the final reactor cycle of 1984.

Co-ordinator:
W.G. Stirling

The new triple-axis spectrometer IN20 set up for testing in the "hall d'essais".



INSTRUMENT GROUP TIME-OF-FLIGHT HIGH RESOLUTION AND DIFFUSE SCATTERING

- IN4: Time-of-flight spectrometer on thermal tube H12.
- IN5: Multichopper spectrometer on cold guide H16.
- IN6: Focussing time-of-flight spectrometer on cold guide H15.
- IN10: Backscattering spectrometer on cold guide H15.
- IN11: Spin-echo spectrometer on cold guide H141.
- IN13: Backscattering spectrometer for short wavelengths on thermal guide H24.
- D7: Diffuse scattering spectrometer on cold guide H15.
- D11: Small angle and diffuse scattering spectrometer on cold guide H15.
- D17: Low-q high resolution SAS on cold guide H17.

INTRODUCTION

The completely rebuilt D7 with polarization analysis is now routinely available. The reconstruction of IN4 is progressing to schedule. The multidetector bank for IN11 is almost completed.

Several other improvements were implemented during the reactor shut-down. These included the installation of extra memories, electronics, computer control and shielding improvements on most of the instruments.

IN4 TIME-OF-FLIGHT SPECTROMETER

(A.P. Murani, W. Langel and A. Key)

During the reactor shut-down from February to August some of the ageing instrument electronics have been replaced; in particular the driving and phasing units for the rotating monochromators as well as those for their linear movements. Instrument tests in September confirmed a markedly improved performance and stability. Subsequently very little experimental time has been lost from causes arising from these sources and the overall performance of the spectrometer has been quite satisfactory. It is also envisaged to replace, in due course, the high tension modules for the He³ detectors received late in the year, to extend the Camac memory to 256 K and to replace the time-of-flight analyzer unit. Besides the electronics replacement a new data acquisition and instrument control programme developed by H. Schwab has also been installed (in parallel with IN5). This permits a greater flexibility and ease of instrument operation and has proved to be quite reliable.

For the future development of the spectrometer, orders for the construction of two choppers on horizontal axes, supported on magnetic bearings, have been given out. One of these will be a heavy steel chopper with 25% duty cycle (on/off ratio) and will have rotation speeds up to 15000 rpm. The second chopper will also be made of steel but will have a smaller diameter and incorporate a 1.5° collimator for fine pulsing of the beam. It is hoped to complete the installation of the choppers before Summer 1984 and to perform tests in the single monochromator configuration before the long shut-down in September 1984.

IN5 MULTICHOPPER SPECTROMETER (TOF)

(F. Douchin, G. Kearley, J.P. Beaufils, S. Jenkins)

Twenty scheduled experiments and three tests were carried out on IN5 in 1983 (6 months of beam-time). The major part (12) were chemical investigations. A beryllium filter in the secondary beam has been successfully tested for intensity gains in quasi-elastic measurements (100% at 6 Å, R. Lechner, HMI). Another successful development in TOF methods is the use of several wavelengths in the incoming beam (2 or 3 choppers) or even white beam pulses (1 chopper) (G. Kearley).

The computer control of IN5 has been thoroughly improved during the six months reactor shut-down. A third terminal can be linked either to the instrument computer or to the general DEC NET of the ILL, facilitating the data reduction and permitting quicker access to all instrument programs and instructions ("Informatic User's Manual").

A completely new acquisition and control program has been implemented (H. Schwab). It is also applicable to IN4 and has the same features and commands as IN6, thus achieving a semi-standardisation of the three TOF instruments. It is fully time-sharing and modular and permits the step-by-step introduction of a completely automatic control of the instrument. A survey program allows for a first stage of remote control. A chopper prototype with magnetic bearings for the full speed range (< 2000 rpm) has been completed at KFA-Jülich. It will be installed on IN5 during the forthcoming long reactor shut-down. In the meantime the chopper electronics have been overhauled and partly rebuilt by a team from ISPRA (Euratom).

IN6 FOCUSSING TIME-OF-FLIGHT SPECTROMETER

(A.J. Dianoux, M. Bée, Y. Blanc)

Despite the long reactor shutdown 23 experiments had been performed by the end of December. The demand for experimental time has increased considerably this year, raising the overload factor to about 4. A sizeable amount of time has been allocated to College 4 for magnetic and crystal field splitting studies.

Some improvements have been implemented during the year:

- The new evacuated sample box with its radial oscillating collimator gives much less parasitic scattering.

- The level of unchopped parasitic neutrons arriving on the detectors has been considerably reduced by improved shielding around the Be-filter and the choppers.

- A new heating and cooling loop using the gas from a liquid nitrogen reservoir offers a continuous temperature range between 90° and 600° K.

- An ILL high precision temperature controller was delivered in October. It has performed with the cryostat, using manual control, very satisfactorily, giving a temperature stability of a few hundredths of a degree. The control by the IN6 computer has already been tested and will be implemented shortly.

IN10 BACKSCATTERING SPECTROMETER

(A. Magerl, C. Poinignon, P. Joubert)

The shutdown period has been used extensively to reconstruct the software system of IN10. Most significant from the users' point of view is the new command structure for making the start-up of an experiment both more transparent and more flexible. The same command structure has been installed at the second backscattering instrument IN13. The speed of the Doppler machine determining the energy window of IN10 is now computer-controlled. A standard option is a continuous change of the Doppler velocity during a run. In this way particular statistical weight can be put on certain parts of the energy spectra.

IN10 has now been adapted to the standard ILL data format. This greatly facilitates data filing and data retrieval. Also the large number of programs for data inspection and data analysis can be used more easily.

A high temperature furnace has recently been put into operation together with IN13. The temperature range, now easily accessible, extends from 1.5 K to 1800 K. It may be extended below 0.1 K by using an ILL orange cryostat with a dilution insert.

IN10 has been running very reliably during the last year. The main topics were tunnelling spectroscopy and high resolution quasi-elastic measurements of both translational and rotational diffusive motions.

IN11 SPIN-ECHO SPECTROMETER

(J.B. Hayter, F. Mezei, B. Sarkissian, J.P. Varini)

Advantage was taken of the reactor shutdown to implement a number of instrumental improvements. The most significant of these was the installation of a multiplexer system which allows the computer to monitor up to 24 instrumental parameters, in particular the currents in the 18 magnet power supplies, *via* a 6-digit DVM.

Design studies on the first phase of the new multidetector assembly were completed and the major components have been ordered. Preliminary tests are scheduled for Spring 1984. The new detector will allow small-angle neutron spin-echo data to be accumulated simultaneously at 23 Q-values, providing a significant gain-factor over the present single-detector system. This will open the way to studies of physico-chemical systems such as polyelectrolytes, which are at present marginal cases because of the low intensity due to unfavourable form-factors.

The scientific programme restarted with its usual vigour as soon as reactor operation resumed in August, and the experimental backlog is being rapidly cleared. In the domain of chemical physics, a feature has been the number of experiments undertaken in conjunction with light-scattering on micro-emulsions and micellar systems near their critical temperatures.

IN13 BACKSCATTERING SPECTROMETER

(I. Anderson, W. Petry, A. Heidemann, J.F. Barthelemy)

The long reactor shutdown was used to make a number of modifications to the instrument, not least of which was the rebuilding of the control cabin requiring a recabling of the electronics. At the same time the number of detector inputs to the computer was increased from 22 to 44, allowing all detectors to be individually counted and removing the need for hardware grouping at the start of each experiment. A Camac module to control a DANA digital multimeter has been installed to allow control of sample environments using any temperature probe.

A floating point processor was installed in the PDP 11/34 computer together with a new double-density disk unit. The control software has been correspondingly updated in conjunction with that of IN10 such that the operation of the two instruments is now similar.

Improvements have also been made to the hardware of the instrument, the main addition being the installation of three small angle angular analysers which are focussed onto 3 detectors mounted close to the incoming beam collimator. A sixth high angle analyser is being constructed which will allow, together with the new hard wiring of the detectors, simultaneous measurement over the whole of the available Q range ($0.5\text{--}5.5 \text{ \AA}^{-1}$). The cooling circuit for the monochromator has been reconstructed and improved by the installation of a vacuum-isolated tube between the cryostat and the furnace. The low temperature limit of the monochromator has been decreased in this way to $\sim -40^\circ\text{C}$ and modifications to the valve control system have rendered the temperature control of the monochromator furnace more reliable. Further modifications are planned for the beginning of 1984, which should further decrease the low temperature limit.

The IN13 sample furnace ($T_{\text{max}} = 1600^\circ\text{C}$) has been delivered and equipped with a turbomolecular pump. Operation of the furnace has been satisfactory, though modifications are under way to connect the turbomolecular pump directly onto the top of the furnace to improve the vacuum conditions.

Realignment of the focussing graphite deflector allowed the nominal flux at the sample, which had been progressively diminishing, to be regained showing some mechanical inadequacies in the present deflector support assembly. A new support system will be installed next year.

The experimental programme on IN13 can be grouped into two categories: tunnelling spectroscopy and quasielastic scattering at high momentum transfer, and although the available beam-time this year has been restricted, some interesting experiments have been performed. Thus an investigation of the tunnelling in manganese acetate down to low temperatures (40 mK) has shown an interesting inverse temperature dependence of the tunnelling lines. Similarly the tunnelling peak in nitromethane has been investigated as a function of pressure up to 5 kilobars. The corresponding shift of the tunnel frequency cannot be explained by simple theories. In the quasielastic scattering domain the study of enzymes has continued and an investigation of hydrogen motion in single crystal Yttrium has been carried out.

D7 DIFFUSE SCATTERING SPECTROMETER

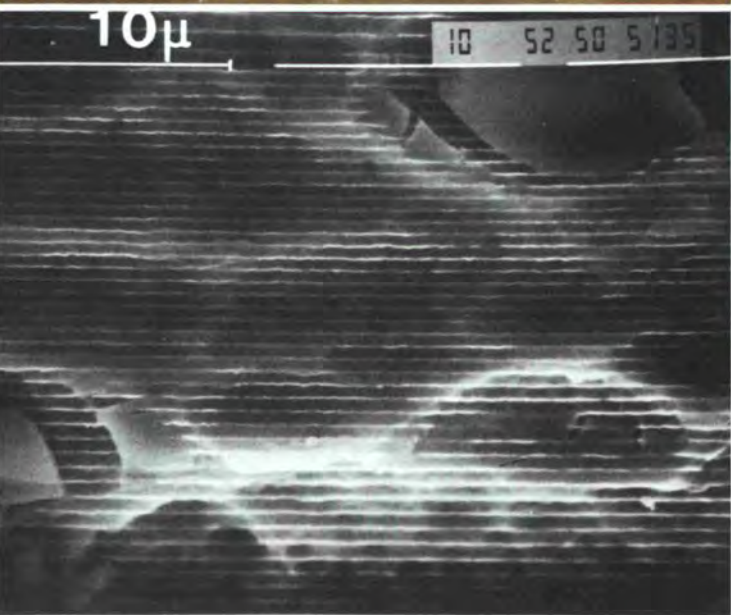
(O. Schärpf, W. Just, R. Rebesco)

During the long shutdown in Spring 1983 the instrument was totally rebuilt. The new monochromator has now ideal neutron beam properties both from a mechanical and an electronic control point of view. The intensity gain by proper focussing in two dimensions is of the order of 4 to 5. Six encoders and 6 step-motors permit the changing of the vertical and horizontal focussing. All adjustments can be implemented via computer control programs with graphical visualization of count-rates and crystal orientation.

The intensities measured at the sample position with gold foil activation are now:

$\lambda(\text{\AA})$	3.1	4.8	5.7
$\Phi = n/\text{cm}^2\text{s}$	1.5×10^7	8×10^6	6.5×10^6

A wavelength change with all adjustments can now be carried out within less than one hour. It turned out, however, that the monochromator shielding will have to be "modified" in order to reduce the interference with other instruments. Following the good experience with the new detector set, all four sets have been built alike. The three horizontal sets can now be equipped with analysers for every second detector.



1

3

2

1. The normal diffuse scattering set-up of D7 in the 4.8 Å position. In the picture it is equipped with a large cryostat and collimator boxes in front of the 64 detectors which are mounted on four separate banks. One bank is mounted vertically, but can be replaced by a horizontal version. A small detector box is also visible containing 16 detectors of 1 cm \varnothing for better Q and TOF resolution (together with an electronic chopper) in a small angular region.
2. Electron microscope image of the cross section of a micro guide produced by the evaporation of 900 layers of 4500 Å aluminium and 500 Å nickel. It is used to strongly deflect neutron beams from their original direction (measured: 40°). Applications of these microguides include polarisers for short wavelengths (0.08 Å–2.5 Å) and for beam curvature over short distances e.g. for use on D17 without loss of the shorter wavelengths.
3. The new small angle analyser of IN13.

Computer-controlled motors for the positioning of the analysers permit an automatic search of the line maximum of the scattered beam. For the movement of the detector banks on air cushions, closed-loop DC motor drives and optical encoders were used. This helps to avoid perturbances caused by the 10 tesla cryomagnet. The central part of the instrument is the sample table. It permits the setting-up of an electromagnet of 1 ton and/or a cryostat, cryomagnet and furnace. The table is rotatable on air-pads encoded with the same closed-loop arrangement. A programmed sample-changer and set-up for the sample rotation is at the disposal of the user. In view of the high reproducibility of the mechanical movements the sample adjustment is not affected by a change of the wavelength setting.

"Microcontrol" optical benches and step-motor drives are available for the adjustment of polarizers, windows, flippers etc. A Be-filter installed outside the shielding can easily be moved in and off the beam. New BASIC programs are routinely operational. They permit an instantaneous check of the results. A new 128 K memory for data storage of TOF with polarization analysis is available. The flux of data has been tremendously increased by the modifications carried out on the machine: the intensity gain of almost 5 by the new monochromators entailed a data flux increase of 10; the doubling of the number of detectors, the storage of data for "spin up", "spin down" and polarization in 3 different directions give another data boost of a factor of 12. For this reason a novel method of data storage has been introduced: a Winchester disk with a capacity of 50 normal disks. Connection with the ILL central computer is ensured.

A new shielding facilitates the task of filling cryostats and furnaces.

D11 SMALL ANGLE SCATTERING SPECTROMETER ON THE COLD GUIDE

(P. Timmins, R. May, R. Oberthür, K. Ibel, J. Torbet, R. Baker)

1983 has seen a number of changes particularly in the automatic control of D11. The change of wavelength is now computer-controlled and may be introduced into a series of measurements with the automatic sample changer. The beam stop is now controlled from the cabin allowing the instrument to be set up more quickly and more easily. The infra-red coding device on the sample changer is being replaced by an optical absolute encoder which should significantly improve its performance.

The exploitation of new sample environments has continued with the building of a stretching machine for cyclic kinetic experiments. The Camac memory has been expanded to 256 K and the acquisition software modified to allow up to 64 time channels together with full 2D information to be used in such experiments.

The scientific program has again been very heavy in 1983 with a particular increase in the number of polymer (chemistry) and material sciences proposals to the detriment of time available for biology.

For the long reactor shutdown of 1984/85 a major modification of the instrument is planned involving a replacement of the current detector tube by a larger one allowing the detector to move on a carriage inside the tube. In addition to allowing a continuously variable sample detector distance of 1 to 38 m this necessitates only one sample position which will be made open and easily adaptable to a range of sample environments. The time for changing detector position should be in the range 1-10 min. It is also envisaged to replace the 10 year old PDP11/40 computer, probably with a VAX 11/730, in order to carry out much more sophisticated on-line data treatment particularly for anisotropic spectra.

D17 LOW-Q, HIGH RESOLUTION SPECTROMETER

(D.L. Worcester, S. Bantle, P. Marie, M. Roth, M. Cruz)

Modifications to the instrument were implemented during 1983 to provide sample-detector distances of up to 3.5 metres, thereby reducing the minimum Q-range to about $3 \times 10^{-3} \text{ \AA}^{-1}$ in small angle scattering experiments. The detector and vacuum chamber, which previously had one fixed support at 2.8 metres, is now fully mobile. Sample-detector distances can therefore be fully optimized for experiments in the low-Q region.

Increasing use of large sample areas resulted in the collimator window being increased in size to 38 mm diameter. Improvements were also carried out on the sample holders and sample changer. A microguide has been developed by O. Schärpf, permitting a beam deflection of 40° on D17 without loss of shorter wavelengths (see photograph).

Several changes of the CAMAC were implemented to standardize the equipment and facilitate positioning of the beam-stop and detector angle, both of which now have digital read-outs.

Co-ordinators: K. Ibel / F. Mezei

INSTRUMENT GROUP DIFFRACTION INSTRUMENTS

- D1A: High resolution powder diffractometer on thermal guide H22.
- D1B: Two-axis diffractometer with multidetector on thermal beam H22.
- D2: High flux 2-axis diffractometer with multidetector on thermal beam H11.
- D2B: Very high resolution powder diffractometer (in preparation).
- D3: Two-axis polarized neutron diffractometer with lifting counter on thermal beam H5.
- D4B: Liquids diffractometer sharing the hot beam H8 with IN1B.
- D5: Three-axis polarization analysis spectrometer on hot beam H4.
- D8: High-flux four-circle diffractometer on thermal beam H11.
- D9: Four-circle diffractometer on hot beam H3.
- D10: Four-circle triple-axis spectrometer on thermal guide H24 (neutron spin echo option).
- T12: Neutron camera on thermal guide H23.
- D15: Four-circle MK6 diffractometer on the inclined thermal beam IH4.
- D16: Four-circle MK6 diffractometer on cold guide H16.
- D19A: 2D multidetector for tests on thermal guide H24.
- D20: High flux multidetector (in preparation).
- S18: Neutron interferometer on thermal neutron guide H25.
- S21: Double crystal diffractometer.

INTRODUCTION

This year the diffraction group was mainly concerned with the necessary exchange of three beam-tubes: H5, H11 and IH4. Four diffractometers (D2, D3, D8 and D15) had to be removed. Owing to the excellent support from many ILL sections, all the instruments in the group are operational again. A new member of the group is D16, which is now equipped with a small two-dimensional multidetector. The new D4B started its routine operation in November 83. The neutron interferometer (formerly D18) has been converted into a special set-up (S18). The experimental programme has been resumed to its full extent with generally improved instrumentation and conditions. The activity of instrument construction was mainly focussed on the H11-project (D2B, D20, D19B), but also some work has been carried out for D9B and a study of the planned transfer of D3 to the hot beam D4 was carried out.

D1A HIGH RESOLUTION POWDER DIFFRACTOMETER

(A.W. Hewat, S. Heathman)

D1A operated for the whole of the reactor time available in 1983, with many users, having only 3.5 days each on average, collecting two or more diffraction patterns per day. This high throughput of experiments, each of which takes perhaps weeks to analyse, meant that the consequences for users of the extended reactor shutdown were minimized. A new rotating sample stick, specially designed for examining the different structures of solid methane, proved very useful for reducing preferred orientation; the programmable temperature controller was often used for such phase transitions. Other interesting experiments included the study of stress in steel welds, the structures and stresses in Nb_3Sn composite superconduction wires, electronic ordering in the $\text{Fe}^{2+}/\text{Fe}^{3+}$ minerals ilvaite and magnetite, conduction mechanisms in Li^+ and H^+ conductors, structure of intercalated zeolites and catalytic metal oxides, phase transitions in molecular compounds and dielectric materials etc. This sustained activity in powder diffraction, which has now been emulated in the US and elsewhere, has resulted in the construction at the ILL of new and better powder diffractometers. Limited manpower in this area will mean that D1A will be phased out of regular operation in 1985, when it will be replaced by D2B. However, D1A will remain available for extended use without ILL support to selected groups.

D1B TWO-AXIS DIFFRACTOMETER WITH MULTIDETECTOR

(J. Pannetier, P. Mangin, A. Dorn)

D1B has continued to work well during 1983. No major changes were made during the last year but the configuration of the instrument (location of the computer and terminals) has been modified to facilitate the treatment of data at the instrument. New computer programs for fast handling and inspection of diffraction data have been developed on the DEC-10; a pseudo-3D plotting program is now available and has been extensively used to visualize chemical reactions, structural and magnetic phase transitions and textures.

D2 HIGH FLUX TWO-AXIS DIFFRACTOMETER WITH MULTIDETECTOR

(J. Bouillot, J. Torregrossa)

At the end of July 1983, the H11 beam-tube was replaced, resulting in a complete dismantling of D2. The rebuilding has been performed very quickly but nevertheless very carefully, so that D2 could go into scheduled operation at the beginning of



September 1983. A new layout of the site was implemented to combine the lowest price (use of the old elements) and the most efficient arrangement (users' convenience) in view of the imminent installation of D20 planned for mid-1985. An oscillating collimator system in front of the multidetector is under way for measurements using sample environments.

D2B VERY HIGH RESOLUTION POWDER DIFFRACTOMETER

(A.W. Hewat, S. Heathman)

D2B will replace D1A, with substantial gains in both resolution and intensity. (High flux reactor beam position, backscattering geometry, large focussing monochromator, 64 detectors covering 160° , high efficiency 5 minute collimators throughout, more powerful computing and electronics systems). While D1A was built with limited finance and resources, D2B is a no-compromise machine based on 10 years' experience. Most of the components have now been bought or made; they will be assembled behind D1A/D1B for test operation at the end of 1983, and scheduled operation on the reactor face in 1985 - together with the new high flux powder diffractometer D20.

D3 TWO-AXIS POLARISED NEUTRON DIFFRACTOMETER WITH TILTING DETECTOR

(F. Tasset, M. Bonnet, K. Ben Saïdane)

Owing to the efficient work of the reactor mechanics the H5 beam-tube liner has been replaced and the corresponding shutter repaired on schedule. This gave plenty of time to rebuild D3 at this position.

One problem arose from the inherent high γ activity of the cobalt monochromator; the removable "cassette" design has proved very helpful enabling us to rebuild all the surrounding parts prior to its installation with no special personnel radiation risks. Consequently the monochromated shielding consisting of "cheap design" concrete blocks was rebuilt with a relatively high degree of precision. This now allows a straightforward change in neutron wavelength without readjusting the orientation matrix. Another important by-product of the better alignment is the good homogeneity of neutron beam polarization. This, together with the outstanding performance of the cryoflipper, ensures excellent ($\sim 98\%$) polarization in both + and - states at every wavelength and without special care.

A further improvement has been the installation of a new pumping line between the Roots unit and the cryomagnet. Despite its large section ensuring a good vacuum of the helium evaporating system it induces no significant torque on the cryostat owing to its original isovolumetric design. It allows easy changing of the diffractometer position and complete freedom of the cryostat rotation. This, together with the application of half shutters of the D15 type permanently attached to the detector slit system, results in a better overall stability of the instrument, allowing more

precise automatic crystal alignment and consequently easier and better data acquisition.

Finally the reliability of the positioning system has been optimized: the Mark VI diffractometer shafts have been checked and renewed where necessary, and new closed loop microprocessor motor drives ("Mumu" ILL system) installed. These changes were entirely satisfactory.

To summarize it should be stressed that the dismantling of D3 during this long shut-down has been an opportunity for solving existing monochromator problems and for improving the overall geometry of the instrument. D3 now offers optimized neutron performances together with easy use. Some problems remain from time to time with the long-term drift of the low sample temperature control ($T < 7$ K) due to the existence of impurities in the liquid helium supply. It is hoped that this deficiency can soon be eliminated by a modification of the cooling system.

D4B LIQUIDS DIFFRACTOMETER ON THE HOT BEAM H8

(P. Chieux, S. Cummings, A. Hawes)

D4B is operational in its standard configuration, i.e. the two 64 cell multidetectors mounted at equal distance from the sample. The instrument has been fully aligned. The new diaphragm and collimator design significantly reduces the background at low angle which is important for multidetector 2θ -scans. The high neutron flux combined with the increase in detection area will allow a statistical precision near one part per thousand to be obtained in many experiments, with roughly the same experimental resolution as on the former D4. Of course this improvement will require a much greater precision in monitoring, multidetector calibration and data corrections. It will take some time before the machine is used to its full capacity.

D5 THREE-AXIS POLARISATION ANALYSIS SPECTROMETER ON THE HOT BEAM H4

(K.R.A. Ziebeck, J. Schweizer, A. Perkins)

During the period in which the reactor functioned D5 was used primarily in the polarisation analysis mode. Approximately 90% of the experiments require polarisation analysis, with the remaining 10% making use of the short wavelengths and the two-axis mode.

Field-changing is now programmable and includes the possibility of switching between vertical and horizontal field configurations. This small innovation has significantly improved the experimental technique employed in paramagnetic scattering experiments. The furnace used for such experiments has been modified to work up to 1700 K.

For single crystal measurements requiring fields up to 17 Koe there is now a variable temperature cryostat available. The new cryostat functions between 1.5 and 300 K and will relieve the heavy demand for the 4.6 T superconducting magnet, for those experiments requiring thermal variation and small fields.

Although 1984 was considered to be the last year in which D5 operated, it now appears that it will continue after the 1984-85 shutdown.

D8 HIGH FLUX FOUR-CIRCLE DIFFRACTOMETER

(G.J. McIntyre, J. Archer, J. Allibon, S.A. Mason)

During the long shutdown the H11 beam tube was replaced by the larger diameter one required for the H11 project. As well, the whole floor surface around D8 was broken up and re-made in preparation for the Tanzboden floor to be laid for the D19 multidetector to be installed at H11 in 1984.

D8 was re-started ahead of schedule in early September thanks to the co-ordinated efforts of many groups. The experiment schedule is particularly tight as the final closing-down of D8 will take place before the long shutdown in 1984 in order to allow realistic tests of the new H11 shielding while neutrons are available.

