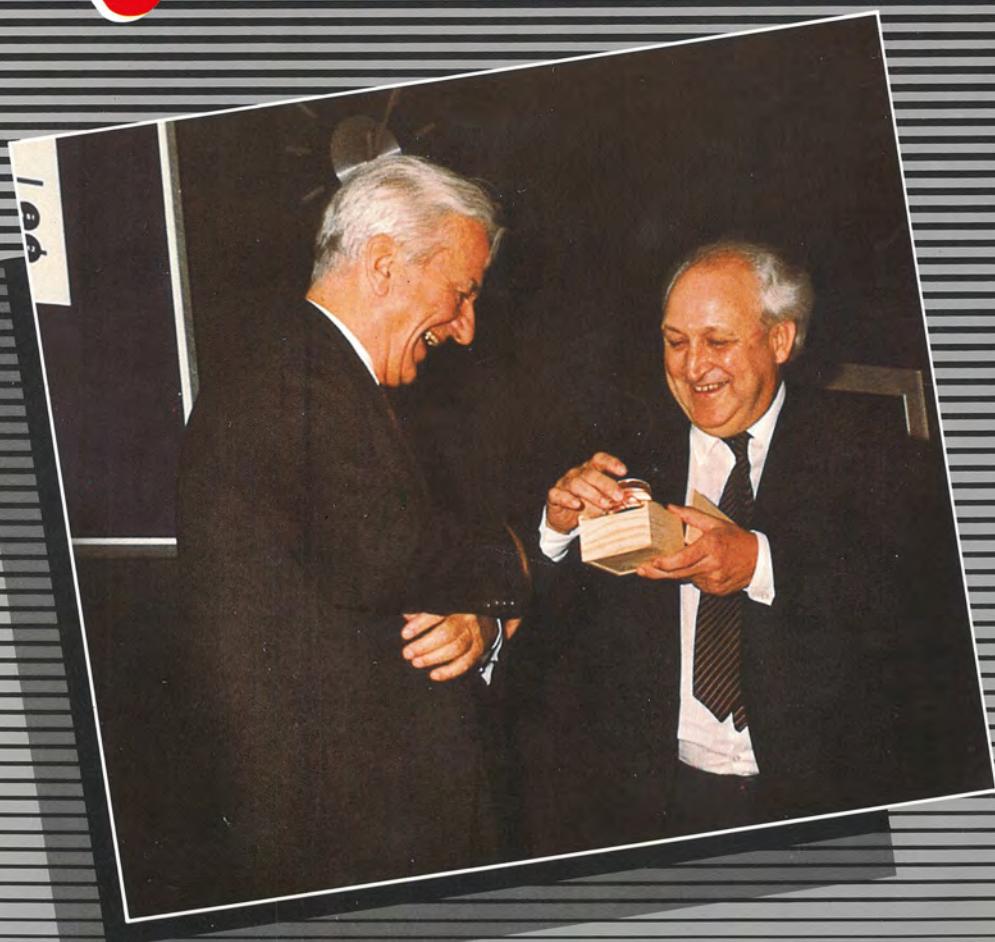


ANNUAL REPORT 04

INSTITUT MAX VON LAUE - PAUL LANGEVIN - GRENOBLE - FRANCE



ANNUAL REPORT 84

INSTITUT - MAX VON LAUE - PAUL LANGEVIN - GRENOBLE - FRANCE

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: Scientific Coordination and 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 F. Cook (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 1984
available from the ILL Library.

Front Cover

The President of the Federal Republic of Germany, Dr. Richard von Weizsäcker visited the ILL on 7 November 1984. He