Cryorefrigerator development is continuing and efforts have been made to improve reliability by improvements to the He compressor and replacement of thermocouples by resistance thermometers. The new four-circle furnace, constructed in Karlsruhe (see D9 report for 1982) has been tested on D8, as has the new standard ILL cryostat controller. In both cases the tests were valuable.

High-quality pyrolytic graphite filters have been obtained for use with a pyrolytic graphite monochromator at 2.36 Å, first on D8, and later on D19.

D9 FOUR-CIRCLE DIFFRACTOMETER WITH SHORT WAVELENGTH

(M.S. Lehmann, W.F. Kuhs, J.R. Allibon, J. Archer)

The instrument has continued to function satisfactorily. During the year the memory of the computer was extended in order to facilitate simultaneous measurement and data reduction coupled with automatic data transfer to the PDP10.

Further tests of the application of a small area detector (bird's eye detector) were carried out. The detector is an Anger-camera and the development work is a collaboration between the Rutherford-Appleton Laboratory, Los Alamos and the ILL. The tests showed that the use of a small detector is feasible, but pointed to severe γ -sensitivity problems.

In the middle of the year the detector arm was rebuilt, and a new module installed for the detector motion. This will allow more flexibility in choosing the detector shieldings. After this a study was made in order to allow the mounting of a two-stage displacer refrigerator on the Eulerian cradle, and a new cradle was ordered towards the end of the year.

Extended tests of the new ILL temperature controller were carried out both during the long shutdown and during the subsequent experiments. They permitted the stability and controllability of the unit to be checked and the parameters for routine operation to be defined.

In connection with the usual development of the cryostats a device for poling crystals has been brought into operation and was successfully used to get mono-domain crystals of ferro-electric materials.

The new monochromator protection which will be the major part of a new instrument, D9B, has been defined, and the offers from industry for the construction have been received. The construction is expected to start in 1984.

D10 FOUR-CIRCLE TRIPLE-AXIS SPECTROMETER

(C.M.E. Zeyen, N. Lehner, R. Chagnon)

The automatic monochromator change became operational this year and will ease the modification of experimental conditions and also reduce frustration for those 4 instruments using the beam transmitted by D10. The full triple-axis software has been extensively used and proved to be very useful in conjunction with the four-circle facility.

Some beam-time was also used on further development of the Triple-Axis Spin-Echo device. Phonon focussing experiments have shown that the present iron-frame magnets are very impractical because of their complicated stray-field pattern. Other types of precession magnets are being envisaged.

D15 FOUR-CIRCLE MK6 DIFFRACTOMETER

(P.J. Brown, S. Wilson, J.M. Reynal)

There is little to report this year since D15 has been out of commission since the last annual report was written. Happily the Lohengrin shielding and the D15 platform have now been reconstructed and re-alignment of the diffractometer is under way. During the period that the instrument was out of commission new motor control modules were installed which should give improved performance.

D16 HIGH Q-RESOLUTION, FOUR-CIRCLE DIFFRACTOMETER IN THE RANGE

$$0.05 \text{ \AA}^{-1} < q < 2.5 \text{ \AA}^{-1}$$

(G. Zaccari, S.A. Wilson, L.F. Braganza, J.M. Reynal)

This year, D16 has become part of the diffraction group. The move reflects the type of work currently being done on the machine. Also, the software philosophy or data collection and treatment is similar to that of other diffraction group instruments. D16 continues to be useful in structural studies which require cold source neutrons, good angular resolution and a large angular range. In addition special environments such as low temperature and high pressure are now being used to study biological structures.

The 2-dimensional multidetector installed last year is working well. Some new features of the instrument include a laser system for sample alignment, encoded motorised slits, a liquid nitrogen cryostat for low temperature membrane studies and a mechanical support system for a hydrostatic pressure cell. An automatic sample changer is being constructed and will arrive next year. Improvements have been made to the software. There is now a new suite of programs for the treatment of powder data and programs for single-crystal multidetector data acquisition and reduction.

D19A FOUR-CIRCLE DIFFRACTOMETER WITH POSITION SENSITIVE DETECTOR

(M. Thomas, R.F.D. Stansfield and M. Berneron)

During the reactor shut-down in early 1983 the ILL's first VAX computer, an 11/750, was installed on D19A. It is remote from the instrument cabin and linked by high-speed data transmission lines. At the instrument site in the guide hall the PDP 11/34 computer controls the instrument, carries out scans of the sample with several Bragg peaks active simultaneously and stores the data prior to transfer. As soon as a scan is terminated the data are automatically transferred to the VAX and reduced to integrated intensities in the regions where Bragg peaks are expected. At the same time a search is made for the presence of extra peaks outside the predicted regions. The results of the analysis are received on a printer at the instrument within a few minutes of the scan being performed.

Software development includes new algorithms for rapid peak prediction in normal-beam geometry and a radically new version of the control program MAD, (formerly LSD), which allows experiments to be performed in equatorial-plane, normal beam or flat-cone geometry.

In late November, experiments were started in earnest, and several experiments on large-unit-cell samples will be performed, in collaboration with outside users, early in 1984.

D20 TWO-AXIS DIFFRACTOMETER WITH PSD AT HIGH COUNTING RATES

(P. Convert, J. Bouillot, J. Torregrossa)

Due to technical difficulties the construction of the ideally suited large multidetector (160° angular range with 0.1° steps) has been postponed. As a first approach for solving these problems it has been decided to equip the diffractometer with an ILL 128-cell PSD (12.8° angular range, ³He gas) which is now almost operational. With this arrangement the "provisional D20" is expected to become operational by mid-85. The decision to build the large "banana detector" can be taken at a later stage and after testing the various possible solutions.

THE H11 PROJECT

The H11 beam-tube liner was replaced in July 1983. The diameter of the in-pile part is now 200 mm, twice as large as the previous one. In the mean-time in order to permit the two instruments D2 and D8 to be reinstalled, the old shutter has been temporarily revised.

The new shielding for H11 was ordered in November 82 and February 83. The delivery is due for the various parts in the period December 83 to March 84. The first part of the shielding will be installed on the site in early Summer 84 to enable a real neutron test before the long reactor shut-down. To be realistic this test needs the complete installation of the various in-beam devices (diaphragms, Soller Slits, monochromators, vacuum lines, etc.). The new shutter, equipped with appropriate collimators and graphite shield, will have to be put in place prior to the shielding.

S18 NEUTRON INTERFEROMETER

(U. Kischko, T. Wroblewski)

Most of the measuring time was used for experiments on fundamental physics. Thus the quantum mechanical laws of transformation in noninertial frames and of spin superposition could be verified. New interferometers for future experiments have been successfully tested. Measurements of several scattering lengths have been carried out.

For 1984 several external users have proposed experiments. We think that they can carry out their experiments without difficulty. Except for some problems with the electronics the instrument is in good shape now.

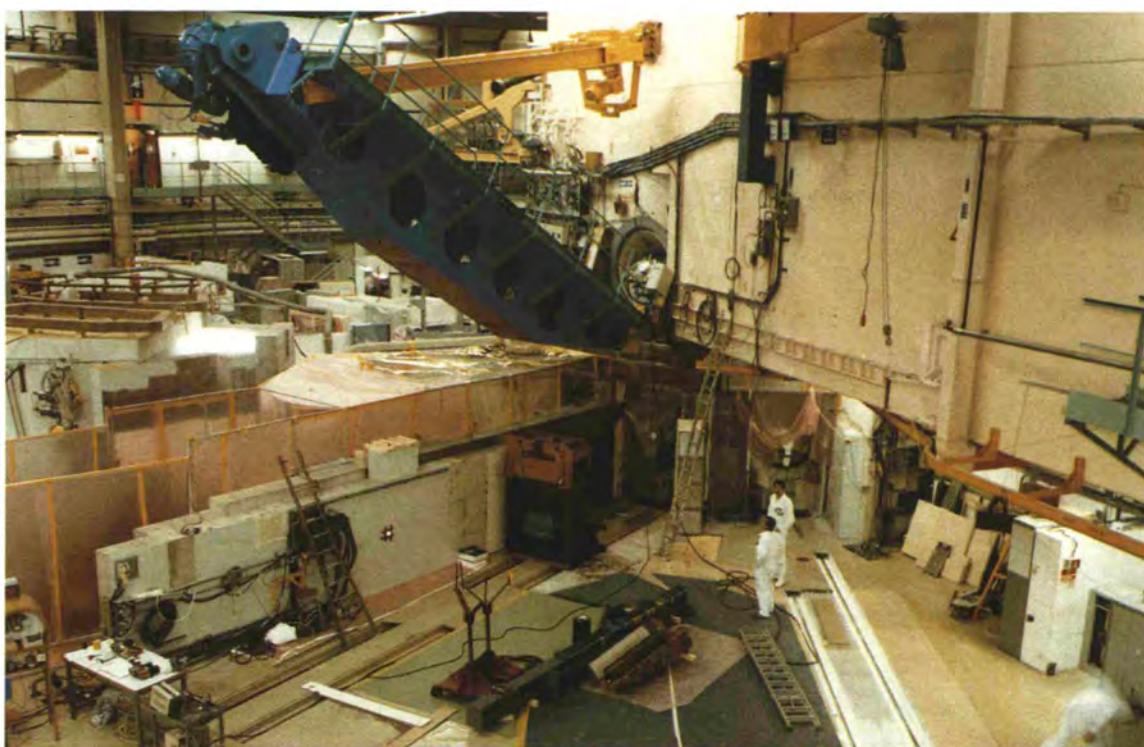
S21 DOUBLE CRYSTAL DIFFRACTOMETER

(C.M.E Zeyen, R. Chagnon)

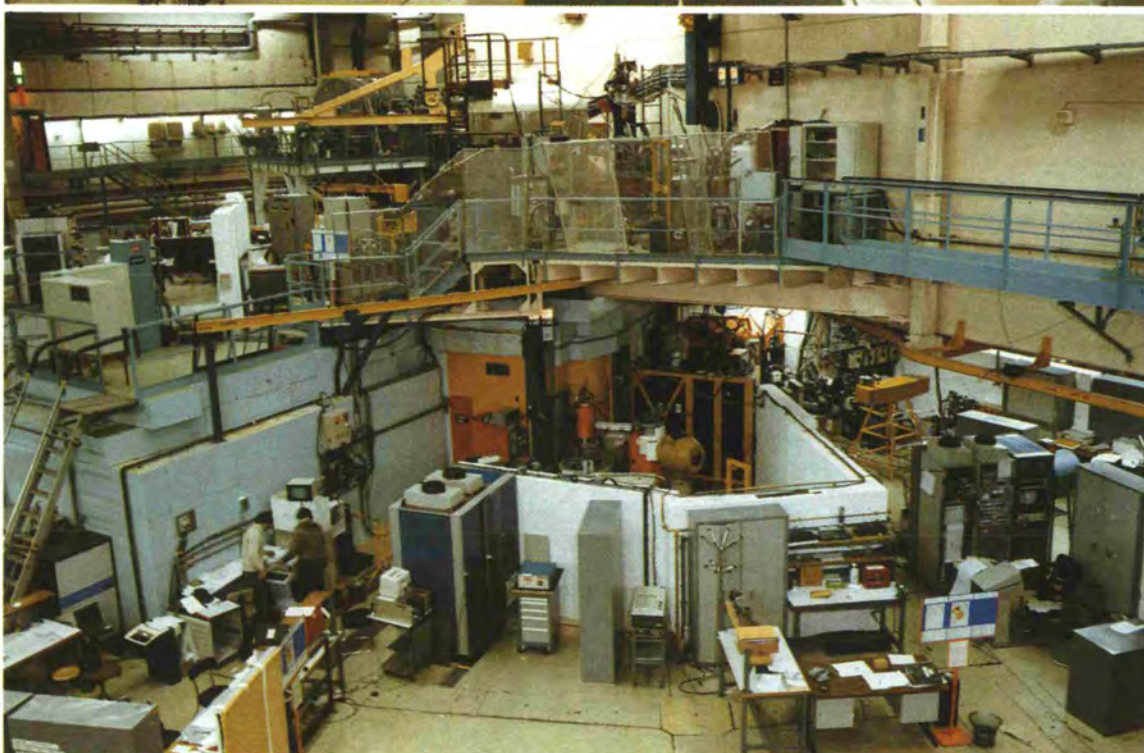
The electronics of this instrument have been replaced this year and the software implementation is currently being completed. A study has been undertaken to install an on-line γ -diffractometer (Ir¹⁹² source) which will allow simultaneous determination, on the same crystal, of lattice constant variations and rotations of lattice planes due to shear for example. The γ -diffractometer should be operational by early 84 and measurements are planned to study such effects as electrostriction or magnetostriction around certain structural phase transitions.

Fundamental physics experiments on dynamic effects in neutron optics and spin interactions will also be initiated.

Co-ordinator: F. Tasset



The zone around the beam-ports H10-H11-TH4 during the reactor shut-down (above) and after the reassembly of the instruments and associated equipment.



3

**EXPERIMENTAL ACTIVITIES
IN 1983**

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**WORKSHOPS
AND CONFERENCES**

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PUBLIC RELATIONS

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**SCIENTIFIC COORDINATION
AND PUBLIC RELATIONS OFFICE**



3

The Office has 3 main tasks:

- Coordination and management of the experimental programme.
- Organisation of ILL workshops and conferences.
- Public Relations.

Prior to the start of the routine operation of the new D4 the machine was thoroughly tested. In the picture is P. Chieux who makes final checks of the equipment.



EXPERIMENTAL ACTIVITIES IN 1983

Due to the continuing implementation of the reactor renewal programme only 3 reactor cycles were possible during 1983. Technical difficulties concerned with the removal of the accessible part of the D_2O suction nozzle prolonged the shut-down until 8th August thereby considerably reducing the neutron beam-time available for the scientific programme. Consequently, the considerable back-log of experiments arising from the two previous Scientific Councils of October 1982 and March 1983, had to be compressed into the remaining reactor time up to April 1984 and to avoid further congestion no sub-committee meetings were held in October 1983. Exceptionally, a dead-line of 1 December 83 was imposed for a further submission of proposals; sub-committee meetings in February 84 will decide on the allocation of beam-time until the end of that year and the commencement of the long reactor shut-down to complete the remaining work still outstanding under the renewal programme. (A record number of 640 proposals were received for adjudication bringing to over 5300 the number of experimental submissions which have been made during the last 5 years).

The instrument availability during 1983 is given in the following:



The impressive poster board of SCAPRO for scheduled experiments.

TABLE 5

Beam-time Allocation and Instrument Statistics

Following the long shut-down which commenced on 1 February 1983 the reactor operated for 107 days, the first 19 days of which were devoted to instrument re-commissioning.

For the period 1st January 1982 to 1st February 1983, the relevant allocations and statistics can be found in the Annual Report 1982 (page 25).

Instrument	Scheduled Operating Time (days)	Coll. 3	Coll. 4	Coll. 5	Coll. 6	Coll. 8	Coll. 9	Instrument test, experiment change-over and minor repairs	Comments
IN1 (3-axis)	20		20					6	Time-sharing BeF + D4
IN1 (BeF)	13				5		8	5	Time-sharing 3-axis + D4
IN2	66		48		11		7	22	
IN3	60		42		4		14	28	Installation of dedicated computer
IN4	70		23		14		33	18	
IN5	72				15	5	52	16	
IN6	69		31		10	7	21	19	
IN8	66		52		14			22	
IN10	68				19		49	20	
IN11	72		27		7	13	25	16	
IN12	66		50		16			22	
IN13	67				7	7	53	21	
D1A	65			60	4		1	23	
D1B	66			32	9		25	22	
D2	72			19	41		12	16	
D3	65			65				23	
D4	35				35			9	Time-sharing 3-axis + BeF
D5	75		29	46				13	
D7	44		17	8	12		7		26 days backlog from instr. rebuild
D8	63			63				25	
D9	68			68				20	
D10	39			39				49	N.S.E. feasibility tests
D11	72			9	6	24	33	16	
D15	30			30				58	Re-installation of instrument after beam-tube changes
D16	58						36	22	Mono. tests, detector checks and programming
D17	75			3	12		38	22	
PN1	60	60						28	Machine adjustments after re-construction
PN2	71	71						17	Mag. field and detector calibration
PN3/4	80	80						8	
PN6	88	88						0	
PN8	88	88						0	Instrument commissioning experiments

During 1983 it was decided that 5 reactor cycles could be made available in the following year and these are as follows:

Reactor Cycles 1984

Cycle 1-84 3/1 1984 8°°h - 16/2 1984 8°°h
 Cycle 2-84 28/2 1984 8°°h - 12/4 1984 8°°h
 Cycle 3-84 24/4 1984 8°°h - 7/6 1984 8°°h
 Cycle 4-84 19/6 1984 8°°h - 2/8 1984 8°°h
 Cycle 5-84 14/8 1984 8°°h - 27/9 1984 8°°h

A further aspect of the scientific activity is in the area of special beam experiments and although they were limited in the same way by constraints on the period of reactor operation, opportunity was taken to either rebuild or improve the often considerable experimental set-up: Table 6 shows the experiments that were either completed or in progress.

TABLE 6

Special Beam Experiments carried out, in Progress or under Preparation during 1983

Experiment No.	Beam Position	Proposed by	Title	Time Allocated
3-07-007	H142	Univ. Heidelberg	β -decay of polarized and unpolarized neutrons	3 cycles
3-07-006	H142	ISN, Harvard	Further search for parity violation in neutron-proton capture	4 cycles
7-04-008	H16	Berlin, Munich	Determination of range profiles and lattice positions	long-term
	H17	R.A.L., ILL	Commissioning of superthermal UCN source	2 cycles
8-08-11	H18	Rouen Univ., Uppsala, CENG	Boron-labelled probes in physiology and oncology	30 days
01-003	H21	Braunschweig	Experimental determination of h/m	long-term
3-13-49	H22	CEN-Mol	Systematic studies of n-alpha and n-fission reactions	77 days
3-13-51	H22	Darmstadt, Bordeaux	Multiparameter measurements of light charged particle-associated fission	60 days
7-03-232	H24	Stuttgart	Macroscopic and microscopic thermal expansion studies	2 cycles
7-04-005	H25	Munich University	Concentration profiles by (n, γ) and (n, p) reactions	long-term
	H25	Marburg University	In-beam NMR	long-term
	H25	Dortmund University	Neutron interferometry studies	long-term
	IH3	Sussex Univ., Harvard, Munich	Magnetic neutron bottle	long-term
	IH3	Sussex Univ., Harvard Univ.	Search for the EDM of the neutron	long-term
3-05-033	IH3	T.U. Munich	Test of neutron microscope	2 cycles

WORKSHOPS AND CONFERENCES

The Office organised 2 workshops in 1983: (1) on "3d Metallic Magnetism" together with K. Ziebeck and D. Givord (CNRS) on 25 and 26 March 1983, (2) on "The Use of Neutrons in Applied Chemistry" together with J. Hayter and J.P. Beaufils from 27-28 October 1983. A third workshop on "Reactor-based Fundamental Physics" was organised by F. Gönnewein from 7-10 November 1983 in collaboration with the Secretary of the German Co-Director. All three events have been a considerable success.

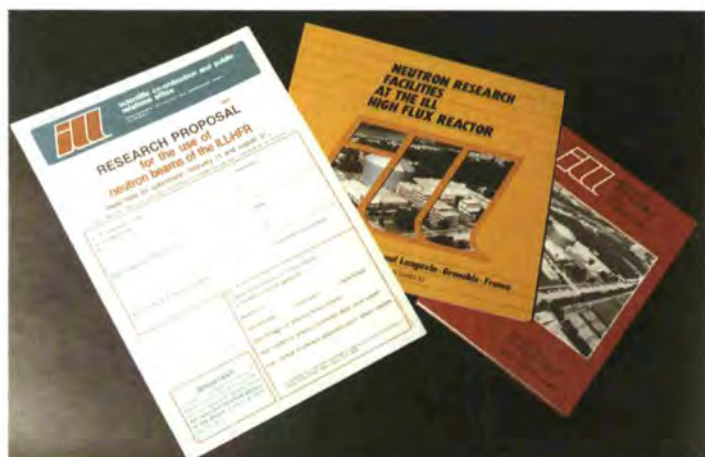
In 1984 the Office will organise the following workshops:

- (1) "Sample Environments", 13-14 February 1984 (Responsible: C. Vettier).
- (2) "Semiclassical Methods in Nuclear Physics", 5-8 March 1984 (Responsible: R.W. Hasse, ILL; P. Schuck, ISN).
- (3) "Water", 16-18 April 1984 (Responsible: A. Dianoux, P. Chieux, ILL; J. Teixeira, LLB Saclay and G. Zaccari, CNRS-Grenoble).
- (4) "Powder Diffraction", 2-3 August 1984 (Responsible: A. Hewat).

In 1985 an International Conference on "Structure of Non-Crystalline Materials", (Responsible: C. Janot) will be held at the ILL from 8-12 July.

PUBLIC RELATIONS

The Office is also responsible for ILL Public Relations and has edited a new brochure "ILL Neutron Beam Facilities Available for Users" (January 84 edition). In addition, the brochure "Guide-lines and Regulations for Reactor Users, Long-Term Visitors and New Scientific Staff" was compiled together with the Translation Office. This is the first document of its kind, giving information on the ILL infrastructure and will be available in April 1984.



1. One major activity in 1983 of the Scientific Coordination and Public Relations Office was the compilation of two new brochures.

2. The organizing committee for the Workshop on "Water" at work. From left to right K. Mayer-Jenkins, A. Dianoux, G. Zaccari and P. Chieux).

4

INSTRUMENTS AND METHODS

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GENERAL SERVICES

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The construction of the new (second) guide hall extending from the SW direction of the reactor hall was started in Autumn 1983 and is expected to be completed in Summer 1984. ▶

TECHNICAL DEPARTMENT



4

Introduction

From 1 January 1983 the Technical Department has had a dual function. The first of these - the Department of Instruments and Methods - with the aid and advice of several scientists, consists of supporting and continuing past efforts in the field of equipment to develop measuring methods with neutrons (monochromators, high performance choppers, multidetectors sensitive to the position of the neutron detected, neutron optics etc.).

The department assists the Directors in the best utilisation of the limited funds devoted to special beams and instruments (the majority of the time under contracts with laboratories or universities).

Finally the DIM is required to raise to the best possible level, or to maintain at this level, the facilities of the ILL for the technical design and construction of experimental instruments to be made available to visitors. This is the function of the Mechanical Construction and Electronics Groups.

In 1983 many projects were associated with the long reactor shut-down, including the beam-tube replacement programme, which necessitated the dismantling and reinstallation, followed by the commissioning of various instruments (IN8, D2, D8, D15, PN1), or gave the opportunity for major modifications,

as on D7 or IN3, which was separated from the former CARINE control system.

Under new instruments, the following may be mentioned:

— Commissioning of IN1B, D4B, D7B

— Assembly of IN20 in a test position permitting the continued scientific operation of IN2 (more than 6 months were thus gained), and at the same time guaranteeing the best conditions for final assembly on the site (anticipated gain approximately 3 months).

— Finally a new evaporator for the production of supermirrors was commissioned in 1983, while work has started on the construction at ILL of a workshop for the production of multidetectors.

The second function, General Services, is the preventive or corrective maintenance to keep in an operational state all the technical installations or buildings apart from the reactor. This function is covered by the Building Services and Maintenance Group and its various workshops, which also provide support for new projects and for the infrastructure at experimental instruments.

Einleitung

Seit 1. Januar 1983 sind der technischen Abteilung zwei Aufgabenbereiche zugeteilt worden.

Der erste Aufgabenbereich besteht darin, die Abteilung "Instrumente und Methoden", mit Unterstützung und Beratung durch verschiedene Wissenschaftler, die bisher unternommenen Anstrengungen auf dem Gebiet der Instrumentierung aufrechtzuerhalten und weiterzuführen, um Messmethoden mit Neutronen weiterzuentwickeln (Monochromatoren, Hochleistungschopper, ortsempfindliche Multidetektoren, Neutronenoptik...).

Die Abteilung unterstützt die Direktion bei der bestmöglichen Nutzung der begrenzten Mittel für Neutronenstrahlen und Spezialinstrumente (grösstenteils im Rahmen von Verträgen mit Laboratorien oder Universitäten). Schliesslich hat die Abteilung dafür zu sorgen, dass die bestmögliche Nutzung der Mittel, über die das ILL verfügt, erreicht oder gehalten wird, um die Experimentiereinrichtungen technisch zu entwickeln und herzustellen. Dies ist Aufgabe der Gruppen Konstruktion und Elektronik.

Viele Arbeiten mussten 1983 in Zusammenhang mit dem längeren Reaktorstillstand vorgenommen werden. Das Erneuerungsprogramm für die Strahlrohre erforderte den Ab- und Wiederaufbau, sowie die Wiederinbetriebnahme zahlreicher Instrumente (IN8, D2, D8, D15, PN1) und bot eine gute Gele-

genheit zu grösseren Änderungen wie an D7 oder an IN3, welches vom alten Kontrollsystem CARINE getrennt wurde.

Im Bereich der neuen Instrumente ist folgendes zu erwähnen:

Inbetriebnahme von IN1B, D4B, D7B.

Aufbau des IN20 in der Versuchshalle, wodurch gleichzeitig der weitere Betrieb von IN2 ermöglicht wird (mehr als 6 Monate wurden somit gewonnen) und wobei gleichzeitig die besten Voraussetzungen für die endgültige Montage am Reaktor garantiert werden (erwarteter Zeitgewinn: 3 Monate).

Ausserdem wurde 1983 eine neue Aufdampfanlage für die Produktion von Superspiegeln in Betrieb genommen und die Bauarbeiten für die Werkstatt zur Herstellung von Multidetektoren wurden begonnen.

Der zweite Aufgabenbereich, Allgemeine Technische Dienste, betrifft die Gewährleistung der Funktionsbereitschaft durch Routine- und Bedarfswartung an allen technischen Einrichtungen oder Gebäudeinstandhaltung ausserhalb des Reaktors. Dieser Aufgabenbereich wird durch den "Service Aménagement Entretien" und seine verschiedenen Werkstätten erfüllt, die darüber hinaus für die neuen Projekte und die Infrastruktur der Experimentiergebäude zuständig sind.

Introduction

Depuis le 1^{er} janvier 1983 le Département Technique s'est vu confier une double mission.

La première, avec le Département Instruments et Méthodes consiste, avec l'aide et les conseils de plusieurs scientifiques, à soutenir et poursuivre sur le plan des équipements les efforts accomplis dans le passé pour développer les méthodes de mesures avec neutrons (monochromateurs, machines tournantes de hautes performances, multidétecteurs sensibles à la position du neutron détecté, optique du neutron...).

Le Département aide la direction pour le meilleur emploi des moyens limités consacrés aux faisceaux et instruments spéciaux (la plupart du temps dans le cadre de contrats avec des laboratoires ou universités).

Enfin, le DIM est chargé de porter à leur meilleur niveau possible, ou à maintenir à ce niveau les moyens dont l'ILL dispose pour concevoir techniquement et réaliser les dispositifs expérimentaux qui seront mis à la disposition des visiteurs. C'est le rôle des services de construction mécanique et électronique.

De nombreuses interventions ont été liées, en 1983, à l'arrêt prolongé du réacteur dont le programme de remplacement des doigts de gant a exigé le démon-

tage et le remontage, puis la remise en route de nombreux instruments (IN8, D2, D8, D15, PN1), ou a offert l'opportunité de grosses modifications comme sur D7 ou sur IN3, qui a été séparé de l'ancien système de contrôle CARINE. Dans le domaine des nouveaux instruments, on peut citer:

Mise en service de IN1B, D4B, D7B.

Montage en plate-forme de IN20 permettant à la fois le maintien en fonctionnement scientifique de IN2 (plus de 6 mois ont ainsi été gagnés) tout en garantissant les meilleures conditions pour le montage définitif sur le site (gain attendu = 3 mois).

Enfin un nouvel évaporateur en vue de la production de supermiroirs a été mis en service en 1983, tandis qu'un chantier a été ouvert pour la réalisation à l'ILL d'un atelier pour fabrication des multidétecteurs.

La deuxième mission, de Service Général, concerne le maintien en état de fonctionnement par entretien préventif ou correctif de toutes les installations techniques ou bâtiments hors réacteur. Cette mission est assurée par le Service Aménagement Entretien et ses différents ateliers qui apportent en outre leur support aux projets nouveaux et à l'infrastructure des sites d'expériences.

INSTRUMENTS AND METHODS

CONSTRUCTION AND MECHANICAL MAINTENANCE

This group has also seen various changes.

Personnel: The retirement of 2 employees in the Assembly and Workshop Groups permitted the recruitment of a German technician and a British turner.

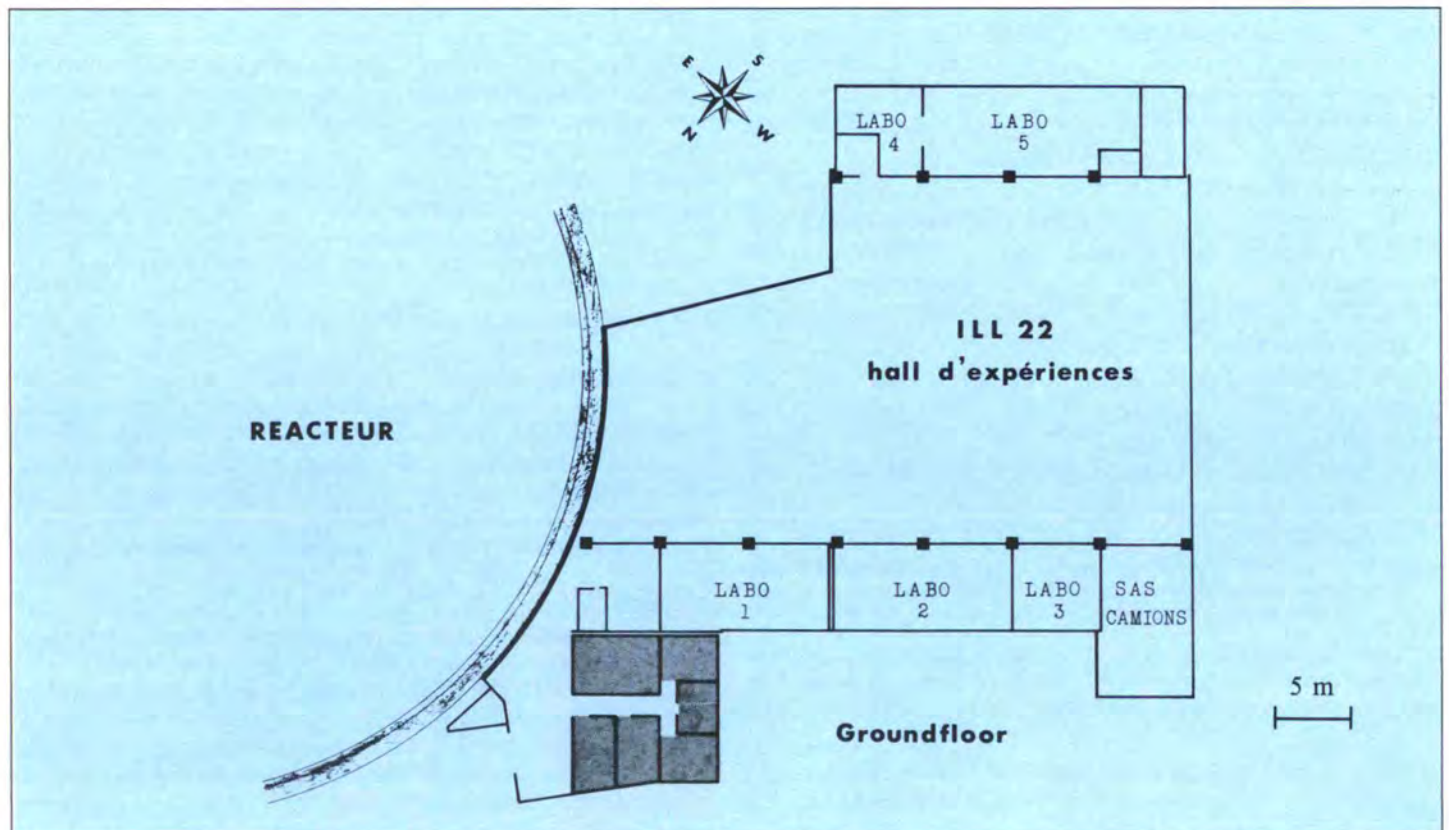
Design: The Drawing Office has specified the secondary items for the spectrometers D19B, D2B, D20, IN20. The studies for the equipment of instruments IN1B, D4B and IN1Be, which were completed during the first half of the year, permitted their experimental start-up. The additional equipment for D7B with its prototype chopper on air bearings has also been completed.

For 1984 the invitations to tender for the IN4B choppers, shielding for D9B, and small angle spectrometer D11C should make it possible to place the contracts with industry at the beginning of January 1984.

Production: The sub-contracting group has forwarded 218 specifications to industry, including an increasing number in the United Kingdom. The Workshop Group has dealt with 190 specifications, mainly for the reactor and the equipment of instruments with sensitive characteristics.

Assembly and tests: The activity of this group covers the measurements and checks required by the reactor in parallel with the commissioning of instruments IN1B, D11B, IN1Be, D7B. In addition, the complete assembly on the platform of the spectrometer IN20 with electronic cabling and tests should result in a gain of at least 3 months on the duration of installation on site (planned for Spring 1984).

The special products laboratory, with the specific aim of producing neutron-absorbent materials for the construction of neutron shielding or collimation, has recently been reinstalled in a more suitable area and its equipment has been improved.



The picture shows the ground floor of the second guide hall. The hatched areas are offices. The first floor will house one additional lab and 20 more offices.

ELECTRONICS

The work is divided into 3 groups, which work relatively independently.

The group responsible for all the triple-axis spectrometers had a particularly difficult year in 1983, as the majority of these instruments were subjected to major modifications at the same time.

IN1B and its analyser with Beryllium filter started their scientific programme in Autumn 1983.

IN8 was completely dismantled to permit the replacement of beam-tube H8, and also restarted in the autumn.

IN3 was finally disconnected from the CARINE system and connected to a Solar computer. On this occasion, new control electronics based on the solutions adopted for the other triple-axis instruments were installed.

However IN2 will not require any work, as its replacement IN20 has been assembled, connected and tested on a test platform away from the future site of the instrument.

In the triple-axis field a considerable effort is still required to ensure complete homogeneity of the instruments, including IN12. This will be the main subject of our reflections in 1984.

The group dealing with the majority of the time-of-flight instruments and in general with the high rate data acquisition from the multidetectors has carried out:

- the reconstruction of PN1
- the commissioning of the rebuilt D4B and the improved D7B (adoption of the "tanzboden" and extension to 64 detectors)
- replacement of the control electronics of the IN4 choppers in connection with computerisation of this type of control
- the standardisation of the CAMAC controllers on PN1, IN4, IN5, D7, D11, D17 and D19
- the design and construction of a data acquisition system by MACAMAC for the prototype of D20 with a 128 cell detector
- finally this group undertook a study of the possibilities of a future replacement of this CAMAC standard in the fields where this now imposes intrinsic limits

The third group, currently more oriented towards automatic controls (of movement, or of experiment parameter, such as temperature or magnetic fields) has done replacement or improvement work on PN2, PN3, IN10, IN11, IN13, S3A, S3C, S21, D3 and D8.

It has also undertaken the design and construction of the biology diffractometer DB21, to be built in collaboration with EMBL, which should be designed and built in one year and tested with neutrons during 1984.

MONOCHROMATORS

Instruments:

D 13A: Neutron double-crystal diffractometer on thermal guide H24.

D 13C: Neutron double-crystal instrument on thermal guide H23

LI 2A: X-ray double-crystal diffractometer

LI 2B: X-ray orientation unit

LI 3: Gamma-ray diffractometer
Laboratory for crystal preparation.

Status of the Instruments

D13 A has the advantage of high flexibility because of the easy monochromator change, even during experiments, due to its large angular range. Thus D13 A is suitable not only for sample orientation and routine tests of mosaicity and crystal reflection properties but also for short diffraction experiments in connection with more extended studies on other instruments. This year these possibilities and the rapid access were also appreciated by many users. In addition to the set of perfect monochromator crystals several mosaic crystals are now available for cases where more intensity is needed. A small programme permits automatic setting of the detector, ω and ω - 2θ scans and the calculation of peak position, reflectivity and width. All important movements are now equipped with encoders.

D13 C had the highest number of instrument days in 1983 because it had been transferred to the CENG's Siloë reactor at the beginning of the ILL's neutronless period. Thus it was possible to continue the monochromator production with only minor delays. The assistance of our colleagues of the CENG Neutron Diffraction Section is gratefully acknowledged. D13 C was almost exclusively used for crystal tests and monochromator assembling.

The X-ray double-crystal facility LI 2A is being rebuilt and will use the same air cushion technique as do neutron instruments but on a smaller scale. The main reason for this major modification is the future preparation of beryllium monochromators. The very small absorption of X-rays by this material permits the bulk of rather thick crystals to be topographed as with neutrons but faster and with better resolution. Be monochromator assembling will also be carried out on LI 2A so that the whole production process will be neutron-independent. A further application of LI 2A may be the testing and development of large perfect crystals for X-ray monochromatisation.

The gamma-ray facility LI 2 was completely rebuilt during 7 months of this year. Two γ -ray sources, ^{198}Au and ^{137}Cs , are housed in a separate building and deliver γ -radiation to five independent diffractometers. The somewhat lower flux of the Cs radiation ($\gamma = 0.0187 \text{ \AA}$) is compensated for by the permanent availability of the source: its half-life is 30 years compared to 2.7 days for Au. In addition, the reflectivity of thick Cu and Ge crystals is higher for 0.0187 \AA than for the 0.0301 \AA radiation of Au because of less absorption which is also of advantage when environmental cells are used. On the other hand, Au is preferable for high resolution and small samples, so both sources are complementary. The first diffraction unit accommodates the Bridgman furnace for in-beam controlled growth of big copper crystals which just produced its first monocrystalline ingots. The second diffractometer is mainly used for in-beam plastic deformation at high temperatures producing the desired mosaic spread. The third and fourth units are intended for both monochromator testing and physics experiments with high and medium resolution, respectively. The fifth diffractometer has been installed by the crystal growth laboratory of the LETI/CENG but is, for part of its time, also available for ILL users. Three of the five units are computer-controlled.

Monochromator production and development

The production team has been reinforced in 1983 by the recruitment of one more technician. Most of the time and effort was spent on the construction of the huge IN1/D4 monochromator unit consisting of three composite crystal systems (Cu 200, 220 and 311), vertically focussing with variable curvature. A total of 165 crystal plates of uniform and anisotropic mosaic spread were produced and assembled to 33 slabs by soldering. They cover a surface of 1200 m^2 and weigh about 10 kg. For the first time, the transfer of the lamellae to the mechanical support was carried out without direct control of orientation by neutron diffraction. The excellent results of tests performed later on IN1 confirm the high precision and reliability of the new transfer technique which avoids the problem of mounting the big and heavy IN1 monochromator unit on D13 C. The preparation of the four-monochromator device for IN20 including a vertically focussing Heusler alloy polariser went on, as well as the production of a 30 cm high focussing Ge monochromator for D2 B. The doubly focussing pyrolytic graphite monochromator of the instrument D7 has been replaced by an improved system which completely satisfies the precision, reproducibility and stability required for beam definition.

An intercalated, highly oriented, pyrolytic graphite monochromator (IHOPG) $50 \times 30 \times 2 \text{ mm}^3$ in size has been produced for the biology diffractometer DB21. This RbC_8 compound enclosed in a thin-walled quartz container has a lattice spacing of 5.65 \AA and gives a peak reflectivity of 70% for 8 \AA neutrons at a mosaic spread of 2° . Its high transparency for other than Bragg-reflected neutrons permits the transmitted beam to be used at other instruments. The production of mixed $\text{K}_{1-x}\text{Rb}_x\text{C}_8$ compounds for a focussing composite monochromator with an 8% variation in d-spacing is under preparation. These developments are carried out in conjunction with the Ecole d'Electrochimie, INPG, Grenoble-St-Martin d'Hères. A new type of filter for reducing higher order contamination has been developed because for wavelengths $\lambda \geq 8 \text{ \AA}$ the $\lambda/2$ neutrons are outside the Be filter range. This HOPG multicrystal system can be used as an efficient and tunable $\lambda/2$ filter also for the range $2.4 \text{ \AA} < \lambda < 8 \text{ \AA}$.

The excellent results reported last year on the growth of high quality beryllium crystals in the newly constructed mirror furnace at the Max-Planck-Institute for Metals Research, Stuttgart, are reproducible. Several oriented specimens of about 1 cm^2 cross-section and 5 to 10 cm length have been prepared and currently serve for the construction of a new monochromator for D9. While the problems of crystal growth and the subsequent production of any desired mosaicity by means of plastic deformation have finally been solved, the bottleneck for routine production is purification, because the high purity feed material is no longer commercially available. Zone refining is possible but needs time and additional investment. After many years of development the ILL now has asked all potential users for participation in a common Be project. At present there is a fair chance that a large number of Be crystals will be produced in the near future.

Following up the Jülich conference on beam-defining devices where the need for closer collaboration and better information was confirmed (and on the occasion of the 10th anniversary of the ILL's monochromator group) several specialists were invited to a discussion meeting on neutron monochromators. The subjects discussed were: the present state of material development, strongly bent perfect crystals compared to mosaic crystals, the understanding of diffraction mechanisms in monochromator crystals, and the development of computer programs calculating intensity and resolution taking into account crystal diffraction properties.

Co-ordinator: A. Freund

4

MULTIDETECTORS

Considerable effort was applied, during the reactor shut-down, to the assembly, testing and recommissioning of the instruments IN4 (400 detectors), IN8, D2, D3, D8 and D15, and to the checking and adjustment of the 1200 detectors of IN5. In addition, during the same period, we carried out the final installation work for the instruments on beam-tube H8: IN1 (multiwire detector), IN2B and D4B (2 multidetectors at 15 atmospheres helium). Commissioning of 32 additional detectors on D7 and 5 on IN13, finishing work and neutron testing of the replacement multidetector for D11.

There was also a variety of work on the 8000 cell multidetector of D19 with tests on site to make it available to experimentalists. Complete tests on the multidetector D20 were carried out with a view to acceptance at the beginning of 1984. A replacement 1024 cell multidetector was completed.

Work started on the Gadolinium detector for DB21.

Preliminary studies were carried out on a small angle multiwire detector with circular coordinates for IN4B. A multiwire (80) detector for the study of profiles as a function of (IN1) was completed.

The helium 3 refilling equipment was reconstructed with gas purification and compression systems. Various technological solutions were tested for planes of wires for multidetectors. A low resolution (2 mm) multidetector was constructed on a semi-industrial basis.

Preliminary studies were carried out on new logics for multidetectors; the processing of amplitudes with the aid of a fast microprocessor should make it possible to obtain position-sensitive detection close to 1.5 mm compatible with the new gas mixtures.

SPECIAL INSTRUMENTS

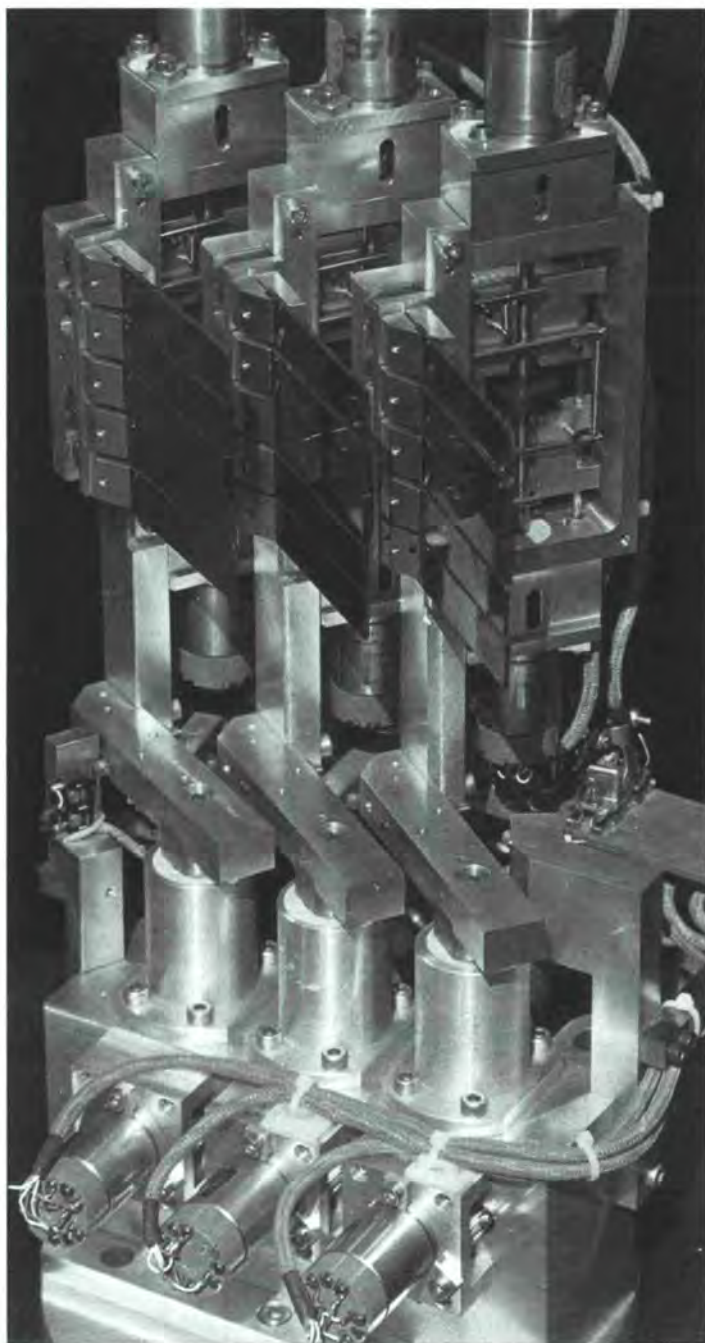
In mid-1983 the Special Instrument Group was established to centralise the technical aspects of special instruments and of tests at ILL and thus to make possible the optimum scientific utilisation of these instruments (now more than 20). The preparation, planning and budgeting of the work is done in collaboration with the Project Office, and their construction with the assistance of the technical departments and groups at the ILL (Instrument Operation Department, Department of Computing, Technical Department).

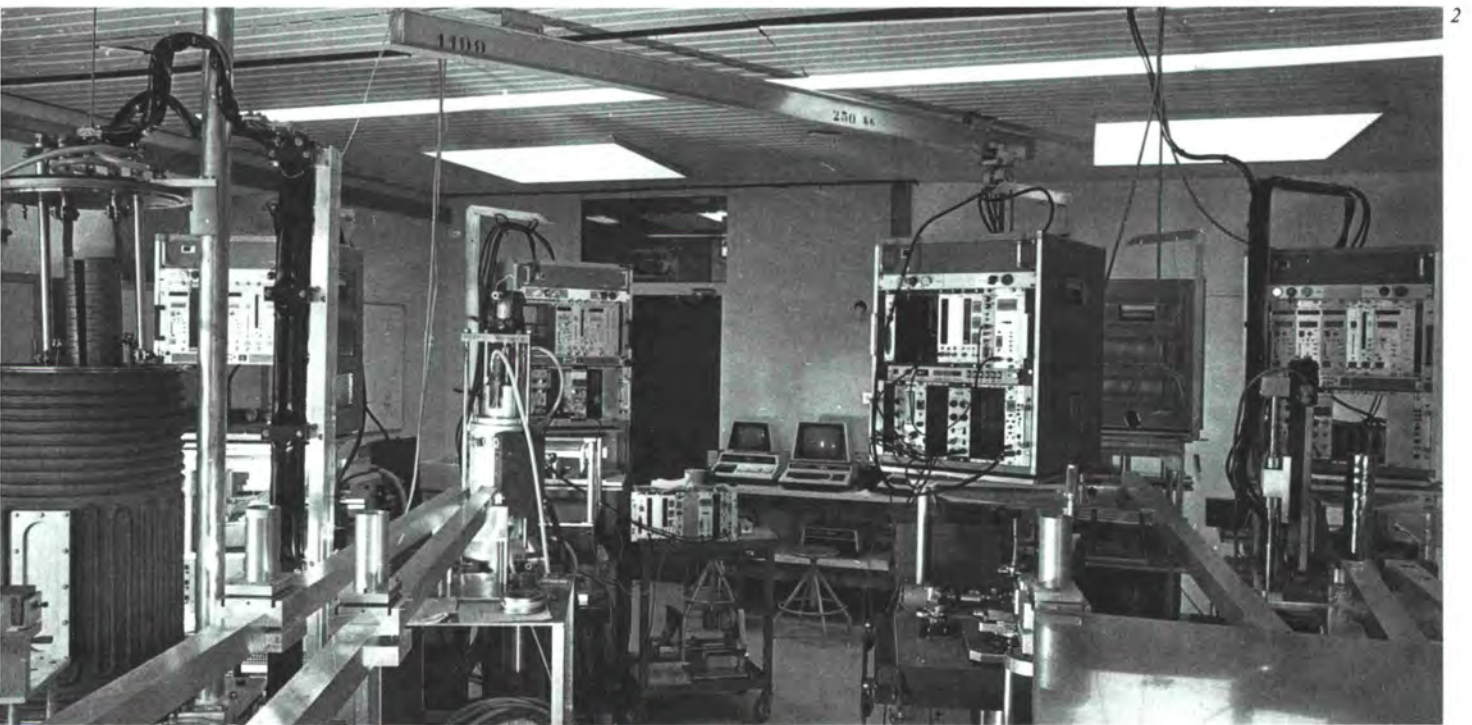
Major work was carried out in 1983 on:

S1, S6, S18, S20, S21, S50, S51, T16, H6 and H16, permitting on S6 in particular a gain of a factor close to 2 in neutron intensity, and an improvement in safety conditions on SN7 and S51.

In addition, intervention work was necessary on a number of occasions to assure the operation of S and T instruments.

In addition to work on the existing S and T instruments, the ILL is continuing a number of projects in this field, including:





1. Composite focussing monochromator of the ILL type (A. Freund).
2. The five γ -ray diffractometers. On the left the crystal growth facility.
3. The new fully automatic evaporator for super-mirror production.

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- the installation of a “neutron turbine” for the production of an intense beam of ultracold neutrons (Steyerl, Munich Technical University)
- the installation of a second generation instrument for the investigation of nn oscillations (international collaboration)
- the possibility of installing a very high resolution time-of-flight diffractometer on the second cold source (Steichele, Munich Technical University).

GENERAL SERVICES

BUILDING SERVICES AND MAINTENANCE

Facilities available

The group comprises 32 persons divided as follows:

Central Services	2 staff
	+ 1/2 secretary
Drawing Office, building and follow-up of works	2 staff
Technical preparation and maintenance	4 staff
Miscellaneous: maintenance and self-service production workshop	19 staff

The group also cleans the experimental halls (with 4 ILL staff) and organises the cleaning (by contract) of the buildings.

Maintenance work

This may be divided into two functions:

Basic function: the main work of the group. Maintenance or repair of buildings, equipment and technical installations, and elimination of any risks. Minor modifications to this equipment to deal with any problems which arise, or at the request of users. Distribution of power.

Additional functions:
Maintenance of stock of handling equipment.
Monitoring power supplies.

Providing logistical support for events in the life of the ILL.

The maintenance of certain technical installations and repetitive intervention work (requiring regular rounds) are entrusted to specialist external firms under maintenance contracts.

In 1983 priority was given to the organisation of preventive maintenance work including the following reconstruction work and improvements:

- reconstruction of toilets ILL4
- reconstruction of terraces at ILL 2
- work on the ILL 2 overhead crane
- replacement of electrical racks for IN2
- commissioning of the second mains water supply.

New work

The group has been assigned two functions:

- design of new installations (internally or in conjunction with engineering consultants);
- follow-up of work carried out by ILL workshops or external firms;

The main jobs in 1983 were:

- completion of work on buildings ILL 2 and ILL 23
- installation of maintenance workshops in ILL 3 and transfer of self-service workshop to ground floor of ILL 2
- completion of renovation of building ILL 4
- reconstruction of rooms for Works Committee in ILL 9
- reconstruction of the ILL 4 foyer
- reconstruction of the 4th floor conference room ILL 4
- construction of a store for dangerous products (ILL 24)
- assistance with studies for the new guide hall (ILL 22).

Technical assistance to other groups

Three main areas may be distinguished, depending on the work of the person requesting:

1. Workshop services

- the self-service mechanical workshop is available for ILL staff with some experience of machine tools, to permit them to modify or make certain parts at short notice

the main sheet metal workshop produces items which are difficult to sub-contract (prototypes, items requiring fitting on the spot or very urgent items), and its very varied equipment makes it possible to machine the majority of steels and lightweight alloys.

Main jobs in 1983:

- construction of a storage platform for ILL 5
- assistance with preparatory work for the replacement of beam-tubes
- production of biological shielding (PN8, PN4, T16)
- production and installation of metal parts in connection with the equipment of buildings.

2. Services for external organisations

This concerns EMBL (European Molecular Biology Laboratory), which shares the site and has a contract with ILL for maintenance and supplies.

In addition to maintenance of buildings and technical installations and minor modification work, the group also carries out studies for the equipment of laboratories and monitors the construction work.

3. Equipment of instrument positions

On the basis of requests from the Instrument Operation Department or the Project Office, and in collaboration with the Reactor Department and the Construction and Maintenance Group, the group organises the construction and assembly of biological shielding and other equipment (electricity, air-conditioning, handling, infrastructure) for new and existing instruments.

The most important jobs in this field in 1983 were:

- assembly of the storage platform in ILL 5
- preparation of the H11 area for D19 and D20
- dismantling and assembly of shielding for beam tube replacements (D3, IN8, PN1, D15)
- construction of instrument positions T16, TEM and GAMS 4
- improvements to the power supply distribution in ILL 7.

5

REACTOR OPERATION 1983

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OPERATION OF THE SUB-ASSEMBLIES

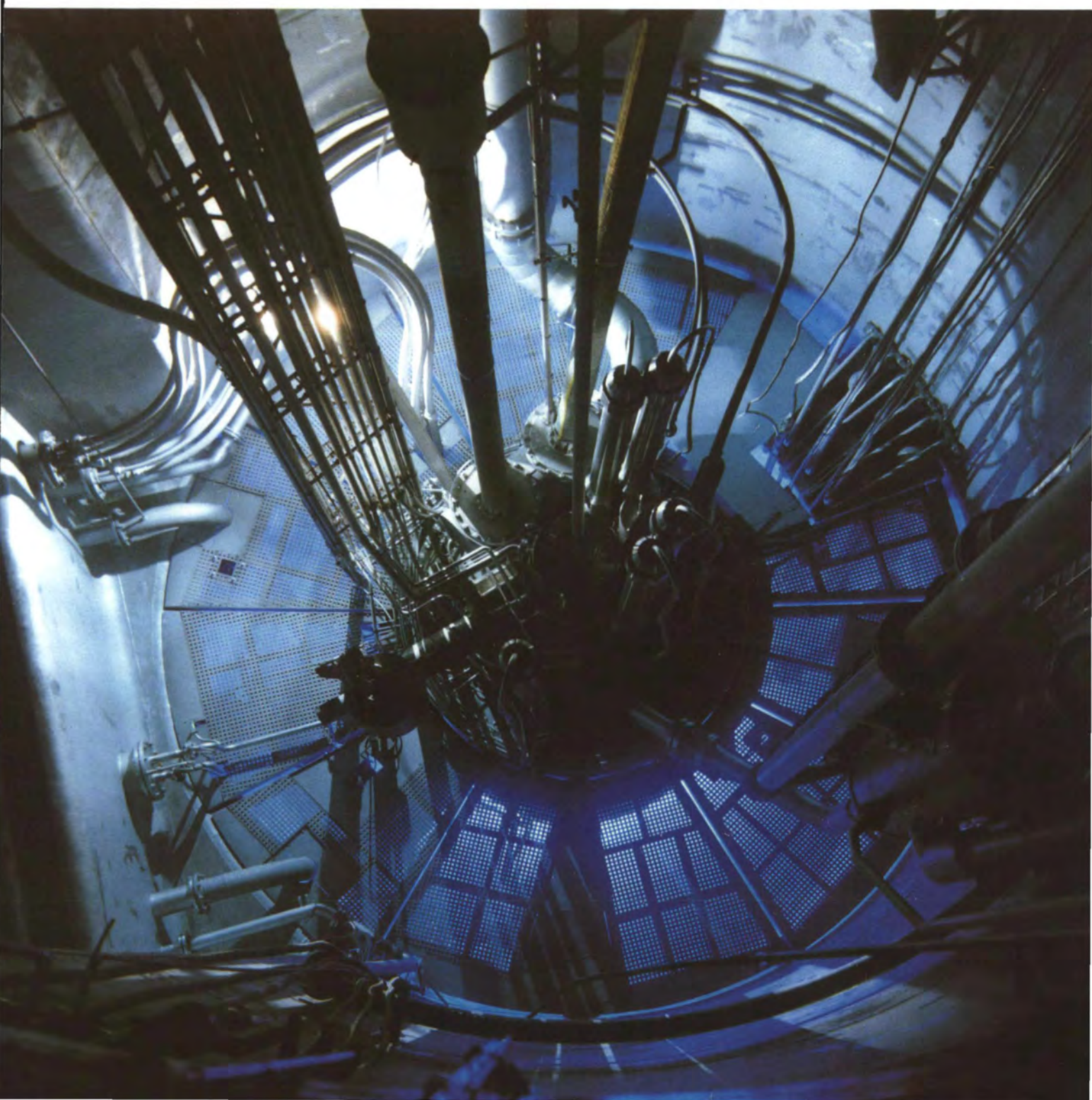
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RELATIONS WITH THE SAFETY AUTHORITIES

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A view on top of the D₂O vessel of the HFR. The blue light is Cerenkov radiation. ►

REACTOR OPERATION DEPARTMENT



5

Introduction

The regular operation of the reactor, based on 6 cycles of 44 days each per year, was interrupted in 1983 from 1 February to 8 August, particularly to permit the replacement of 5 beam-tube liners and the removal of the damaged part of the heavy water collector in the reflector tank.

Apart from the shut-down, the reactor operation programme covered 3 cycles with a total of 140 days operation.

Einleitung

Der normale Betriebsrhythmus des Reaktors von 6 Zyklen pro Jahr mit je 44 Betriebstagen pro Zyklus ist 1983 vom 1. Februar bis 8. August unterbrochen worden, um 5 Strahlrohre neu einzusetzen und um den beschädigten Teil der Schwerwassersammelleitung im Reflektortank zu entfernen.

Von diesem Stillstand abgesehen umfasste das Reaktorbetriebsprogramm 3 Zyklen mit insgesamt 140 Betriebstagen.

Introduction

Le rythme de fonctionnement habituel du réacteur, basé sur 6 cycles de 44 jours de marche par an, a été interrompu en 1983 du 1^{er} février au 8 août, pour procéder, notamment, au remplacement de 5 doigts de gant des canaux et pour découper la partie fissurée du collecteur de reprise de l'eau lourde dans le bidon réflecteur.

En dehors de cet arrêt, le programme de fonctionnement du réacteur a comporté 3 cycles totalisant 140 jours de marche.

REACTOR OPERATION 1983

End of cycle 5/82

Uninterrupted operation until 1 February 1983. The schedule was respected and the cycle was completed without any notable incident.

Cycle 1/83

Operation from 8 to 29 August. The scheduled dates for this cycle were respected despite 2 shut-downs resulting from operating incidents which prevented the reactor from operating from 11 to 13 August and from 21 to 23 August.

Cycle 2/83

Operation from 13 September to 27 October. The scheduled dates were respected and the cycle was completed without any notable incident.

Cycle 3/83

Operation from 8 November to 22 December. The scheduled dates were respected and the cycle was completed without any notable incident.

Data for 1983

No. of days originally scheduled	140
actual No. of days of operation	136
No. of equivalent days of full power	134.57
actual operating time	37.3%
actual operating time in relation to time scheduled	97.1%
No. of fuel elements used	3
No. of fuel elements actually dispatched for processing	6
No. of new fuel elements received	6
No. of unscheduled shut-downs	4
including: brief shut-downs	2
shut-downs with Xenon poisoning	2

OPERATION OF THE SUB-ASSEMBLIES REACTOR BLOCK

In 1983 the major operations were carried out during the reactor shut-down:

- partial removal of the heavy water collector in the reflector tank; this was done by electro-erosion under heavy water, necessitating the design and construction of remote-controlled equipment
- replacement of beam-tube liners for beam-tubes H5, H9, H10, H11 and IH4
- dismantling of beam-tube liner IH2 and insertion of a plug
- replacement of safety rods nos. 1 and 2 and of the control rod
- inspection and maintenance of the natural convection valves, safety rod mechanisms, control rod and the integrated experimental instruments (H9 and H6/H7)
- recommissioning of instrument H9.

CIRCUITS

In addition to the assistance to the reactor block group on cutting operations for the heavy water collector, the long shut-down was used for carrying out systematic checks of the circuits for ventilation, production of compressed air and various cooling operations.

On the heavy water circuits, items to be noted include the replacement of main pump n° 2, the inspection of the D₂O/H₂O exchanger tubes, and the replacement of valves which were no longer leak-proof.

The gas leak detection circuit (DRG) was completely replaced.

ELECTRICITY

The network "Normal-emergency - 22 V Reactor Control" was completely replaced from generation (rectifiers, static inverters and batteries) to the distribution racks.

The moving and modernisation of the health physics panel in the control room necessitated major cabling and relay work. The processing of data from the control panels is now carried out by modern technology.

ELECTRONICS

The design and implementation of the reconstruction of the health physics control panel were the biggest jobs, along with the change in the gas leak detecting circuit. During the shut-down all the thermodynamic measures were calibrated and all

the leak detection plugs in the beam-tubes were checked.

DETRITIATION

At the end of the tests on the model of the future horizontal cold source, the detritiation plant was returned to the normal configuration and the processing of heavy water was resumed: 3800 l from the reactors at Harwell (UK)

360 l from the reactor Mélusine (CEN Grenoble)
approximately 30000 l from the HFR.

RELATIONS WITH THE SAFETY AUTHORITIES

Following incidents which occurred in 1982 on the reactor (fracture of the heavy water collector and leak on beam-tube liner H12), the "Service Central de Sûreté des Installations Nucléaires" (French nuclear safety authority) authorised the reactor to operate until February 1983 and imposed certain conditions for the authorisation to restart after this shut-down:

1. The origins and consequences of the fracture of the heavy water collector must be determined.
2. A programme of work on the heavy water collector must be carried out.
3. The replacement programme for beam-tube liners must be speeded up.
4. An up-to-date summary must be prepared of the experimental results on the behaviour of materials subject to irradiation used in the reactor.
5. A programme must be prepared for the replacement of the various components of the reactor block.
6. A formal quality control organisation must be set up.

These different requirements have resulted in major studies, which have had to be carried out by the reactor department. The corresponding documents were submitted to the safety authorities at the beginning of January 1983.

However the discovery at the end of February 1983 of a change in the state of the heavy water collector led to a decision to remove part of this unit before the reactor restarted.

It was necessary to submit further documents when proposing this modification.

The dossiers submitted by the ILL were the subject of a study in April 1983 by the permanent group of experts on nuclear reactors.

Following this study, the safety authorities accepted the great majority of the ILL proposals, and the life-time of the various components of the reactor was determined.

The work of replacing the beam-tube liners not yet replaced and the removal of the central part of the heavy water collector will be carried out during the next shut-down, due to commence at the end of 1984.



2



1. A formidable array of electronic and mechanical facilities as well as considerable teamwork was required to cut off the deficient part of the "collecteur de reprise" in the D_2O circuit of the HFR (June 1983). This was carried out by means of an electro-erosion facility, able to operate under water. The whole operation, a unique and pioneering venture, was performed without any incident within 4 days. The photograph shows the transport of the facility to its operational position.

2. The picture shows a last inspection of the cutting head (with the electrode) by the reactor experts.

3. A series of TV screens and electronics ensured visualisation and the remote control of the operation. In the picture is Dr. Bauer who was responsible for the operation.

4. Several shapes of electrodes were required to achieve the work.

5. Astruc, one of the engineers responsible for the construction of the new vertical Cold Source, with the provisional set-up of the source in the reactor hall (level D).



4



5

6

**AUTOMATION
AND
DATA SERVICE (SAD)**

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**CENTRAL
COMPUTING
SERVICE**

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COMPUTING DEPARTMENT



6

Introduction

The start of 1983 saw a major reorganisation, the electronics and detector sections of what had been up till then the Computing and Electronics Department being transferred to the Technical, Instrumentation and Methods Department. The sections which remained became the Computing Department, and the opportunity was taken to make some organisational changes amongst them.

All activities not forming part of the Central Computer Service have been combined to form the new Automation and Data Service (SAD), with the aim of emphasising the unity of the various information handling activities. For example, some stages of the treatment of experimental data are carried out on the instrument control computer and need to be taken into account when data acquisition is being planned. Similarly the Management Information Systems Group (MIS) normally uses the same hardware as the instrument systems and is linked to them through the ILL internal network, JUDAS, for the purpose of transferring information files.

SAD thus comprises 5 groups:

- Software A: crystallographic instruments
- Software B: other neutron scattering instruments
- Software C: nuclear and particle physics instruments (including most special instruments)
- Management Information Systems
- Computer Hardware Maintenance.

It will be noted that the responsibilities of the three software groups are defined in terms of Instrument Groups. This was done with the aim of achieving standardisation of systems, and particularly the user interface, amongst groups of instruments having the same clientele. It may well take several years before one sees the full benefit of this, but already useful standardisation has been achieved between IN4, IN5 and IN6.

Amongst the principal achievements within SAD one should note

- arrival and installation of VAX 11/750 for D19B
 - rapid progress on the development of the IN20 system, following the choice of the TSX operating system
 - considerable user satisfaction with the network providing local data handling for β - and γ -spectrometers
 - introduction of wordprocessing facilities using standard hardware.
- The Central Computer Service has seen a year during which the DEC 1091 has performed with notable reliability. The level of use has risen considerably, which might seem surprising in view of the long reactor shut-down, but many scientists took advantage of their freedom from routine duties to work on the analysis of data from past experiments.

Much of the work done by the Service is concerned with small but steady improvements to the operating system, or resolving users' problems, and is difficult to highlight in this brief summary. But one should note that Fortran 77 was introduced for evaluation and is almost certain to become the default option for Fortran in the near future. Also in the field of high level languages, the Service is trying to encourage scientists and engineers to try out some of the mathematical preprocessors that are now available for operating directly on problems presented in symbolic form.

A number of communications projects, which by their nature tend to cut across the boundary between the two Services, are coming to fruition. The internal computer network, JUDAS, is effectively complete and operational. Most instrument computers now use this for data transfer to the Central Computer. The MICOM terminal switch is also operational, permitting a terminal to be logged on to any of a number of computers. ILL's connection to Transpac, the French national package switching service, via which access can also be gained to Germany and the United Kingdom, is scheduled for early in 1984.

Einleitung

Anfang 1983 wurde eine grössere Umorganisation in Angriff genommen. Die Elektronik- und Detektorabteilungen des damaligen Informatik- und Elektronikdepartments wurden in das Department für Instrumentierung und Methoden übernommen. Die Abteilungen, die übrigblieben, wurden zum Departement für Informatik zusammengefasst und diese Gelegenheit wurde dazu benutzt, einige organisatorische Änderungen innerhalb dieser Abteilungen vorzunehmen. Alle Aktivitäten, die nicht zum Rechenzentrum gehören, wurden zur neuen Abteilung für Automation und Datenerfassung (SAD) zusammengefasst mit dem Ziel, die verschiedenen Informationsverarbeitungsaktivitäten mehr zu vereinheitlichen. Zum Beispiel werden einige Phasen der Verarbeitung von Experimentdaten auf dem Instrumentcomputer durchgeführt und müssen in Betracht gezogen werden, wenn eine Datenaufnahme geplant wird. Auch benutzt die Gruppe für Büroinformatik die gleiche Hardware wie die Instrumentensystemgruppe und ist an sie durch das ILL-interne Verbundnetz, JUDAS, zum Zweck der Weiterleitung von Informationen angeschlossen.

Die Abteilung für Automation und Datenerfassung (SAD) besteht somit aus 5 Gruppen:

- Software A: Instrumente für Kristallographie
- Software B: andere Neutronenstreuinstrumente
- Software C: Instrumente für Nuklear- und Elementarteilchenphysik (einschliesslich "S-Instrumente")
- Management Information Systems
- Computer Hardwarewartung.

Der Verantwortungsbereich der drei Softwaregruppen ist durch die Instrumentengruppen definiert. Dies hatte zum Ziel, eine Vereinheitlichung der Systeme und besonders der Benutzerschnittstelle innerhalb von Instrumentengruppen mit gleichen Experimentatoren zu erreichen.

Es wird wohl einige Jahre dauern bevor der gesamte Nutzen sichtbar wird, aber eine brauchbare Standardisierung wurde bereits für IN4, IN5 und IN6 erreicht.

Unter den wichtigsten Leistungen innerhalb der Abteilung für Automation und Datenerfassung (SAD) sind folgende anzuführen:

- Anlieferung und Installation der VAX 11/750 für D19B.
- schneller Fortschritt bei der Entwicklung des IN20 Systems, aufgrund der Wahl des TSX-Betriebssystems.
- beachtliche Zufriedenheit der Benutzer mit dem Verbundnetz, das

lokale Datenverarbeitung für Beta- und Gamma-Spektrometer ermöglicht.

— Einführung von Textverarbeitungssystemen unter Benutzung der Standard-hardware.

Das Jahr 1983 war für das Rechenzentrum ein Jahr, in dem die DEC 1091 mit bemerkenswerter Zuverlässigkeit gearbeitet hat. Die Benutzung des Rechners hat sich beachtlich ausgeweitet, was erstaunlich erscheinen mag im Hinblick auf die lange Reaktorstilllegung; aber viele Wissenschaftler nutzten diese Zeit ohne Routinarbeiten dazu, an der Analyse von Daten von früheren Experimenten zu arbeiten.

Ein grosser Teil der von dieser Abteilung durchgeführten Arbeit betrifft kleine aber ständige Verbesserungen des Betriebssystems, oder die Lösung von Benutzerproblemen und ist zu umfangreich, um in dieser kurzen Zusammenfassung dargestellt zu werden. Es ist zu beachten, dass Fortran 77 probeweise eingeführt wurde und sehr wahrscheinlich bald die Standardversion für Fortran sein wird.

Ebenso versucht die Abteilung auf dem Gebiet der hochentwickelten Sprachen die Wissenschaftler und Ingenieure dazu zu ermutigen, einige der mathematischen Preprozessoren zu testen, mit denen man jetzt in symbolischer Form dargestellten Probleme direkt bearbeiten kann.

Eine Anzahl von Kommunikationsprojekten, die naturgemäss dahintendieren, die beiden Abteilungen zu überlappen, zeigen erste positive Resultate. Das interne Rechnernetz, JUDAS, ist fertiggestellt und betriebsbereit. Die meisten Instrumentenrechner benutzen nun dieses System für die Übertragung von Daten zum Zentralrechner. Auch die MICOM-Terminal-Schaltstelle ist betriebsbereit und ermöglicht den Anschluss eines Terminals an eine ganze Reihe von Rechnern. Der Anschluss des ILL an Transpac, dem nationalen französischen Datenübertragungssystem, über das man Verbindung nach Deutschland und Grossbritannien bekommen kann, ist für Anfang 1984 vorgesehen.

Introduction

Suite à une réorganisation importante début 1983, les sections électronique et détecteurs de l'ancien Département Informatique et Electronique ont été transférées au Département Technique, Instruments et Méthodes. Les autres sections sont devenues le Département Informatique, et on a profité de cette occasion pour apporter quelques modifications d'organisation entre elles.

Toutes les activités hormis celles du Service Calcul Scientifique ont été rassemblées dans le nouveau Service Automatisation et Données (SAD), dans le but d'accentuer l'homogénéisation des différentes activités de manipulation des données. Par exemple, plusieurs étapes du traitement des données expérimentales sont effectuées sur l'ordinateur de contrôle de l'instrument et devraient être prises en compte lorsque l'acquisition des données est prévue. De la même façon le groupe Management Information Systems (MIS) utilise en général le même matériel que les systèmes des instruments et y est lié par le réseau interne de l'ILL, JUDAS, afin de permettre le transfert de fichiers d'informations.

Le SAD comprend donc 5 groupes :

Logiciel A : instruments de cristallographie

Logiciel B : autres instruments de diffusion neutronique

Logiciel C : instruments de physique nucléaire et de particules (y compris la plupart des instruments "S").

"Management Information Systems"

Entretien du matériel informatique.

On notera que les responsabilités des 3 groupes "logiciel" sont définies en fonction des groupes d'instruments. Ce système a été mis en place afin d'obtenir une standardisation des systèmes — en particulier de l'interface utilisateur — pour les groupes d'instruments qui servent les mêmes clients. Un niveau utile de normalisation a déjà été atteint entre IN4, IN5 et IN6, mais plusieurs années seront probablement nécessaires avant qu'on en perçoive les résultats.

Entre les réalisations principales au sein du SAD il faut noter

— l'arrivée et l'installation du VAX 11/750 pour D19B

— le progrès rapide du développement du système IN20, d'après le choix d'un système d'exploitation TSX

— une très grande satisfaction des utilisateurs pour le traitement local des données pour les spectromètres β et γ

— la mise en place d'un système de traitement de texte basé sur du matériel standard.

Le service Calcul Scientifique a vécu une année pendant laquelle le DEC 1091 a fonctionné avec une fiabilité notable. Le niveau d'utilisation a augmenté de façon importante, ce qui pourrait paraître étonnant étant donné l'arrêt prolongé du réacteur; cependant de nombreux physiciens ont profité de leur disponibilité vis-à-vis des travaux de routine pour analyser les données des expériences antérieures. La plupart du travail du Service consiste à apporter des améliorations petites mais progressives au système d'exploitation, ou à résoudre les problèmes des utilisateurs, choses qui sont difficiles à souligner dans ce bref résumé. Mais il faut noter que le Fortran 77 a été introduit pour évaluation et que cette version deviendra presque certainement l'option par défaut pour le Fortran dans un proche avenir. Egalement dans le domaine des langages de haut niveau, le Service encourage les physiciens et ingénieurs à essayer sérieusement quelques-uns des préprocesseurs mathématiques actuellement disponibles comme outils immédiats, pour l'utilisation directe sur les problèmes présentés sous forme symbolique.

Plusieurs projets de communication, qui par leur nature ont tendance à dépasser la limite entre les deux services, sont en train d'aboutir. Le réseau interne d'ordinateurs, JUDAS, est pratiquement complet et opérationnel. La plupart des ordinateurs d'instruments l'utilisent désormais pour le transfert des données à l'ordinateur central. L'aiguilleur de terminaux MICOM fonctionne également et permet à un terminal d'être connecté à n'importe lequel des ordinateurs faisant partie de ce réseau MICOM, le branchement sur Transpac, le service national français de commutation de paquets, par lequel on peut également accéder aux services allemand et britannique, est prévu pour début 1984.

AUTOMATION AND DATA SERVICE (SAD)

SOFTWARE A (CRYSTALLOGRAPHIC INSTRUMENTS)

The group is responsible for software for the instruments D1A, D1B, D2, D3, D4, D5, D8, D9, D10, D15, D16, D18, D19, D20, DB21, LI4. For historical reasons it is also responsible for the CARINE system, but following the transfer of IN3 to its own Solar computer, there remains only IN2 on that system. The group also has responsibility for the organisation of the JUDAS computer network.

A key activity during the year has been concerned with the instrument D19. The definitive version of D19B will have a PDP 11/34 (used already on D19A) for instrument control and data acquisition and a VAX 11/750 for on-line data reduction. The installation of the VAX and its connection to the PDP 11 took place during the year. As the first VAX to be acquired by ILL, there was considerable effort needed for familiarisation with the VMS operating system and user interface. In addition, the program package on the PDP 11 has been completely revised and the new version tested.

As regards other new instruments, work has progressed normally on D2B, but on D20 has been held up awaiting a decision on the choice of detector system. The new biological diffractometer, DB21, will follow the D19B design and a PDP 11/24 has been selected for instrument control. The VAX for data reduction will also serve as general scientific computer for the EMBL outstation.

Elsewhere, instrument modifications have required changes to the control programs. The new ILL temperature controller, installed on D1A, D5, D8, D9, uses a microprocessor which has had to be interfaced to the PDP 11. The rebuilt D4B uses a PDP 11/23 and was brought into operation in the Autumn. The D9 program was adapted to permit tests of the "fly's eye" detector.

The 3 PDP 11s which serve as communication nodes for the ILL computer network, JUDAS, are the responsibility of this Group, which therefore has a key role in the operation and maintenance of the network. All the connections were essentially completed in time for the Reactor restart in August.

SOFTWARE B (OTHER NEUTRON SCATTERING INSTRUMENTS)

In January the Group was assigned the responsibility for development of control software and assistance in data treatment for instruments in the THREE-AXIS and VERCORS instrument groups, namely D7, D11, D17, IN1, IN3, IN4, IN5, IN6, IN8, IN10, IN11, IN12, IN13, IN20. The long shutdown enabled the software on all instruments to be studied. During this period a major effort has been expended on rationalising and simplifying control programs, and unifying data formats. This now permits easier maintenance and common use of routines.

The principal activities on the THREE-AXIS spectrometers were the adaptation of the standard control programs to operate IN1 and IN3 using individual SOLAR computers. A large effort was expended on the detailed optimisation of the dialogue with the micro-processor-controlled motors and counting system. A similar counting system was installed on the operational spectrometer IN8. An ILL precision temperature controller is under installation on the SOLAR computer of IN12. After study of available operating systems, TSX, a simple but flexible monitor, was selected for the PDP 11/24 acquired to operate the new spectrometer IN20. A new user interface was designed, written and tested by the project physicist within three weeks.

Most of the inelastic spectrometers in the VERCORS group were subject to extensive revision during the long shutdown. Complete revision of the electronics on IN4 and IN5 prompted a complete rewrite of all programs for these instruments, incorporating a number of features already found useful on IN6, and benefiting from the CAMAC routines and utility programs already in regular use on the small-angle scattering spectrometers (run on). For the user the commands have been greatly simplified, and the surveillance of detector count rates has been incorporated during the scheduled recording onto disk. This is especially useful for these two instruments where the detectors are frequently recabled and individual cable failures have been common.

Both back-scattering spectrometers IN10 and IN13 had extensive modifications to implement new hardware, improve the user-command interface and to format data in a similar fashion to the time-of-flight instruments, allowing standard programs to be shared more easily.

The low-Q spectrometers D11 and D17 were little modified during the year except to introduce means to follow rapidly changing kinetic experiments using the large CAMAC memories recently installed on the instruments.

The Group has ensured maintenance of existing projects outside its present formal responsibilities; these include vital programming for PN1, and programs for the MACAMAC controllers on the D4 spectrometer and D20 detector test facility.

The one year visit of an engineer from Los Alamos permitted completion of a number of closed projects for data treatment, such as a general raw data manipulation package common to the backscattering and time-of-flight instruments, which is available both on the instrument computers and the Central Computer.

SOFTWARE C (NUCLEAR PHYSICS AND SPECIAL INSTRUMENTS)

The principal instruments involved here are PN2, PN3 (GAMS 1, 2, 3, 4), PN4, PN6, PN8, with some support for SN5, SN7, S20, S21, S34, S52. An effort is being made to give more assistance to the S instruments than in the past.

The computer systems on these instruments show considerable variations. Some of them, having originated outside the Institut, do not follow ILL standards for either hardware or software.

An important achievement during the year has been the establishment of the Nuclear Physics Data Concentrator, a PDP 11/23 equipped with a wide range of peripherals, especially for the plotting of spectra from the β - and γ -spectrometers, and which is linked to both the instrument computers and the Central Computer. This has enabled a three-stage sequence of data handling to be introduced:

- (1) on the instrument computer, if resources permit
- (2) on the Concentrator, for fast access to special peripherals, in cases where only limited processing is required
- (3) on the Central Computer for large calculations, and for archiving of both raw and treated data.

Some data treatment program packages are necessarily specific to one instrument, but common software is used in cases where standardised procedures apply, such as list-mode and matrix operations.

The Group is also responsible for the management of the PDP 11/55, formerly the hub of the Nicole network, which is still much in demand as a medium-sized data handling machine, and for developing for the electronics section a microprocessor software development system on a PDP 11/24.

MANAGEMENT INFORMATION SYSTEMS AND OFFICE AUTOMATION

An automated information handling service based on a PDP 11/34 has been in existence for several years serving principally — scientific coordination and public relations office — library — travel section — radiation dose records — project office — telephone directory.

It has been extended during 1983 to include — information on presence of short-term visitors (instrument users) — management of radioactive sources — broadcast news service (chiefly for instrument users) — address lists.

With improvements being continually made to the established facilities the system resources are rapidly reaching saturation, and it will not be possible, without further investment, to undertake any new projects.

A start on a limited scale was finally made in 1983 to the introduction of word processing. By choosing the centralised system OS11, which runs on DEC hardware, and reactivating an ancient PDP 11/40, it has been possible to offer a service to 4 secretariats. Because of the high scientific and technical content of documents produced, the workstations are equipped with Sanders S700 printers which offer a wide range of fonts and characters, alongside the Word Processing version of the VT100 terminal. One of the advantages of the system, however, is that by means of the network and the MICOM switch, it can receive text input from any VT100 or equivalent terminal, or text files held in any computer.

The secretaries involved have adapted well to the new mode of working, despite some inconveniences due to the limited sums available for investment. The full benefits of a centralised system will only be gained when all secretariats are equipped, but with the present budgetary constraints this is not expected to be achieved for several years.

COMPUTER HARDWARE MAINTENANCE

ILL being an organisation with a service role, efficient maintenance of operational equipment is essential. To look after an ever increasing amount of equipment on a constant budget is not an easy task, despite a general improvement in reliability of components.

The key to the problem is to decide which equipment should be maintained under contract and which by in-house technicians. The latter solution is usually more cost-effective for standard equipment principally because in-house staff are more familiar with the total environment within which the equipment operates. For equipment which is used in limited number, however, the cost of holding spares may well change the balance.

Maintenance of non-standard equipment, such as exists on some S instruments poses severe problems. Whilst the formal position is that the Department cannot guarantee support for such equipment, in practice every effort is made to try and get all instruments running again with a minimum of delay.

CENTRAL COMPUTING SERVICE

Apart from the basic function of operating the DEC 10 and assisting the scientists in the use of this machine, the main activity of this service has been devoted to the continuation of certain projects started in 1982, which have necessitated new developments during this year: for example the DECNET system, the system of terminals linked to a switching concentrator, the PDP 11/24 system which front-ends the DEC 10 for data support media for which there is no standard connection to the DEC 10.

OPERATION AND USE OF THE DEC-10

The DEC-10 operated very satisfactorily during 1983 with a remarkable stability of equipment, operating system and environment: the availability rate was approximately 98.5%.

As in the past, the computer operated 24 hours per day, with operator cover on Mondays from 5.30 a.m. to 9.30 p.m., Tuesday to Friday from 6.15 a.m. to 8.45 p.m., Saturday from 9. a.m. to 5 p.m. and the remainder of the time in self-service mode.

The reactor shut-down from February to August 1983 did not result in a reduction of activity as regards the use of computing power except during the months of March and May, when there was a reduction of the order of 25%. There was an increase in the requirement for batch work starting in April, when certain restrictions were introduced in the use of programs in interactive mode. This demand has become particularly high since July for applications in crystallography and biology. During these last four months the central processor has been active for more than 95% of the real elapsed time.

SYSTEM WORK

Towards the middle of the year a new version of the operation system and the accompanying utilities was introduced; this operation is accompanied by a certain number of modifications, the aims of which are to adapt the system to our own requirements.

Various projects started the previous year were continued in 1983: these cover in particular access to archive files, distribution of messages, the improvement of the performance of Versatec graphic outputs on the 11/24 frontend of the DEC-10. Data transfer programs or procedures to or from other organisations on magnetic or other supports such as floppy disks or cartridges have been developed on the DEC-10 and the associated PDP 11/24.

A new system is currently under test for the control of queuing for printers, graph plotters and batch work and for checking magnetic tape labels; this new product should be efficient and should provide users with easier access when the machine is in self-service operation.

COMMUNICATIONS

Work on the DECNET system has continued this year, in collaboration with SAD, with a view to increasing the number of instrument computers on this system, introducing new functions for the transfer of standard files to different destinations (disk, printer, batch), and improving the operational reliability of this system.

During the reactor shut-down the terminal switching concentrator was installed; the terminals and computers have been progressively linked to this equipment which currently makes it possible to access the majority of the ILL computers from a considerable number of terminals.

During the current year an application has been submitted to the Direction Générale des Télécommunications (French Telecommunications authority) for connection to Transpac; the necessary purchases of equipment have been made and this new service for ILL users should be available before the end of this year.

GRAPHICS

There has been no major development in this area apart from normal maintenance and the regular improvements necessary for all software.

However, a preliminary study has been carried out jointly with SAD and certain scientists on the ILL's general requirements for a more sophisticated graphic system than the graphic terminals currently in use at ILL. Such a system would be particularly useful for applications in crystallography and biology. The action to be taken following this study is still under consideration.

MATHEMATICS

A certain number of software packages are available for scientists:

- data presentation software (HBOOK), prepared at CERN and incorporating smoothing facilities and the capacity for histograms

- CERN mathematical library (CERLIB)

- minimisation software developed at CERN (MINUIT)

- modelling software (MLAB) developed at the National Institute of Health (USA) covering much of numerical analysis and statistics

- two high-level languages permitting the easy formulation of mathematical or statistical problems (MATH and STAT/PROTRAN) (the preprocessors translate the PROTRAN language into FORTRAN, incorporating subroutines from the IMSL library)

- a new version of REDUCE offering new facilities in the field of formal calculation (integration, factorisation).

The version of Fortran 77 is currently under test and may be used by anyone wishing to take advantage at this stage of the new specification of this standard; this test phase permits users to assess the difference in results due to a new library of more precise elementary mathematical functions. This new Fortran should facilitate the exchange of programs between the different ILL computing systems and more generally between the various research centres.

7

**SAFETY
AND HEALTH PHYSICS GROUP**

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LIBRARY

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**SECRETARIAT
OF PHYSICISTS**

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The ILL Library.

In the insert: Control unit of the Radioprotection Group for checking the tritium content in the atmosphere at the ILL's detritiation plant. ►

OTHER SECTIONS



7

SAFETY AND HEALTH PHYSICS GROUP

The year 1983 saw major work around the reactor, including in particular 6 replacements of beam-tube liners and the work on the heavy water collector for the reactor tank. The Safety and Health Physics Group has thus been closely associated with this work as regards the definition of working conditions, monitoring during the work, decontamination and control of waste.

Other events in 1983 included:

the commissioning of the storage and decontamination part of building ILL 22 (this building improves the working conditions of the decontamination staff)

the introduction of computerised control of radioactive sources and of the dosimetry of guest scientists

the inspection of all X-ray equipment following displacement

the continuation of the health physics calculations associated with new experiments, and in particular with the future cold source

the safety studies for the experiments involving risks, such as those using liquid hydrogen (S1) or counters filled with methane (S51), experiments using radioactive sources in cryostats, and those using equipment under very high pressure

in collaboration with the Works Doctor the group participated in studies on safety at working positions, as it has done since the establishment of the Institut.

The radioprotective arrangements for the extraction of thimbles. In the picture is the working and dressing area of the technicians.



LIBRARY

The increase in the price of scientific literature continues to be the main concern and was still higher than anticipated: scientific journals, which represented 49% of the total budget in 1982, rose to 56% in 1983 despite the considerable increase in the budget.

The books and serial publication acquisition remained almost steady and covered the needs expressed (460 items of which 130 are deposited with departments) while binding and reprints were most affected by financial pressure.

The library's budget in 1983 was 542 KF.

An experiment to encourage the extended use of literature retrieval systems showed that the existing facilities at the C.E.N.-G. covered the current needs, while some requests have been satisfied with the ILL publication data base (there are now at the ILL about 1800 references of publications related to neutron measurements).

The programs developed and intercomputer connection will permit this year direct reproduction without reprinting of the lists at the end of this volume (experiments performed and publications).

SECRETARIAT OF PHYSICISTS

This secretariat is in charge of the typing of scientific publications and the mail of the ILL physicists and long-term visitors.

Typing of research proposals and reports (submitted to the Scientific Council) is also done by this section.

The secretariat is also involved in the preparation of the list of ILL publications for the annual report of the Institute in collaboration with the library.

The group contributes to the preparation of external conferences and workshops and regularly sends reprints of ILL publications for which there is a high level of demand from very many laboratories.

The introduction of a word processor for the secretariat of the physicists (ILL 19) has proved very successful in terms of both quality and efficiency. It is foreseen that this service will soon be extended to the benefit of the full secretariat (ILL 4 + ILL 1).



PERSONNEL

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WELFARE

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FINANCE

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The sculpture by Ipusteguy in front of the ILL main building. ►

ADMINISTRATION DEPARTMENT



8

Introduction

The Administration Department covers

- the Personnel Group for the approximately 500 ILL staff
- the Finance and Purchasing Section
- the Groups Training, Welfare, Schools and General Services (post, drivers, reprography, reception, cafeteria, ILL flats)
- the Works Doctor (regular monitoring of employees' health, particularly where there is danger to irradiation risks)
- the Translation and Interpreting Office
- the Secretariat of the Steering Committee and its Subcommittees.

The previous head of the department, Dr. Wolfgang Grillo, left ILL in May 1983 to take up a new post in Germany. His successor is Christoph Eitner. On 30 June 1983 the Director and the CFDT, CGT and FO unions signed the new Collective Agreement, which is valid for 5 years. The CGC union did not sign this Agreement, wishing to express its reservations on the current position on limited term contracts for scientists. The Management

Einleitung

Die Verwaltungsabteilung umfasst

- das Personalbüro für die rund 500 ILL-Angestellten
- den Sektor Finanzen und Einkauf
- die Bereiche berufliche Fortbildung, betriebliche Fürsorge, Schulfragen sowie verschiedene Infrastruktur-Dienste (Post, Fahrbereitschaft, Vielfältigung, Empfang, Cafeteria, Gästewohnungen)
- den Werksarzt (laufende gesundheitliche Überwachung der Mitarbeiter, insbesondere soweit sie Bestrahlungsrisiken ausgesetzt sind)
- das Sekretariat des Lenkungsausschusses und seiner Unterausschüsse.

Im Mai 1983 verließ der bisherige Leiter der Abteilung Dr. Wolfgang Grillo das ILL, um in Deutschland eine neue Aufgabe zu übernehmen. Sein Nachfolger wurde Christoph Eitner.

Am 30. Juni 1983 unterzeichneten der Direktor und die Gewerkschaften CFDT, CGT sowie FO den neuen Betriebsarbeitsvertrag. Er hat eine Laufzeit von 5 Jahren. Die CGC gehört nicht zu den Unterzeichnern des Vertrages. Mit der Verweigerung ihrer Unterschrift brachte sie ihre Bedenken gegen die derzeitige Regelung über Zeitverträge für Wissenschaftler zum Ausdruck. Direktion

Introduction

Le département Administratif et Financier comprend :

- Le Service du Personnel, gérant les quelques 500 agents ILL,
- Le Service Financier et Achats,
- Le Service Relations Sociales regroupant la Formation Permanente, l'Assistante Sociale, les questions scolaires et divers services d'infrastructure (coursier, chauffeurs, reprographie, réception, cafétéria, appartements ILL),
- Le Médecin du Travail (surveillance médicale courante des agents, notamment dans les cas de risques d'irradiation),
- Le bureau de Traduction et d'Interprétariat,
- Le Secrétariat du Comité de Direction et de ses sous-comités.

En Mai 1983, l'ancien Chef du Département, Monsieur Wolfgang Grillo, a quitté l'ILL pour prendre de nouvelles fonctions en Allemagne. Son Successeur est Monsieur Christoph Eitner.

Le 30 Juin 1983, le Directeur et les syndicats CFDT, CGT et FO ont signé la nouvelle Convention d'Entreprise. Celle-ci est conclue pour une période de cinq ans. Le syndicat CGC ne figure pas parmi les signataires de cette Convention. De cette façon il voulait exprimer ses réserves concernant le règlement actuel au sujet des contrats à durée limitée pour les physiciens.

and Associates of the ILL maintain the principle of the 5-year limited term contracts for the majority of the scientists, despite the intention of the Management to convert some additional limited term posts to permanent posts over the next few years.

The implementation of the 1983 budget was characterised by additional expenditure for repair work on the reactor, and the placing of the contracts for beam-tubes H1/H2 and H6/H7, and for the construction of the second neutron guide hall. The ILL was also obliged to request the Steering Committee to approve additional expenditure because of the increased reprocessing costs for used fuel elements and also because of the considerable increase in the rate of exchange for the US-Dollar.

Over the next few years the Institut is likely to have diminishing room for manoeuvre in both the personnel and financial field, which poses a difficult problem for the Institut to nevertheless maintain its leading position in the world in the development of instruments and methods in neutron research.

und Gesellschafter des ILL halten jedoch am Prinzip der 5-jährigen Zeitverträge für die Mehrzahl der Wissenschaftler fest, unbeschadet der Absicht der Direktion, in den nächsten Jahren einige weitere Zeitvertragsstellen in Dauerstellen umzuwandeln.

Die Abwicklung des Haushalts 1983 war gekennzeichnet durch die Mehrausgaben für Reparaturarbeiten am Reaktor und die Auftragsvergabe für die Strahlkanäle H1/H2 und H6/H7 sowie für den Bau der 2. Neutronenleiter-Halle. Ferner musste das ILL wegen der erhöhten Wiederaufarbeitungskosten für seine abgebrannten Brennelemente sowie wegen des stark gestiegenen Wechselkurses für US-Dollar den Lenkungsausschuss um Zustimmung zu Mehrausgaben bitten.

Für die kommenden Jahre zeichnet sich ein zunehmend enger werdender Spielraum des Instituts sowohl im personellen als auch im finanziellen Bereich ab, der das Institut vor das schwierige Problem stellt, trotzdem seine Spitzenstellung in der Welt bei der Weiterentwicklung von Instrumenten und Methoden der Neutronen-Forschung zu bewahren.

Cependant, la Direction et les Associés de l'ILL maintiennent le principe des contrats à durée limitée de cinq ans pour la plupart des physiciens, malgré l'intention de la Direction de transformer quelques postes à durée limitée en postes permanents au cours des prochaines années.

L'exécution du budget 1983 a été caractérisée par les dépenses supplémentaires pour les travaux de réparation dans le réacteur, ainsi que par la passation des contrats pour les canaux H1/H2 et H6/H7 et pour la construction du deuxième hall conduits de neutrons. En plus, l'Institut a dû demander l'accord du Comité de Direction pour des dépenses supplémentaires en raison de l'augmentation du coût de retraitement des éléments combustibles usés ainsi que du taux de change considérablement accru du dollar.

Pour les années à venir la marge d'action de l'Institut deviendra de plus en plus étroite dans le domaine du personnel et dans le domaine financier ; ceci place l'Institut devant le problème difficile de maintenir néanmoins sa situation de pointe dans le monde en ce qui concerne l'évolution continue des instruments et des méthodes dans le domaine de la recherche neutronique.

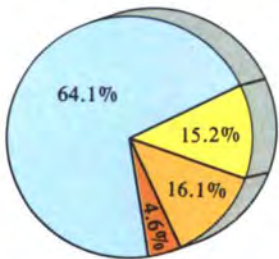
PERSONNEL

The Personnel Section is responsible for recruitment, salaries, staff management, and administrative aspects of external visits and guest scientists. It also deals with the Social Security and the administrative work for the ILL staff "Société Mutualiste".

STAFF

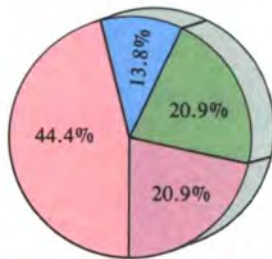
The ILL staff increased by 28 in 1983, mainly because of the incorporation in the staff of 23 employees of external firms working at the Institut, which was completed by May 1983. The main changes which have taken place in the non-cadre personnel are essentially due to the premature retirement of 10 employees, which is a result of the "Solidarity contract" signed by the Institut in December 1982.

1. Nationality



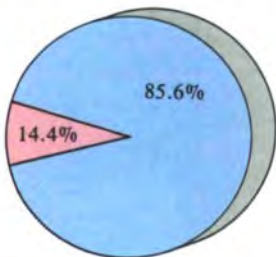
French	322
German	76.5
British	81
Others	23
Total	502.5

2. Category of work



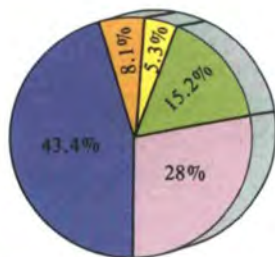
Scientists	105
Technicians	223
Admin. & Secretaries	69.5
Others	105
Total	502.5

3. Sex



Women	14.4%
Men	85.6%

4. Age



Under 25	43.4%
25 to 30	15.2%
31 to 40	28%
40 to 50	8.1%
Over 50	5.3%

Figure 42: Break-down of staff in 1983 by nationality, staff category, sex and age.

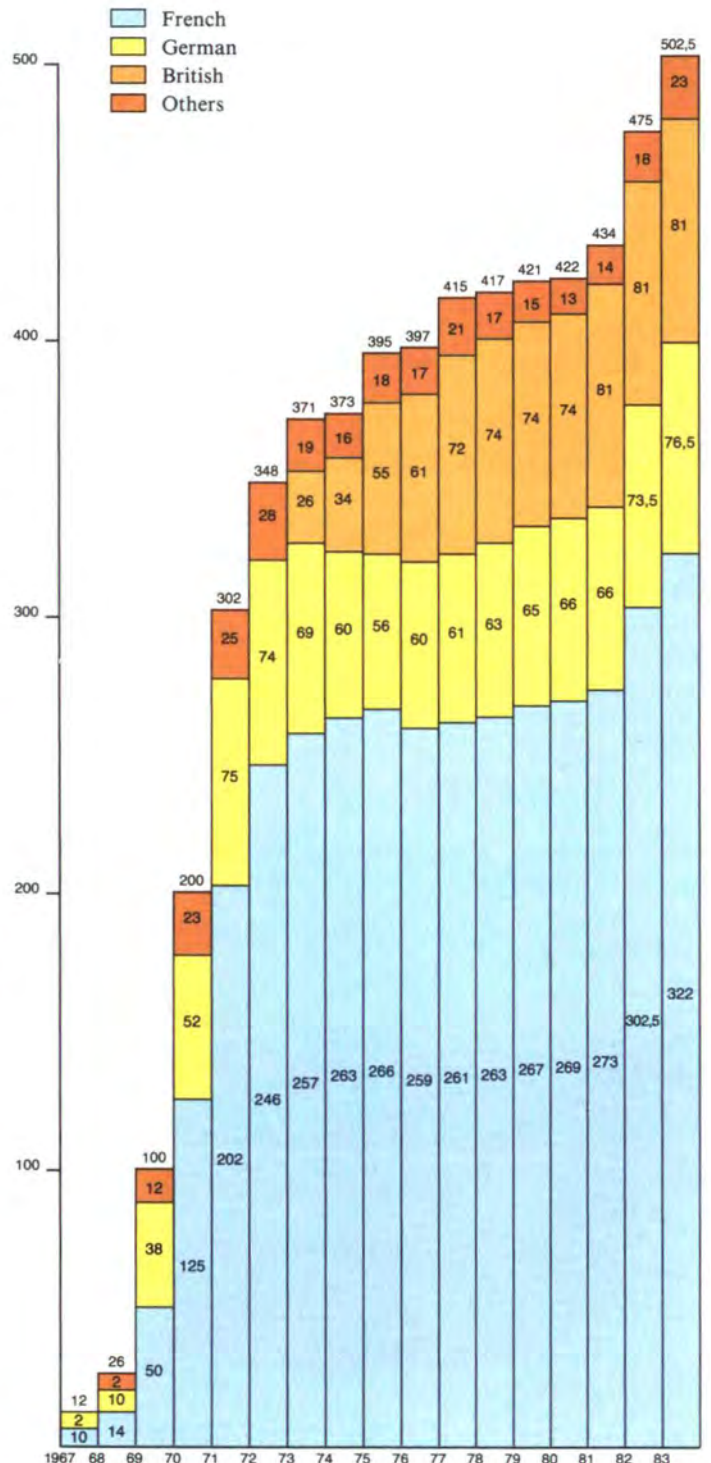


Figure 43: The changes in staff (from the foundation of the ILL) from 1967 to 1983.

TABLE 7
Staff changes in 1983

<i>Categories</i>	<i>Position on 31.12.82</i>	<i>Recruitment</i>	<i>Departures</i>	<i>Difference + or -</i>	<i>Position on 31.12.83</i>	<i>Change % col. 4 compared with col. 2</i>
<i>(1)</i>	<i>(2)</i>	<i>(3)</i>	<i>(4)</i>	<i>(5)</i>	<i>(6)</i>	<i>(7)</i>
1. Scientists	74	11	8	+3	77	10.81
2. Engineers	55	1	—	+1	56	—
3. Other "Cadres"	9.5	2	2	—	9.5	21.05
4. Thesis Students	30	3	5	-2	28	16.67
5. Technicians	166	7	5	+2	168	3.01
6. Others	140.5	36	12.5	+23.5	164	8.9
Total	475	60	32.5	27.5	502.5	6.84

GUEST SCIENTISTS

In 1983 the ILL received a total of 1425 visitors. Due to the long reactor shut-down, the number of visits by guest scientists has shown a reduction of 27% compared with the previous year.

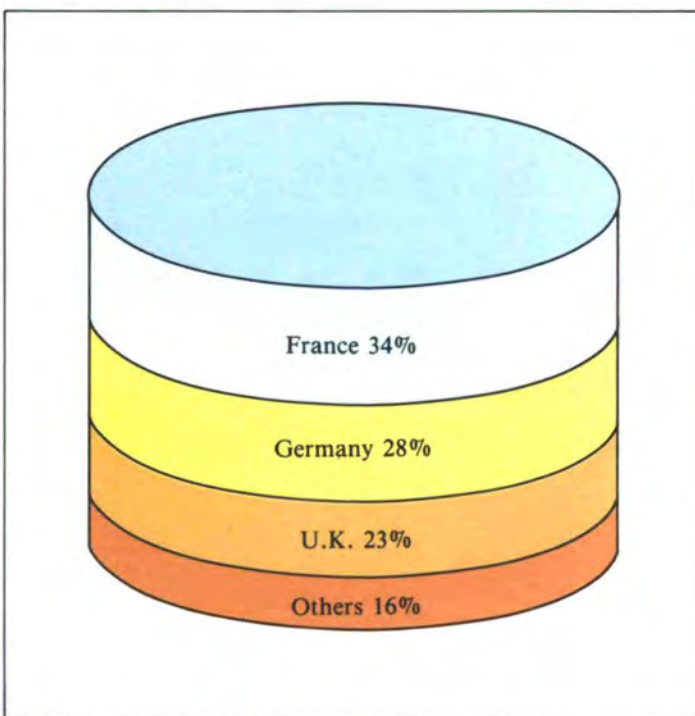


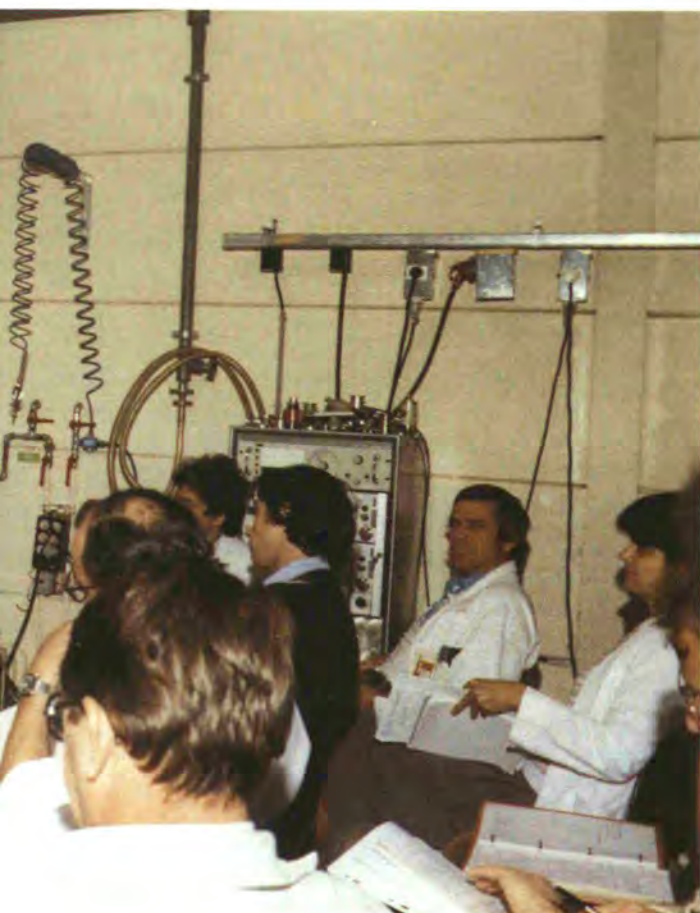
Figure 44: Percentages of guest scientists from the 3 member countries and other states.



WELFARE

The Welfare Section ("Relations Sociales") deals with general services (reception, post, drivers, reprography, cafeteria, etc.) problems of new arrivals, settling-in of families, housing, schools, and staff training.

It also provides administrative support for the medical service and the welfare adviser.



General services

In 1983 the receptionists assisted approximately 1400 people: reactor users, members of the Scientific Council and its sub-committees, seminars, workshops, etc. The formalities for these visits have been computerised, which simplifies them, particularly for the reactor users.

Reprography

The reprography workshop handled 295 originals (technical notes, scientific reports, theses, reactor cycle reports etc.), representing more than 4100 bound documents.

Reception and settling-in of families

Accommodation for staff and guest scientists

The ILL currently has 14 furnished flats, which were sublet to 50 families or groups of visiting scientists for periods of 2 weeks to 8-10 months.

The quest for flats or houses to rent for staff was still very difficult, particularly towards the end of the year. Nevertheless the section was able to assist 42 families.

Nineteen loans (up to 30.11.83) have been provided for a total value of 748 000 F under the "0.9%" law on aid for housing. In 1982 and 1983 9 members of staff obtained flats at a reduced rent in return for the payment of a subsidy by the ILL (average: 45 000 F per flat); four of these obtained houses in small groups outside Grenoble. (The photograph shows a group of houses at St. Jean de Moirans).

Schools

Number of children registered at the beginning of term in September 1983.

Ecole de la Houille Blanche (International Primary School)	64 of English and German mother-tongue, including 34 children of ILL staff and guest scientists.
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Collège d'Enseignement Secondaire and Lycée des Eaux Claires (Secondary Schools)	59 children of English and German mother-tongue, including 18 children of ILL staff and guest scientists.
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In the framework of staff training a series of courses on vacuum techniques was held at the ILL. In the picture is M. Rocco, engineer at the CENG, giving lectures in one of the ILL laboratories.

The ILL provides 9 teachers for these schools (including 6 part-time).

Children, teachers and parents bring a happy international atmosphere to the traditional christmas party at the international primary school (see photo).

Staff training

Each year the ILL prepares a programme of training courses for the staff. Approximately 250 to 270 requests for training (including French as a foreign language), are received and considered for the organisation of technical, language or general courses.

About 60% of the courses are in the *technical field*. A number of these are organised and/or given by ILL engineers or technicians, for example:

- an introduction to programmable control devices, under the responsibility of a reactor engineer
- an introduction to electronics, done completely by a young electronics engineer
- two sessions on vacuum techniques given on ILL premises by an engineer from the adjacent Centre d'Etudes Nucléaires de Grenoble, the practical work being done by the specialist technicians of the ILL Instrument Operation Department (see photograph).
- two computing courses have been run jointly by a professional computing instructor and an engineer from the ILL Computing Department.

The staff are very interested in advanced technology and request specialist courses on micro-computing, micro-electronics, programmable control devices, health physics techniques, etc. About 30% of the training covered *language courses*:

- in October 1983 beginners' and advanced courses in French as a foreign language covered 55 persons (including non-French scientists or technicians working at CNRS, CENG and IRAM). The courses are organised by ILL.
- English courses are based mainly on conversation connected with work (approximately 35 persons per year).
- 10 persons attend German classes.

General training

This covers activities such as car servicing, woodwork, health problems, etc, amounting to approximately 10% of the budget. The interest of ILL staff in their work is also shown by their desire to learn about or give instruction on their work environment. The organisation of a course entitled "Research around a large instrument" bears witness to this: three ILL scientists, in conjunction with the training group, organised this course for non-scientific staff, based on two themes:

- design and construction of an instrument
- planning and carrying out an experiment.

They called on members of staff representing various ILL activities, who collaborate on a construction or experiment project, who explained their work and where they fitted in, and arranged visits to their working areas.

A first course totalling 40 hours was enthusiastically attended by 14 staff. Eighteen persons are registered for the second course, which started in October 1983 and includes both new staff and others who have been at ILL for many years.

Medical service

ILL staff and long term guest scientists are subject to a close medical surveillance. Depending on where they work, each individual is required to attend one or two regular medical examinations per year, plus special examinations or analyses. This service works closely with the Safety and Health Physics Group, which helps to provide a good knowledge of work stations.



A group of houses at St-Jean-de-Moirans, 20 km from the ILL, available for staff and guest scientists.



The annual festival at the school "La Houille Blanche": a jolly international ambience.

FINANCE

The 1983 budget was authorised with an inflation rate of 8%, plus an additional reserve of 2%, and a further reserve of 2 000 000 F to cover the exchange rate risk associated with the fuel element budget. Apart from staff costs no real growth was possible despite the need to finance certain increases in expenditure associated directly with operation, such as electricity, tax on nuclear installations, heating, etc. From the beginning of 1983 the ILL Management, in accordance with French legislation, continued and completed the process of incorporating the contract staff. Of these 35 were incorporated in the ILL staff in 1982, and 23 during the first half of 1983.

The reduction in the number of reactor cycles from 5 to 4 resulted in a series of economies, mainly in the fields of energy, liquids and guest scientists, amounting to a total of approximately 1.6 MF. This sum was completely devoted to the financing of equipment for cutting off the damaged parts of the heavy water collector in the reactor.

During the last quarter of 1983, the initial work for the construction of a second neutron guide hall was started. In 1986 this building is due to accommodate the instruments on the new horizontal cold source. This new building will be financed under section 21 (buildings) in the Normal Budget and the Modernisation Programme Budget. For 1983, the sum of 3.1 MF was provided for this.

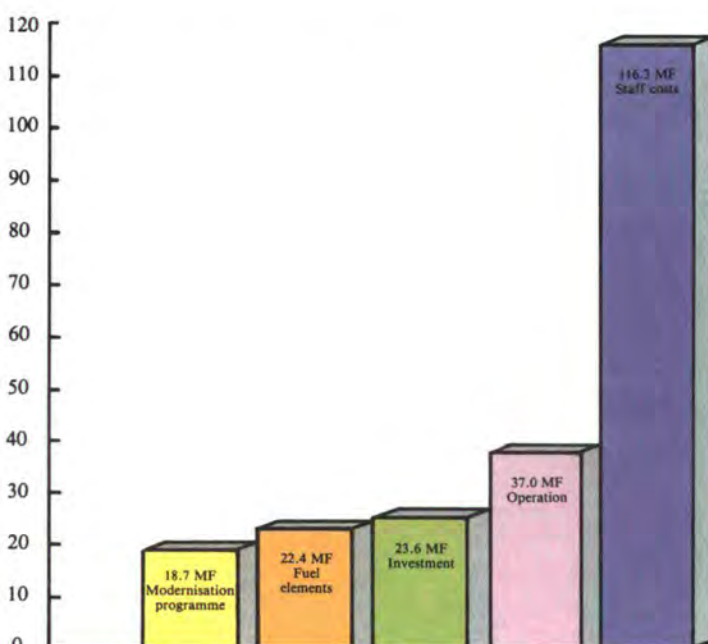


Figure 45: Associates' contribution 1983: 218 Million F.

The total expenditure for 1983 amounted to 228 MF excluding taxes (Normal and Modernisation Programme Budgets), of which 217.8 MF were financed by the Associates and 10.2 MF from ILL's own income (cf Fig. 45).

Implementation of the 1983 budget

Normal Budget

In 1983 the Normal Budget provided for 206.6 MF expenditure excluding taxes of which 199.2 MF were financed by grants from the Associates.

According to the provisional annual accounts to 31.12.83, the expenditure situation under the normal budget in comparison with 1982 was as follows (excl. taxes):

TABLE 8
Comparison of expenditure in 1983 and 1982

	1982		1983	
	(× 1000 F)	% of total	(× 1000 F)	% of total
<i>a) Operation</i>				
Consumable materials	13 006	7.2	14 063	6.8
Fuel elements	20 879	11.5	22 259	10.8
Staff costs	96 449	53.2	116 295	56.3
Taxes	701	0.4	936	0.5
Long term service and supply contracts	13 728	7.6	15 287	7.4
Other work, supplies and services	10 740	5.9	8 166	3.9
Transport, removal and travel expenses	1 600	0.9	1 733	0.8
Miscellaneous administrative costs	4 200	2.3	4 285	2.1
Total operation	161 303	89.0	183 024	88.6
<i>b) Investments</i>				
Buildings	487	0.3	1 160	0.6
Equipment	4 595	2.5	6 852	3.3
Experimental instruments	11 037	6.1	11 519	5.6
Other investments	3 738	2.1	4 042	1.9
Total investments	19 857	11.0	23 573	11.4
Total expenditure	181 160	100.0	206 597	100.0
<i>c) Income</i>				
ILL's own income	5 828	3.2	7 412	3.6
Grants from Associates	175 332	96.8	199 185	96.4
Total income	181 160	100.0	206 597	100.0

In comparison with the preceding year, the operation expenditure increased from 161.3 MF to 183 MF (+ 13.4%). If the expenditure on staff costs and fuel elements, for which steps were taken to finance the effects associated with inflation and the increases in the dollar and the DM, are excluded from this comparison, there is a reduction of 3.5 MF in real terms in the operation budget in comparison with 1982.

The investments increased by 7.9% in real terms in 1983.

Modernisation Programme Budget

The complete Modernisation Programme as scheduled from 1979 to 1985 was evaluated at 104.2 MF at 1979 prices, (cf Fig. 46). At the end of 1983, 73.8% of the aims had been achieved at a cost of 101.8 MF (76.9 MF in 1979 Francs).

The construction of a second neutron guide hall, the replacement of some of the beam-tube liners, the design and construction of the new second cold source are the main investments initiated in 1983, which will be continued in 1984-85.

The 1983 instalment of the Modernisation Programme Budget amounts to 21.8 MF, of which 3 117 000 F are covered by ILL's own income and 18.68 MF by the Associates' contributions.

The expenditure may be broken down by sections as follows:

TABLE 9
1983 Budget for the Modernisation Programme (excluding taxes)

	1983 (1000 F)	% of total
<i>a) Operation</i>		
Consumable materials and small equipment	298.5	1.6
Staff costs	3 944.0	21.1
Long-term service and supply contracts	308.0	1.6
Other work, supplies and services from third parties	3 215.5	17.2
Transport, removal and travel expenses	143.0	0.9
Miscellaneous administrative costs	173.0	0.9
Total operation expenditure	8 082.0	43.3
ILL's own income	3 117.0	-16.7
Total operation	4 965.0	26.6
<i>b) Investments</i>		
Buildings	1 994.0	10.7
Experimental instruments	11 721.0	62.7
Total investments	13 715.0	73.4
Total expenditure	18 680.0	100.0

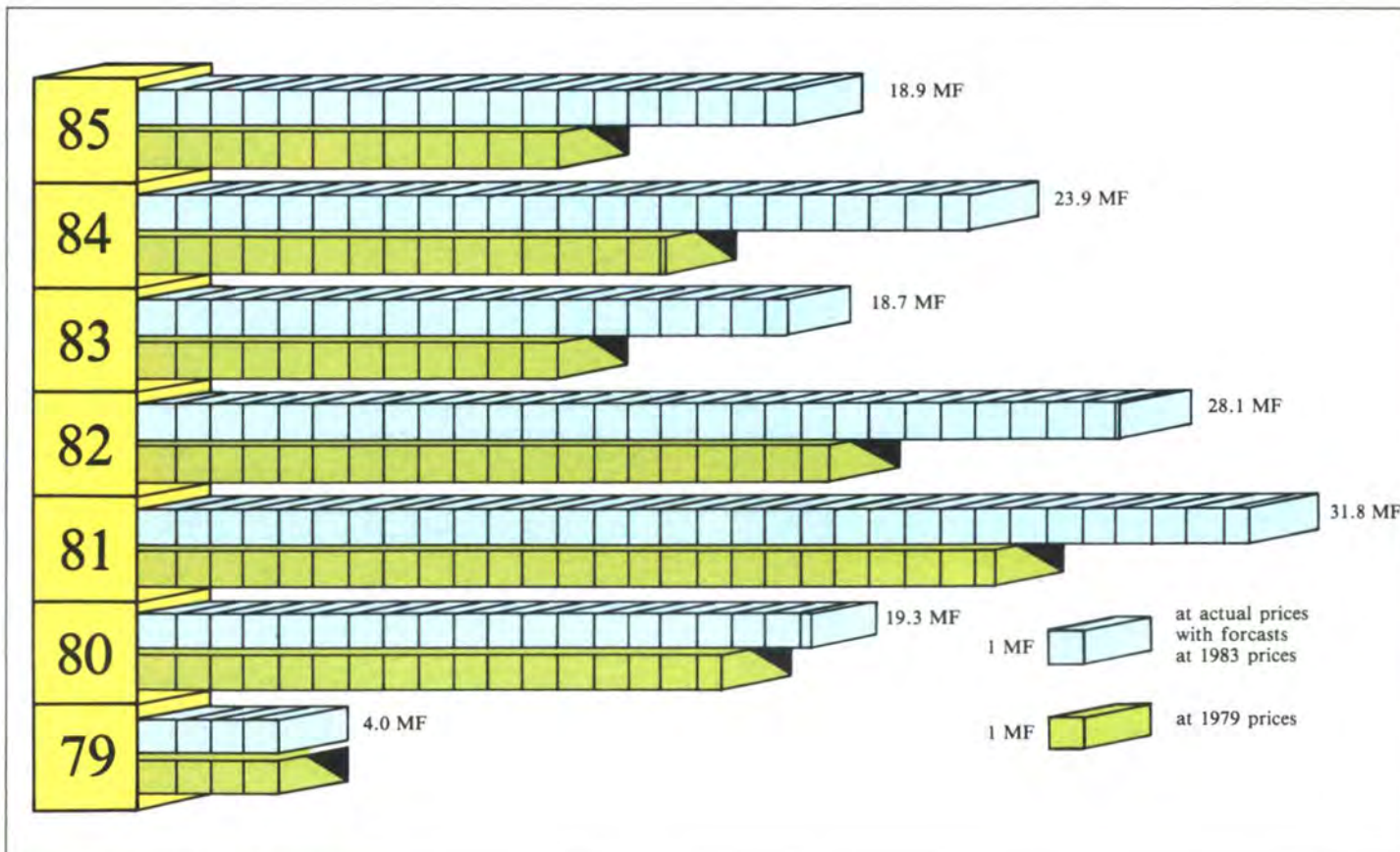


Figure 46 : The Modernisation Programme.

ILL budgets 1967-1983 and outlook for 1984-1987 (1983 prices)

The graphs of the ILL budgets from its foundation (1967) show the various phases of the Institut's development (cf Fig. 47). From 1967 to 1971 there was the construction phase for the buildings, the reactor and its associated installations, leading up to the reactor going critical in December 1971, which was followed by normal operation from 1972 to 1979.

In 1979 the ILL's Associates decided to implement the Modernisation Programme with a financial plan up to 1985. For the next few years, the ILL Management has planned to undertake a major programme of renovation of the reactor and of investments for the new instruments which will be installed on the new cold source. In addition to the financial problems resulting from inflation and the increases in the dollar and the DM in relation to the Franc, budgetary difficulties appear inevitable from 1986 in pursuing the proposed scientific aims and the financing of expenditure resulting from the end of the Modernisation Programme.

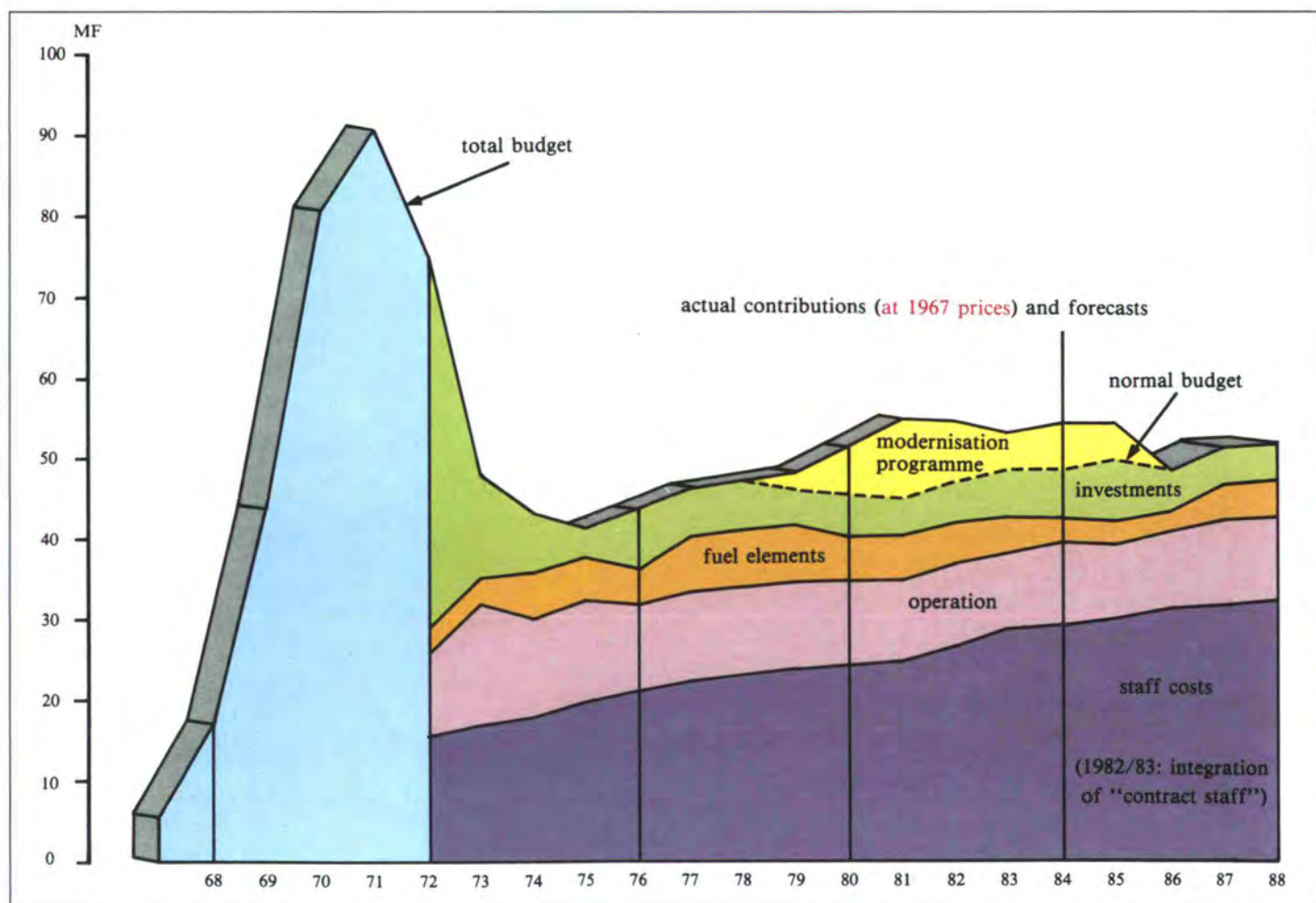


Figure 47: ILL Budgets 1967 to 1988 at 1967 prices.

Purchasing

The investment programme continued with a large number of important purchases in 1983. Orders were placed for the replacement of beam-tubes H1/H2 (5.1 MF to Neyrpic, Grenoble) and H6/H7 (0.9 MF to Interatom, Bergisch-Gladbach). The contract for the construction of a second Neutron Guide Hall was keenly contested and eventually placed with Negro, Grenoble at 5.8 MF. Noell, Würzburg, was awarded the contract for the design and construction of a remote control device for the reactor at 1.8 MF.

The ILL continued its efforts to maintain relationships with British and German companies, and to establish contacts with new suppliers. During the year several of these firms have visited the Institut and ILL scientists and engineers have travelled to production sites particularly in the three member states to inspect and test new equipment.

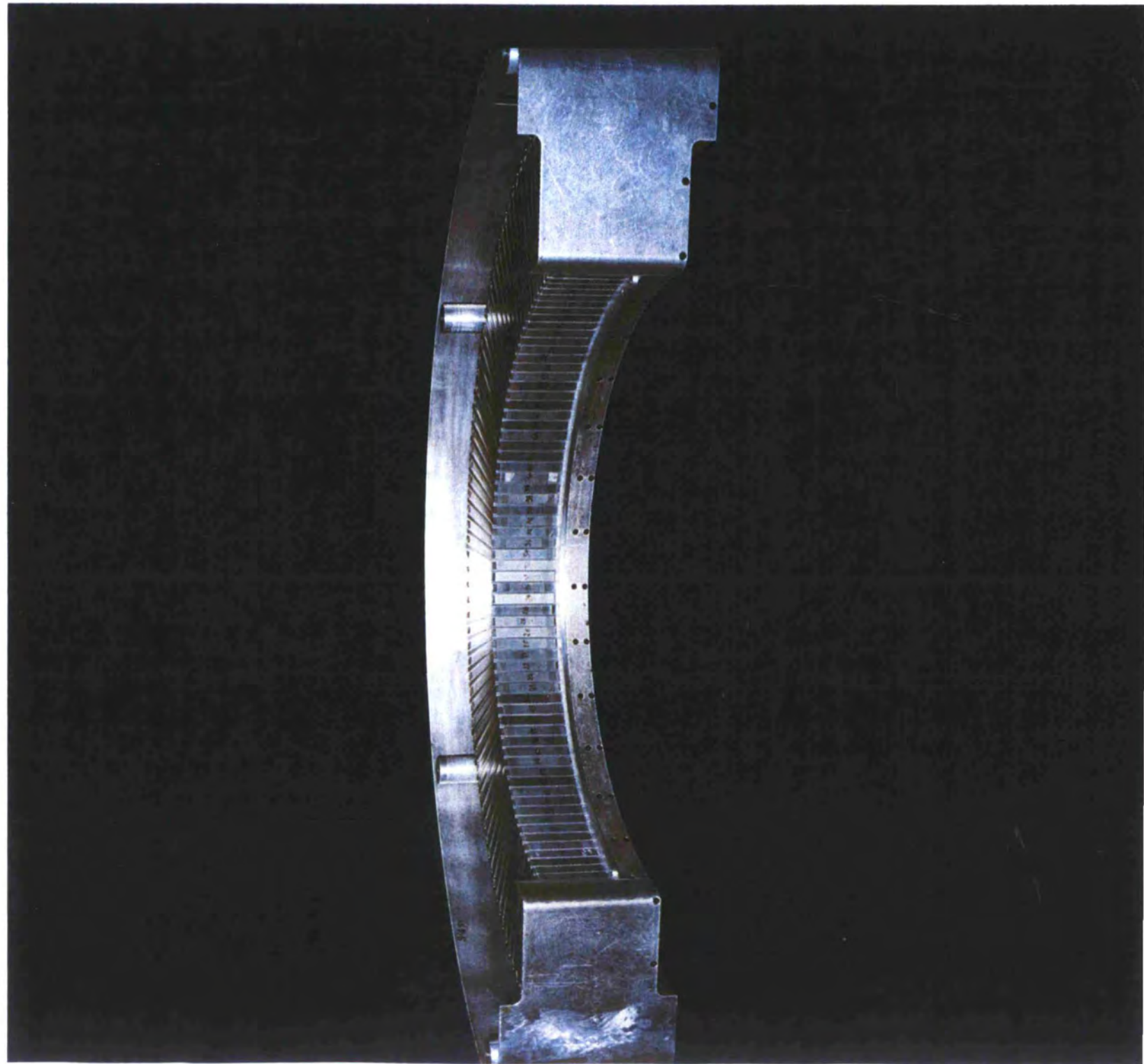
For all major purchases, firms of the three member states were consulted and the KFK and SERC also assisted by suggesting suitable suppliers in their respective countries. However, various factors, for example unfavourable exchange rates have caused British and German Companies to be less competitive with their tenders than French companies. As a result, the distribution of ILL's "free" purchases* in 1983 was as follows:

TABLE 10
Distribution of ILL's "free" purchases

	1983		1982
	MF	%	(for comparison) %
France	16.2	60	40
Germany	5.8	21	29
United Kingdom	2.3	8	18
Other	2.9	11	13
Total	27.2	100	100

* "Free" purchases means that a free choice of suppliers was possible, excluding therefore the fuel cycle, electricity and small purchases of less than FF 50 000.

The multidetector of the new very high resolution powder diffractometer D2B under construction.



MISCELLANEOUS

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05-81	Matrix protein : channel structure in a protein spanning the outer membrane of Escherichia coli. BUELDT G., ROSENBUSCH J. (Berlin).	D16	*9-03-319	Rotational transitions of H2 in condensed material. LANGEL W., BEAUFILS J.P. (ILL).	IN 5
05-85	Location of retinal in purple membrane protein. JUBB J. (Cambridge). WORCESTER D., ZACCAI G. (ILL).	D16	9-03-320	High resolution study of the tunneling spectrum of CH4 at very low temperatures. PRESS W. (Juelich). NEUMAIER K. (Garching). MORRISON J., LUSHINGTON K. (Hamilton). HEIDEMANN A. (ILL).	IN 5
05-89	Neutron diffraction study of the light triggered cascade reactions in retinal rod outer segments. CHABRE M., PFISTER C. (CEN-Grenoble). MINH-VUONG T. (Stanford). WORCESTER D. (ILL).	D11	9-03-326	Search for translational tunnelling in hydrogen bonded systems. HEIDEMANN A. (ILL). DYER M., THOMAS R.K. (Oxford).	IN13
05-91	Neutron scattering of cytochrome reductase. PERKINS S.J. (Heidelberg). WEISS H. (Duesseldorf).	D11 D17	9-03-330	Proton dynamics study in H3O+ClO4-. POTIER A., PHAMTI M. (Montpellier). DIANOUX A.J., POINSIGNON C. (ILL).	IN 6 IN10
05-95	Structure of the cholesteryl ester core of human plasma low density lipoproteins. Selective deuteration and neutron small-angle scattering. LAGGNER P. (Graz).	D11	9-03-332 9-03-338	Mechanism of hydrogen diffusion in HUP (hydrogen-uranyl phosphate). FENDER B.E.F., POINSIGNON C. (ILL).	IN 5 IN13
05-97	Study of the structure and molecular weight of the ADP/ATP carrier protein from beef heart mitochondria. LAUQUIN G., BLOCK M., VIGNAIS P. (CEN-Grenoble).	D11	9-03-334 9-03-338	Dynamical disorder in a two-dimensional ice : CsOH . H2O. DACHS H., JACOBS H.E., LECHNER R.E. STAHN M. (Berlin). SEE 9-03-332	IN 6 IN13
06-30	The structure of cauliflower mosaic virus. WITZ J., KRUSE J. (Strasbourg). TIMMINS P. (ILL).	D11	9-03-341 9-03-347	The rotational tunneling of the spherical top molecule NH3D. PRAGER M., PRESS W. (Juelich). HEIDEMANN A. (ILL). Fast hopping of CD3. CLOUGH S., ZELAYA F.O. (Nottingham). CAVAGNAT D. (Bordeaux/ILL). LASSEGUES J.C. (Bordeaux).	IN10 IN 5

COLLEGE 9 : CHEMISTRY

9-03-349	CH ₃ tunneling in Mn-acetate at temperatures below 1.2 K. HEIDEMANN A. (ILL). MCDONALD P., CLOUGH S. (Nottingham). NEUMAIER K. (Garching).	IN13	TABONY J., HAYOUN M. (CEN-Saclay).	
9-03-350	Proton tunnelling in tropolone. WHITE J.W., JACKSON I.P. (Oxford). LASSEGUES J.C. (Bordeaux).	IN13	9-05-352 Molecular motions in micelles and microemulsions. TABONY J., LLOR A., DRIFFORD M. (CEN-Saclay).	IN 6 IN10
9-03-351	Dynamics of hydrogen bonds in carboxylic acid dimers. ERNST R.R., MEIER B.H. (Zuerich). FURRER A., STOECKLI A. (Wuerenlingen). HEIDEMANN A. (ILL).	IN13	9-05-352 Molecular motions in micelles and microemulsions. TABONY J. (CEN-Saclay).	IN 6
9-03-355	Reorientations in the different phases of norbornane, norbornylene and norbornadiene. BEE M. (ILL). JOBIC H. (Lyon).	IN 6	9-05-354 Microémulsions fluorées. RAVEY J.C., DELPUECH., STEBE (Nancy).	D17
9-03-356	Rotational motions in trimethyloxosulfonium halides. BEE M. (ILL). SOURISSEAU C. (Bordeaux). JOBIC H. (Lyon).	IN 5	9-05-354 Micro-emulsions with non ionic surfactants. RAVEY J.C., BUZIER M. (Nancy).	D17
9-03-357	Reorientational motions and dimerization in trimethylacetic acid. LONGUEVILLE W., AMOUREUX J.P. (Lille). BEE M., POINSIGNON C. (ILL).	IN10	9-05-357 Solvent effects on the structure of water-in-oil microemulsions. DORE J.C., TOPRAKCIOGLU C. ROBINSON B.H. (Kent).	D17
9-03-358	Reorientational motions in NH ₃ SO ₃ and C ₄ H ₄ SCr(CO) ₃ . LUCAZEAU G., BOCQUET J.F., CHHOR K. (Villetaneuse).	IN 6	9-05-360 Critical scattering from microemulsions. TABONY J., DRIFFORD M., GEYER A. DE (CEN, Saclay).	D17 D11
9-03-359	SEE 5-22-232		9-05-363 Hydrodynamic interactions in colloidal dispersions. CEBULA D.J., HAYTER J.B. (ILL). MARKOVIC I., OTTEWILL R.H. PUSEY P.N. (Bristol).	IN11
9-04-299	Vibrations of molecular species chemisorbed on rutile (TiO ₂). THOMAS R.K., HUNT G.M. (Oxford).	IN 6	9-05-368 SEE 9-05-347	
9-04-301	Test of model of methyl dynamics for high hindering barriers. CLOUGH S. (Nottingham).	IN 4	9-05-371 Critical concentration fluctuations in binary lipid alloys. KNOLL W., SCHMIDT G., SACKMANN E. (Muenchen). IBEL K. (ILL).	D11
9-04-303	Phonons in mixed-valency antimony (III,V), M(III) Sb(V) and SN(IV) hexahalide salts. DAY P., PRASSIDES K. (Oxford).	IN 6	9-05-375 Concentration effects on structure of unilamellar vesicles. HIGGINS J.S., CUMMINS P.G. MUDDLE A.G. (London).	D11
9-05-304	Ion distribution and electrostatic potential in the aqueous phase between charged phospholipid bilayers. BUELDT G. (Berlin). OBERTHUER R.C. (ILL).	D17	9-05-377 Critical reflection to study black films. THOMAS R.K., HIGHFIELD R.R. CUMMINS P.G., WILLITT A., MINGINS J. GREGORY D.P. (Oxford).	D17
9-05-330	Solubilisation in ionic micelles. HAYTER J.B. (ILL). PENFOLD J. (Rutherford).	D17 IN11	9-06-388 Rotational tunnelling of hydrogen in porous aluminosilicates. THOMAS R.K., COLLINSON S. (Oxford).	IN 6
9-05-336	Micelles of mixed hydrocarbon and fluorocarbon surface active agents. CEBULA D.J. (RHEL/ILL). OTTEWILL R.H. (Bristol).	D17	9-06-398 Dynamics of H ₂ O molecules absorbed in synthetic A zeolite. CARRU J.C., AMOUREUX J.P. TABOURIER P. (Lille). BEE M. (ILL).	IN 5
9-05-345	Critical reflection from fatty acid monolayers. THOMAS R.K., MINGINS J. HIGHFIELD R.R., HUMES R.P. (Oxford). GREGORY D.P., CUMMINS P.G.	SP.BE (S 3)	9-06-425 The tunnelling of CH ₃ D on graphite. THOMAS R.K., BALL P., ROSER S.J. (Oxford).	IN 5 IN10
9-05-347	Magnetic colloids.	D11	9-06-434 Quasielastic neutron scattering on LiC ₆ . MAGERL A. (ILL). ZABEL H. (Illinois).	IN10
9-05-368	CEBULA D.J. (Rutherford). CHARLES S.W., POPPLEWELL J. (Bangor).	D17	9-06-437 Fine structure in the tunnelling of H ₂ in graphite intercalates. WHITE J.W., JACKSON I.P. (Oxford). BEAUFILS J.P. (ILL).	IN 5
9-05-350	Internal structure of micelles. CABANE B. (Orsay). DUPLESSIX R. (Strasbourg). ZEMB T. (Saclay).	D17 D1B	9-06-442 Dynamics of CH ₃ OH in ZMS-5 zeolite. RENOUPREZ A., JOBIC H. (Lyon). POINSIGNON C., BEE M. (ILL).	IN 6 IN10
9-05-351	Structure of cationic micelles. TABONY J., DRIFFORD M. (CEN, Saclay).	D16 D17	9-07- 42 Deuterium ordering in graphite intercalates. NAYLOR G.R.S., WHITE J.W. (Oxford).	D 1A D16
*9-05-351	Structure of cationic micelles. TABONY J. (CEN-Saclay).	D16	9-07- 45 Liquid-structure factor of ³⁶ Ar on graphite. LAUTER H.J. (ILL). OBERMAYER P. (Regensburg). TIBY C. (Mainz).	D 2
9-05-351 9-09- 26	Local structure of surfactant (alcohol mixed micelles).	D16	9-07- 60 Island sizes in graphite intercalation compounds.	D11

	WHITE J.W. ,TROUW F. (Oxford). MAGERL A. (ILL).		9-13- 29	A neutron small angle scattering study on molecular conformation of polyethylene terephthalate.	D11
9-07- 64	Localization of benzene in the network of a Y-zeolite. RENOUPREZ A. (Villeurbanne). JOBIC H. ,FITCH A.N. (ILL).	D 1A		ZACHMANN H.G. ,FISCHER E.W. ,HAHN K. KUGLER J. (Mainz). WISWE (Hamburg).	
9-07- 71	SEE 9-07- 60		9-13- 30	Conformation of molecules in semi-crystalline polymers.	D 1B
9-07- 73	Structural studies of the intercalation compound TiS ₂ .(CD ₃ NC)0.5. FENDER B.E.F. ,COCKCROFT J.K. (ILL).	D 1A	9-13- 35	Structural studies of highly conducting doped polyacetylenes by inelastic neutron scattering.	IN 4
9-08- 15	Study of the rotational diffusion in the rotator phase of n-alkanes. DOUCET J. (Orsay).	IN 6	9-14- 23	Conformation of chain molecules in oriented amorphous polymers.	D17
9-09- 8	Rod-like nonionic micelles in a shear gradient. RAVEY J.C. ,STEBE (Nancy). OBERTHUER R.C. ,LINDNER P. (ILL).	D11	9-14- 24	Observation of separated retraction and disengagement processes in strained polystyrene films.	D11 D17
9-09- 9	Structure of amphiphilic aggregates in isotropic micellar phases. HENDRIKX Y. ,CHARVOLIN J. (Orsay). OBERTHUER R.C. ,LINDNER P. RAWISO M. (ILL).	D11	9-14- 25	"Network effect" of long chains in shorter chemically identical chains.	D11
9-09- 11	Test of a q ³ behaviour of critical concentration fluctuation in a 3-component microemulsion. TEIXEIRA J. ,FARNOUX B. (LLB,Saclay). CHEN S.H. (Cambridge,US).	IN11	9-14- 45	FROELICH D. ,PICOT C. ,MULLER R. (Strasbourg).	D17
9-09- 26	SEE 9-05-351		9-14- 26	Radius of gyration in anisotropically swollen networks.	D11
9-11- 53	Study of the effect of pressure on the dynamics of polymer chains. HIGGINS J.S. ,MA K.T. ,ROOTS J.E. (London).	IN10	9-14- 32	Conformation and interaction of isolated polymer coils in a shear gradient (9-14-32) block allocation with (9-12-15):SANS-investigation of the ordering of an unscreened polyelectrolyte solution in a shear gradient.	D11
9-11- 60	Conformation of styrene-methyl methacrylate b block copolymers in selective solvents. RICHARDS R.W. ,EDWARDS C.J.C. (Strathclyde).	D11 D17	9-12- 15	LINDNER P. ,OBERTHUER R.C. (ILL). KIRSTE R.G. (Mainz).	
9-11- 66	Dynamics of bulk polymers. HIGGINS J.S. ,ROOTS J.E. (London).	IN10	9-14- 35	Separated retraction and disengagement process in strained polystyrene films :universal time behaviour.	D11 D17
9-11- 74	Thermodynamic properties and conformation of polymers in solution under high pressures. LECHNER M.D. ,EXELER N. VENNEMANN N. (Osnabrueck). BANTLE S. ,OBERTHUER R.C. (ILL).	D11	9-14- 37	Dimensions of a polymer chain in a crosslinked network.	D11 D17
9-12- 13	Dynamics of flexible polyelectrolyte solutions and electrostatic length. NALLET F. ,NIERLICH M. ,COTTON J.P. (CEN-Saclay). HAYTER J.B. (ILL).	IN11	9-14- 43	Conformation study of labelled paths in dry and swollen networks.	D11 D17
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9-13- 18	Oriented solution grown crystals of isotactic polystyrene. SADLER D.M. ,SPELLS S.J. (Bristol). GUENET J.M. (Strasbourg).	D11	9-14- 45	"Network effect" of long chains in shorter chemically identical chains.	D17
9-13- 21	Chain conformation in crystals of low molecular weight PEO. FISCHER E.W. ,BORN R. ,HAHN K. (Mainz).	D17 D 1B	9-14- 47	Dynamic relaxation in polydimethylsiloxane networks.	D11
9-13- 21	Chain conformation in crystals of low molecular weight PEO. FISCHER E.W. ,BORN R. (Mainz).	D11	9-15- 26	Conformation in two-phase polymeric systems.	D17
9-13- 23	Near range order in amorphous and semicrystal. polymers studied by neutron scattering from partly deuterated molecules. FISCHER E.W. ,BORN R. (Mainz). KUGLER J. (ILL).	D16	9-15- 67	HIGGINS J.S. ,CARTER A.J. TOMLINS P. (London).	
9-13- 27	Neutron powder diffraction on doped organic polymers. HAESSLIN H.W. (Basel). RIEKEL C. (Hamburg).	D 1B	9-15- 32	Conformation of copolymer molecules embedded within a homopolymer matrix.	D11 D17
			9-15- 48	GALLOT Y. ,DUPLESSIX R. ,RAMEAU A. SELB J. ,MARIE P. (Strasbourg).	
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9-15- 53	SANS-Investigations on electrically conducting polymer systems. RIEKEL C. (Hamburg). HAESSLIN H.W. (Basel).	D17	9-15- 70	SEE	9-15- 32	
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9-15- 69	Self-organization of synthetic polymer molecules. KIRSTE R.G. ,SCHMITT B.J. SCHMITT-STRECKER S ,OHM H. (Mainz).	D11	9-15- 83	Kinetics of phase separation in polymer blends. HIGGINS J.S. ,TOMLINS P. ,HILL R. (London).		D11
9-15- 69	Self-organization of synthetic polymer molecules.(Supplement) KIRSTE R.G. ,SCHMITT B.J. SCHMITT-STRECKER S ,OHM H. (Mainz).	D17	9-15- 89	Segregation and chain conformation in polyurethanes. FISCHER E.W. ,STRUTH U. ,HAHN K. (Mainz).		D17

I.L.L. WORKSHOPS AND CONFERENCES

WORKSHOPS ORGANIZED BY THE I.L.L. IN 1983

Workshops on "COSI FAN TUTTE" (organized by F. Gönnerwein)	I.L.L. February 8, 1983
Workshop on "3d Metallic Magnetism" (83Z118T) (organized in collaboration with the Laboratoire Louis Néel of the CNRS Grenoble by D. Givord and K.R.A. Ziebeck)	I.L.L. March 25-26, 1983
Workshop on "Data Treatment for Studies of Concentrated Polymer Solutions and Colloids" (organized by R.E. Ghosh, J.B. Hayter, R.C. Oberthür)	I.L.L. March 29-30, 1983
"Lectures on the IBA Model" (83SC11T) (organized by K. Schreckenbach)	I.L.L. May 10-11, 1983
Workshop on "Use of Neutrons in Technologically Important Problems in Powders, Gels and Colloids" (organized by J.P. Beaufils and J.B. Hayter)	I.L.L. October 27-28, 1983
Workshop on "Reactor Based Fundamental Physics" (organized by B. Desplanques, F. Gönnerwein, W. Mampe) (Proceedings to be published in Journal de Physique)	I.L.L. November 7-9, 1983

WORKSHOPS SPONSORED BY THE I.L.L. IN 1983

Workshop on "Beam Definition Devices : Neutron Monochromators, Mirrors, Polarizers, Choppers" (organized by T. Springer and H.H. Stiller, sponsored by the I.L.L.) (Lectures published by KFA 1983)	IFF/KFA Jülich June 9-10, 1983
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I.L.L. WORKSHOPS PUBLISHED IN 1983

"The Impact of Polarised Neutrons on Solid-State Chemistry and Physics" Journal de Physique-Colloque 43, C7 (1982). International Conference sponsored by the European Physical Society, la Société Française de Physique, the Institute of Physics, die Deutsche Physikalische Gesellschaft (organized by P.J. Brown, R. Lemaire, J. Schweitzer), and held at the I.L.L., October 15-19, 1982 (Les Editions de Physique 1983).
"Position-Sensitive Detection of Thermal Neutrons" P. Convert, J.B. Forsyth Eds. (Academic Press 1983). Based on the Proceedings of the Workshop on Position-Sensitive Detection of Thermal Neutrons, held at the I.L.L., October 11-12, 1983.

I.L.L. SPONSORED WORKSHOP PUBLISHED IN 1983

"The Neutron and its Applications, 1982" P. Schofield Ed. (Conference Series Number 64, The Institute of Physics 1983). Plenary and invited papers from the Conference to mark the 50th Anniversary of the Discovery of the Neutron held at Cambridge, September 13-17, 1982, sponsored by the I.L.L.

THESES

The experimental work of which was carried out at I.L.L.	
Jean-Pierre AIME	Thèse de Doctorat ès Sciences Physiques Université de Paris VII (novembre 1983). Etude de la réaction topochimique en phase solide d'un diacétylène (pTS) par diffraction des neutrons.
Peter BOPP	Inaugural-Dissertation zur Erlangung der Doktorwürde der Naturwissenschaftlich-Mathematischen Gesamtfakultät der Ruprecht-Karls-Universität Heidelberg (1983). Die Beta-Asymmetrie im Zerfall des freien Neutrons.
Pierre CENEDESE	Thèse de Doctorat d'Etat, Université Pierre et Marie Curie Paris VI (décembre 1983). Ordre à courte distance dans les solutions solides métalliques.
Claude COMTE	Thèse de Doctorat ès Sciences Physiques, Université Louis Pasteur de Strasbourg (janvier 1983). Etude de la condensation de Bose de paires électron-trou sur toute la gamme des densités.
Bernard CROSET	Thèse de Doctorat d'Etat, Université d'Aix-Marseille II, Faculté des Sciences de Luminy (février 1983). Etude de la physisorption par diffraction élastique de neutrons, application à la monocouche de tétrafluorométhane adsorbé sur graphite.
Béatrice GILLON	Thèse de Doctorat ès Sciences Physiques, Université Pierre et Marie Curie Paris VI (mars 1983). Densité de spin dans les radicaux libres. Utilisation de la diffraction neutronique.
Gerhard KIESE	Inaugural-Dissertation zur Erlangung der Doktorwürde der Naturwissenschaftlichen Fakultät der Philipps-Universität Marburg/Lahn (1983). Untersuchung von Legierungssystemen mit und ohne Tendenz zur Verbindungsbildung in der Flüssigkeit. Spin-Gitter Relaxation an ⁶ Li in Li-Na, -Mg, -Pb und -Bi.
Ulrich KISCHKO	Dissertation zur Erlangung des Doktorgrades der Naturwissenschaften der Abteilung Physik der Universität Dortmund (1983). Intensitätsprofile hinter einem fünfstufigen Neutronen-Interferometer.
Eberhard KOGLIN	Inaugural-Dissertation zur Erlangung des Doktorgrades der Naturwissenschaften der Justus-Liebig-Universität Gießen (1982). Halbwertszeiten neutronenreicher Nuklide.

PUBLICATIONS

INTERNAL REPORTS 1983

T = Technical reports
G = General reports

83EP1T
EPAUD F. : Module de visualisation graphique pour le système d'acquisition modulaire Camac - échelle Lecroy 4434. Display driver. (Version 3)(DD.03) TECHNICAL REPORT

83HE2T
HEIDEMANN A. ,MAGERL A. : Proposal for a backscattering spectrometer with increased flux on the second cold source. TECHNICAL REPORT

83LE3G
LEFEBVRE Y. : Expérience IN11. Extensions mises en place pendant l'arrêt annuel. GENERAL REPORT

83CU4G
CURRAT R. ,NAGEL D. : User's guide for IN8. GENERAL REPORT

83CH5G
CHRISTENSEN A.N. ,GHOSH R.E. : Three-D: Display and manipulation of data represented as 3-dimensional surfaces. GENERAL REPORT.

83SC6T
SCHUMACHER M. ,RULLHUSEN P. ,ZURMUEHL U. ,SMEND F. ,BOERNER H.G. ,KERR S.A. : On the use of gamma-ray scattering as a tool for nuclear structure investigations below particle threshold. TECHNICAL REPORT

83NA7G
NAGEL D. : Programmer's guide for IN8. GENERAL REPORT

83BE8T
BEE M. : Analysis of data from time of flight and backscattering experiments : a graph plotting program : "screen". TECHNICAL REPORT

83AG9T
AGERON P. ,ROBERT A. : Preliminary study of the nuclear heating of a liquid hydrogen cold source in the reflector of the FRG 1 reactor. TECHNICAL REPORT

83BA10G
BARTHELEMY A. ,LESOURNE M. : Réseau JUDAS. Notice technique I.L.L./D.I.E. Version 1B. GENERAL REPORT

83SC11T
SCHRECKENBACH K. : Presented view-graphs of 'Lectures on the IBA model' held on May 10-11, 1983 at the ILL, Grenoble, France. TECHNICAL REPORT

83LE12G
LEFEBVRE Y. : Connexion de l'expérience S21 à un ordinateur PDP 11/10. GENERAL REPORT

83BR13G
BRISSOT R. ,DEICHELBOHRER C. ,LEDEBT P. : Data acquisition for PN8. GENERAL REPORT

83MA14T
MAGALLON I. : Mesure de la demi-vie du neutron. Détecteur d'électrons de faible énergie émis lors de la désintégration. TECHNICAL REPORT (Rapport de stage ENSIEG)

83FI15T
FILHOL A. ,BROWN P.J. ,LAUGIER J. : Some computer programs available to aid the indexing of single crystal diffraction patterns. TECHNICAL REPORT

83ST16T
STANSFIELD R.F.D. : EULER program manual. TECHNICAL REPORT

83BE17T
BEE M. : Multiple scattering effects in model systems. TECHNICAL REPORT

83GI18T
GIVORD D. ,ZIEBECK K.R.A. : 3-D metallic magnetism. Proceedings of the workshop on 3-D magnetism held at the ILL 25-26 March 1983. TECHNICAL REPORT

83MA19T
MAGERL A. ,HEIDEMANN A. : Thoughts about the primary spectrometer of IN10B. TECHNICAL REPORT

83NE20G
NELSON R. : Program R. A raw data manipulation program. GENERAL REPORT

83BL21G
BLANC Y. : Le spectromètre à temps de vol IN6 . Caractéristiques techniques et performances. GENERAL REPORT

83TH22G
THOMAS M. ,PIOTTI M. ,MUNNIER J. : Etude de la précision et de la linéarité d'un codeur incrémental "Heidenhain ROD 456" . GENERAL REPORT

83IB23T
IBEL K. ,BOGENBERGER J. ,FOOTE A.M. : A dialysis cell for neutron small angle diffraction experiments. TECHNICAL REPORT

83ST24T
STIRLING W.G. ,KAISER W. : Preliminary technical specifications for triple-axis spectrometer IN14. TECHNICAL REPORT

83FR25T
FREUND A.K. ,JOENSSON S. : Development of beryllium single crystals for neutron monochromators. TECHNICAL REPORT

83HO26T
HOFFMANN H. ,ASTRUC J.M. : Source froide horizontale. Essais de dynamique de fluides sur le modèle modérateur en courant d'eau et d'air. Première partie. TECHNICAL REPORT

83HO27T
HOFFMANN H. : Source froide horizontale. Essais expérimentaux du refroidissement de la cellule - SFH avec azote gazeux. TECHNICAL REPORT

83HO28T
HOFFMANN H. : Source froide horizontale. Les pertes de charge de la maquette D2 avec tubes coaxiaux. Comparaison des résultats de calcul avec les résultats des essais en D2. TECHNICAL REPORT

83PA29T
PATER B. ,GHOSH R. E. : TAPDAT. A program to copy ILL standard raw data files to magnetic tape in IBM or ANSI format. TECHNICAL REPORT.

83JA30T
JACOBE J. : Multidéetecteur pour D20. Essais comparatifs d'un système à gaz et à scintillations. TECHNICAL REPORT

83MA31G
MAIER B. : Neutron beam facilities available for users. (Edition December 1983) GENERAL REPORT.

PUBLICATIONS IN BOOKS, PERIODICALS, CONFERENCE PROCEEDINGS, 1983

I. - Publications with I.L.L. authors and co-authors

(Code number from 101 to 465)

83WA101
WALKER M.B. ,MCEWEN K.A. : Models determining the magnetic structure of neodymium near TN. JOURNAL OF PHYSICS F VOL. 13, PP. 139-144 (1983)

83CH102
CHERNYSHOV A.A. ,DORNER B. ,PUSHKAREV V.V. ,RUMYANTSEV A.YU. : Electron-phonon interactions in magnesium measured by inelastic neutron scattering. JOURNAL OF PHYSICS F VOL. 13, PP. 33-39 (1983)

83HA103
HAYTER J.B. ,PYNN R. ,SUCK J.B. : On the structure of liquid alkali metals. JOURNAL OF PHYSICS F VOL. 13, PP. L1-L6 (1983)

83SU104
SUCK J.B. ,RUDIN H. ,GUENTHERODT H.J. ,BECK H. : Experimental investigation of the dispersion of collective density fluctuations near Q_p in a metallic glass. PHYSICAL REVIEW LETTERS VOL. 50, PP. 49-52 (1983)

83NA105
NALLET F. ,JANNINK G. ,HAYTER J.B. ,OBERTHUER R.C. ,PICOT C. : Observation of the dynamics of polyelectrolyte strong solutions by quasi-elastic neutron scattering. JOURNAL DE PHYSIQUE VOL. 44, PP. 87-99 (1983)

83LY106
LYNN J.W. ,PYNN R. ,JOFFRIN J. ,RAGAZZONI J.L. ,SHELTON R.N. : Investigation of the modulated magnetic phase of superconducting HoMo6S8. PHYSICAL REVIEW B VOL. 27, PP. 581-584 (1983)

83SN107
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HOWE A.T. HOWELLS W.S. HOYLER F.	83HE1021 83KE394 83DA396 83BE143 83PL427 83MA346 83HU369 83HU370 83HU371 83HU395 83MA397 83HU128 83DI151 83MU180 83IB23T 83IB278 83SI311 83KN364 83AR215 83RI243	KEYSER U. KHAMIS H.W. KHAN S. KIESE G.	83KE341 83WI1087 83TR413 83KI120 83AC188 83HE238 83ST1074 83GO272 83BA207 83SU253 83RA265 83KJ195 83ST1049 83KL1008 83FA327 83IB278	LEBET P. LEFEBVRE J. LEFEBVRE Y.	83LE1023 83DU236 83DA1068 83MC209 83DI151 83BE335 83LE1052 83ST1053 83LE1059 83PL427 83BR13G 83EH134 83CH1001 83LE3G 83LE12G 83DU150 83DE368
HUTCHINGS M.T.	83DI151 83MU180 83IB23T 83IB278 83SI311 83KN364 83AR215 83RI243	KILVINGTON I. KISCHKO U.	83ST1074 83GO272 83BA207 83SU253 83RA265 83KJ195 83ST1049 83KL1008 83FA327 83IB278	LEFEBVRE Y. LEFUR D. LEGRAND E.	83CH1001 83LE3G 83LE12G 83DU150 83DE368
IBEL K.	83IB23T 83IB278 83SI311 83KN364 83AR215 83RI243	KJAER K. KJEMS J.K. KLEIN A.G. KLEWE-NEBENIUS H. KLINGHOLZ R.	83KJ195 83ST1049 83KL1008 83FA327 83IB278		
ISHIKAWA Y. IWASAKI S.	83AR215 83RI243				

LEHMANN M.S.	83W1140 83DE368 83HE380 83KU381 83CH464	MARISCOTTI M.A.J.	83MA346 83MA397	MOZE O.	83BU219
		MARMEGGI J.C.	83MA304	MUELLER R.	83MU181
LEHNER N.	83RA162 83FI420 83CH465	MARSEGLIA E.A.	83MA1032 83MA1085	MUELLER-WARMUTH W.	83FU182
		MARTI C.	83PA228	MUENNICH F.	83HE238
LEMAIRE R.	83AL173 83GI183 83BA185 83GI379 83GI411	MARTIN W.	83TH1084	MUENNINGHOFF G.	83MU180
		MARUANI J.	83LA1011	MUENZEL J.	83MU342
			83BO178	MUNNIER J.	83TH22G
		MASON R.	83BO359	MURANI A.P.	83ME137
			83FI1004		83DA164
LEROUX B.	83CA133 83HE410	MASON S.A.	83FI1054		83SO222
			83FI1055		83FI231
LESOURNE M.	83BAL0G		83ER119		83FI262
LEVITIN R.Z.	83BA185		83HO166		83MU314
LEWIT-BENTLEY A.	83RO442 83MO448		83DE245		83MU320
		MASSA N.E.	83BE377	MURRAY A.D.	83HE386
LHOSPICE G.	83HA1073	MATHIOT J.F.	83TH443	MUTTERER M.	83MU388
LIEBERT L.	83HE373	MAUREL M.	83ST445		83BA1042
LIETZKE R.	83NI309 83NI430	MAY R.P.	83RE130		83QU123
			83PL427	NAGEL D.	83HE410
LIN C.	83BL1047		83DJ401		83CU4G
LINDLEY E.J.	83BU219		83DE138	NALLET F.	83NA7G
LITCHINSKY D.	83EG146		83MA261	NASSIF E.	83NA105
LIU D.W.	83PE449		83NI309	NATKANIEC I.	83NA1010
LLOR A.	83TA1093		83SI311	NAUMANN R.A.	83NA333
LOEWENHAUPT M.	83FR352		83SE340	NEILSON G.W.	83DE248
LOIDL A.	83KN132	MAZID M.	83NI430	NELMES R.J.	83NE1091
LONGUEVILLE W.	83BE127	MAZURE-ESPEJO C.	83MA438		83KU367
LOPES L.C.	83LO212		83DA1068	NELSON R.	83ST445
LORBER B.	83MO448		83BA170	NEWNS D.M.	83NE20G
LORENZELLI N.	83MO1095	MCEWEN K.A.	83MA294		83RE274
LOUCHEUX-LEFEBVRE	83LI199		83BA296		83NE378
LU Q.	83AL173		83WA101		83BA428
LUCAS B.W.	83AH271 83AH418		83MC209	NICHOLSON L.K.	83RE429
			83ST220	NIELSEN M.	83HI277
LUCAZEAU G.	83GA109 83SO136 83LU251 83SO336	MCMILLAN P.W.	83MC221	NIEPCE J.C.	83KJ195
		MCTAGUE J.P.	83MC299	NIERHAUS K.H.	83CH459
		MELLEMA J.E.	83WR343		83NI309
LUDI A.	83BR179		83KJ195	NIFENECKER H.	83NI430
LUSHINGTON K.J.	83LU111 83HE358	MELONE S.	83OO1080		83OE122
		MERCIER R.	83CU1082	NOGUERA S.	83DJ401
LUTY T.	83CH1001	MESSOLORAS S.	83ME361	NOGUES M.	83DE402
LYNN J.W.	83LY106 83LY218 83PY330	MEZEI F.	83PO254	NOUET J.	83FI231
			83BE1094	NOWOTNY V.	83BA363
			83ME137		83NI309
MA K.	83HI277		83ME155	NOZIERES P.	83NI430
MAGALLON I.	83MA14T		83ME167	OBERMAYER P.E.	83NO192
MAGERL A.	83HE2T 83MA19T 83MA129 83ZA249 83ZA273 83MA290 83MA349 83ZA374	MIERZEJEWSKI A.	83ME230	OBERTHUER R.C.	83LA196
		MINGINS J.	83WI232		83NA105
MAGID L.J.	83TR321	MIREBEAU I.	83ME258	OED A.	83OB260
MAIER B.	83MA31G	MITCHELL E.W.J.	83ME275		83LI347
MAKI K.	83LU111	MIURA M.	83ME293	OHM H.	83OE117
MAKOSHI K.	83MA282 83NE378 83BR428	MOENKEMEYER C.	83MA294	OKOROKOV A.I.	83OE118
		MOISY-MAURICE V.	83BO303		83OE122
		MOKHLISSE R.	83CO323	OLBRICH H.	83KR263
MALEYEV S.V.	83OK169	MONNAND E.	83CH1001	OLIVEIRA Z.M.DE	83OK169
MALGRANGE C.	83BA1086		83HI414	OLIVER R.A.	83OK406
MAMPE W.	83GO272		83CA1070	OOSTERGETEL G.T.	83GU407
MANES L.	83BO365		83BE1094		83OL462
MANNING T.	83OE118		83CH465	OOSTERGETEL G.T.	83KR263
MARCHAL G.	83JA200 83JA240 83PI287 83JA345		83TO450		83OL405
			83MO1095	OOSTRA S.	83OO1080
MARCHAND A.	83GU1014		83MO1078		83CU1082
MARET M.	83YA284 83YA331	MOOK H.A.	83MO1078		83BL255
		MOON R.M.	83KR263	OSAE E.K.	83VI318
MARIE P.	83SE457	MORAS D.	83HU369	OSBORN R.	83BL356
		MORIN M.	83HU370	OTTEWILL R.H.	83PO1089
		MORIN P.	83HU371		83AB211
		MORIYA T.	83AR215		83CE322
		MORLEVAT J.P.	83BR310		83OT1030
		MORRISON J.A.	83MO448		83OT1031
			83GU124		83HA1075
			83GI1097		83AL1076
			83AR215		83CE1077
			83BO451	OUVRARD G.	83BR313
			83LU111	OXTON I.A.	83KE334
			83HE358	PAHLMANN B.	83KE341
			83MO1092	PALINKAS G.	83KA148
		MOUKARIKA A.	83BR387	PALLEAU J.	83BO216
		MOUTIN M.			

PALMER S.B.	83AL173	PYNN R.	83HA103	ROSENBUSCH J.P.	83ZU1020
	83BA210		83LY106	ROSENMAN I.	83BA193
	83BA1016		83GU124		83SI235
PANNETIER J.	83CO286		83PY145		83SI319
	83RE289		83LY218		83SI375
	83QU417		83PY226	ROSS D.K.	83HA1045
	83LA460		83FR297	ROSSAT-MIGNOT J.	83RO300
PANNICKE J.	83QU123		83PY317		83BO303
	83HE410		83PY330	ROSSET R.	83BE203
PARENTICH A.	83AL1076	QUADE U.	83QU123	ROTH M.	83AL131
	83CE1077	QUILICHINI M.	83QU392		83OK169
PARFONRY A.	83DE368		83QU417		83BE194
PARKIN S.S.P.	83PA228	QUITMANN D.	83SO121		83BE316
PARREINS R.	83EL239		83SO416		83BE344
PATER B.	83PA29T	RADHAKRISHNA P.	83RA301		83RO441
PAUL D.MCK.	83GU168	RAGAZZONI J.L.	83LY106		83RO442
	83CO308		83LY218		83MO448
PAWLEY G.S.	83HU128	RAINFORD B.D.	83BU114		83CA461
	83CH1001		83BU115	ROUDAUT E.	83CO439
PEISL H.	83DO267		83BU116		83MA1032
PEISL J.	83BU376		83AB211	ROUXEL J.	83BR313
PELAUD S.	83RE289		83BU219	ROWE J.M.	83MA129
PENFOLD J.	83HA434	RAMBAUD A.	83JA436		83MA290
PERENTHALER E.	83ZU264		83FE437	RUDIN H.	83SU104
PERKINS S.J.	83LI199	RAMEAU A.	83SE457		83SU385
	83PE1071	RATEL J.	83JA436	RUDOLPH K.	83QU123
	83BO1072		83FE437	RUFIN D.	83BE189
PERNOCK J.B.	83JA436	RAUCH H.	83BA207	RULLHUSEN P.	83SC6T
PERRIN H.	83VO208		83SU253		83RU158
PERRIN P.	83OE122		83RA265		83RU234
	83DJ401		83BA1050		83ZU454
PERRY C.H.	83PE449	RAUH H.	83RA162	RUMYANTSEV A.YU.	83CH102
PETRASCHECK D.	83RA265	RAVAINE D.	83RA154	RUNOV V.V.	83OK169
PEUSCHER M.	83KU433		83RA241	RUPPERSBERG H.	83KI120
PEYRARD J.	83PE217	RAVEAU B.	83LA460		83SO121
PFEIFFER B.	83KR263	RAVOT D.	83BO184		83RU250
	83KE341	RAWISO M.	83HE373		83CO350
	83MU342	RAYMENT T.	83EL237		83RU360
	83PL427	READ N.	83RE274		83SO416
PHAN X.H.	83FI1055		83RE429		83RU421
PHILLIPS R.A.	83NA105	REBEL H.	83FA327		83LA456
PICOT C.	83GU1015	REBIZANT J.	83BO365		83OL462
	83BE1029	REBONATO R.	83BO451	RUSH J.J.	83MA129
	83BE1035	REGNAULT L.P.	83BO303		83ZA249
PIECUCH M.	83PI287	REICH S.L.	83MA346		83ZA273
	83JA345		83MA397		83MA290
PIETRASZKO A.	83FR252	REIMERS W.	83RE163		83ZA374
PINSTON J.A.	83KR263		83RE172	RUSTICHELLI F.	83ME361
PIOTTI M.	83TH22G	REMPP P.	83BE1029		83BO365
PIPER J.	83DA1068	RENARD J.P.	83BO303		83BO451
PLATCHKOV S.K.	83PL427	RENAUDIN J.	83RE289	SACKMANN E.	83KN364
PLUMIER R.	83PL1058	RENKER B.	83RE130	SADLER D.M.	83SA1081
PODO F.	83ST152		83DI151	SAINT-JAMES R.	83PL1058
POINSIGNON C.	83BE127	RENOUPREZ A.J.	83CA246	SALVA-GHILARDUCCI A.	83SA1062
	83SO136		83JO279	SANQUER M.	83BA1003
	83PO254	REY-LAPON M.	83DE139	SARKISSIAN B.V.B.	83SA1002
POPPELWELL J.	83CU126	REYNOLDS P.A.	83FI420	SAUVAJOL J.L.	83AM204
	83CE1017		83FI1004	SCHAERPF O.	83GE176
	83CE1090		83FI1055		83OK406
POUGET J.P.	83GA355	RICHARDS R.W.	83RI1063		83GU407
POULSEN F.M.	83BE377		83RI1064		83HI414
POWLES J.G.	83PO1089	RICHARDSON R.A.	83CE1077	SCHEEERER H.J.	83HU395
PRAGER M.	83HE291	RICHTER D.	83MA129	SCHIRMACHER W.	83CO350
PRANDL W.	83GE176		83MA290		83RU360
PRASSIDES K.	83PR1039	RIEKEL C.	83HA156	SCHLENKER M.	83BA170
PRESS W.	83LU111		83LE1059		83MA294
	83EH134		83RI1083		83BA296
	83HE291	RING P.	83RI243		83BA1016
	83HE358	RIOS JARA D.	83GU124		83BA1086
PRICE R.	83BA1006	RISTORI C.	83OE122	SCHMIDT G.	83KN364
PRINCE J.G.	83PR1043		83DJ401	SCHMIDT H.H.	83HU369
PROKOFJEV P.T.	83BO393	ROBERT A.	83AG9T		83HU370
PRUSSIN S.G.	83KR263	ROBINSON S.J.	83HA108		83HU371
PULITI P.	83ME361		83RO149		83HU395
PUSHKAREV V.V.	83CH102	ROGER M.	83RO315	SCHMITT C.	83QU123
			83RO110	SCHMITT D.	83GI1097
			83RO225	SCHNABEL P.	83DI151
			83RO269	SCHNEIDER E.	83EG146
		ROMBY P.	83MO448	SCHRADER H.	83QU123

SCHRECKENBACH K.	83SC11T	SNELLING D.M.	83SN107	SUMMHAMMER J.	83BA207
	83BL153		83HA108		83SU253
	83MA346		83RO149		83BA1050
	83SC351		83SN283	TABONY J.	83CE322
	83BO393		83RO315		83TA1012
	83KE394	SOFIA H.M.	83MA346		83TA1093
	83HU395		83MA397	TACHEZ M.	83TA244
	83MA397	SOLTWISCH M.	83SO121	TADROS T.F.	83BA1051
	83SC403		83SO416	TARDIEU A.	83CU1009
	83BL455	SOMMERS H.J.	83SO125	TASSET F.	83AL173
SCHROEDER A.	83KR263		83SO165		83BO174
SCHUBERT U.	83SC1028		83US268		83MU180
SCHUCK P.	83GH242		83SO390		83FU182
	83RI243	SOUBEYROUX J.L.	83DA164		83GI183
	83TR338		83SO222		83BA185
	83SC400		83FI262		83GI379
	83HA404		83SO302		83GI411
	83SC408		83BR313	TCHEOU F.	83GU1014
	83HA409	SOUGI M.	83PL1058	TEIRLINCK D.	83JA200
SCHULT O.W.B.	83TO450	SOUQUE D.	83OE118		83JA345
SCHULZ H.	83ZU264	SOURISSEAU C.	83SO136	TEIXEIRA J.	83BO391
SCHULZ H.J.	83SC256		83LU251	TELLGREN R.	83HE380
	83SC337		83SO336	TERLAIN A.	83LA1033
	83SC353	SOUSA J.B.	83BA210	TESSIER C.	83LA1033
	83SC423	SPENCER J.L.	83HO166	TETE C.	83JA200
	83HO424	SPERL W.	83NA1010	THEOBALD F.	83LA147
	83SC431	SPIRIN A.S.	83SE340		83TA244
SCHULZE H.	83NI309	SPIRLET J.C.	83BO365	THEOBALD J.P.	83QU123
	83NI430	SPITS A.M.J.	83BO393		83HE410
SCHUMACHER M.	83SC6T	SPOHR R.	83AL131	THIERRY J.C.	83LI347
	83RU158	SPORTOUCH S.	83JO279	THOLENCE J.L.	83ME137
	83RU234	ST.GREGOIRE P.	83BA363		83FI231
	83ZU454	STAHN M.	83ST1053		83FI262
SCHUSSLER F.	83KR263	STANSFIELD R.F.D.	83ST16T	THOMAS J.M.	83CH1018
SCHWABE D.	83FU182		83TH443		83CH1019
SCHWEIZER J.	83BA170		83ST445	THOMAS M.	83TH22G
	83DE175	STEEB S.	83OL462		83TH443
	83BO177		83NA1010		83FI444
	83BO178		83LA1011		83ST445
	83BO184		83KN1027	THOMAS R.K.	83HI414
	83BE189		83LA1067	THOMASON J.L.	83RI1063
	83BR197	STEIGENBERGER U.	83BA363		83RI1064
	83AB211	STEINER M.	83KA229	THOREL P.	83LA1033
	83BO216		83ST1049		83TH1084
	83BE227	STEPHENS M.E.	83ST257	TIBBALLS J.E.	83KU367
	83DU236	STEWART R.J.	83BE1094		83ST445
	83BA296	STEYTLER D.C.	83BO391	TIBY C.	83LA196
	83SI319		83ST1024	TIMMINS P.A.	83DE285
	83BO359		83ST1046	TINANT B.	83DE368
SCHWITZGEBEL G.	83LA456	STIRLING W.G.	83ST24T	TOKUNAGA Y.	83TO450
SEDELNIKOVA S.E.	83SE340		83HU128	TOMKINSON J.	83HE358
SELB J.	83SE457		83BR144		83GR1088
SEMLYEN J.A.	83HI277		83GU168	TOPERVERTZ B.P.	83OK406
SERDYUK I.N.	83SE340		83ST220	TOURNARIE M.	83BO281
SERKE I.	83KA148		83MC221	TOUZAIN P.	83HA156
SEYFARTH H.	83TO450		83BU288	TREINER J.	83TR338
SHELTON R.N.	83LY106		83ST292	TREUTMANN W.	83RE163
SHIGA M.	83AR215		83FR297		83RE172
SHIRANE G.	83PY145		83MC299	TREWHELLA J.	83TR413
SIBBET G.J.	83SI311		83BO303	TRIOLO R.	83TR321
SICK I.	83PL427		83CO308	TUCK J.J.	83HA1045
SICRE A.	83CA133	STOECKMANN H.J.	83KI120	USADEL K.D.	83US268
SIMON C.	83BA193		83AC188	VACHETTE P.	83CU1009
	83SI235		83HE238	VAN ASSCHE P.H.M.	83BO393
	83SI319		83AC1044	VAN DER MAREL C.	83KI120
	83SI375		83ST1074		83AC188
SIMON J.P.	83SA1062	STRAETLING W.H.	83IB278	VAN MEERSSCHE M.	83DE368
SIMPSON K.	83NI430	STROM R.	83ST152	VAN WUNNIK J.N.M.	83NE378
SINCLAIR R.N.	83WR1022	STROTH U.	83SC400	VANGELISTI R.	83SI319
	83JO1061		83SC408	VARGHESE J.N.	83WI140
SLJUSSAR V.N.	83OK406	STUHRMANN H.B.	83NI309		83FI1054
SMEND F.	83SC6T		83NI430	VARRET F.	83RE289
	83RU158	SUCK J.B.	83HA103	VERGNAT M.	83PI287
	83RU234		83SU104		83JA345
	83ZU454		83SO121		
SMITH J.V.	83CH1018		83EG146		
SMITH R.P.	83FI1054		83SU385		
SMOLANDER K.J.	83AH271		83SO416		
	83AH418				

VETTIER C.	83KN132	WRIGHT A.F.	83RA154
	83MC209		83FI159
	83PE217		83BA233
	83MC221		83EL239
	83BL255		83RA241
	83MC299		83HI298
	83RO300		83DO312
	83MA304		83WR343
	83VI318		83BO365
	83LA339		83EL382
	83BL356		83WR447
VIGNERON F.	83AM1013		83CH464
VILLIERS C.L.	83BO1072	WRIGHT C.J.	83ST1024
VINCENT B.	83BA1051		83ST1046
VIOVY J.L.	83LA1065	WURMBACH P.	83NI309
VISSER R.J.J.	83VI318		83NI430
VITICOLI S.	83FI231	YANG M.S.	83CA461
	83FI262	YASUOKA H.	83AR215
VITTOZ P.	83OL405	YAVARI A.R.	83YA284
VIVIER G.	83OL405		83YA331
VIVIER H.	83LA147	YVON J.	83PO254
VOGT H.	83DU1096	ZABEL H.	83ZA249
VOGT O.	83ST292		83ZA273
	83RO300		83MA349
VOIRON J.	83BL255		83ZA374
	83BE316	ZACCAI G.	83ST152
	83VI318		83LI347
	83BL356		83ZA348
VOLINO F.	83VO208		83GO412
WADDINGTON T.C.	83GR1088		83TR413
WAGEMANS C.	83HO266	ZARZYCKI J.	83BA233
WAGNER C.N.J.	83RU250	ZEIDLER M.D.	83KA148
WALKER M.B.	83WA101	ZEILINGER A.	83BA207
WARNER D.D.	83MA346		83SU253
	83HU395	ZEYEN C.M.E.	83DO112
	83MA397		83BE143
WEBSTER P.J.	83JO171		83FR252
	83BO191		83ZE295
	83ZI205		83FR297
	83ZI206		83ZE305
	83WE224		83ZE306
	83ZI329		83NA333
	83WE362		83LA339
WEDIN R.E.	83BE377	ZHANG Z.Y.	83CA461
WEERTMAN J.R.	83CA461	ZHONG W.L.	83ST445
WEIKARD H.	83KE341	ZIEBECK K.R.A.	83GI18T
WEINGAERTNER K.	83HE410		83BR157
WEISS H.	83PE1071		83JO171
WERNER S.A.	83KL1008		83BO187
WHITE J.W.	83HA1075		83BO191
WIECHERT H.	83LA196		83BR202
WIEDENMANN A.	83WI232		83ZI205
WIESMANN F.J.	83KA148		83ZI206
WIGNALL G.D.	83CA461		83BO213
WILKINS S.W.	83WI140		83BR214
WILKINSON C.	83WI1087		83AR215
WILLIAMS D.E.G.	83WI223		83WI223
	83WI307		83WE224
WILLIAMS G.A.	83FI1054		83BU288
WILLIAMSON S.	83PL427		83WI307
WINNACKER A.	83DU1096		83ZI329
WINTER J.	83GH242		83WE362
WINTER J.	83WI453	ZIEGERT W.	83KR263
WIPF H.	83MA129	ZIMAN T.A.L.	83ZI357
	83MA290	ZINN W.	83BO174
WISSHAK K.	83FA327	ZONG QI LI	83LI199
WITT HUBERTS P.DE	83PL427		83LI347
WOERLE B.	83SC1028	ZUCKER U.H.	83ZU264
WOLFERS P.	83CO439	ZULAUF M.	83ST152
	83MA1032		83ZU1020
WOLLNIK H.	83MU342	ZURMUEHL U.	83SC6T
WRIGHT A.C.	83WR1022		83RU158
	83JO1061		83RU234
			83ZU454

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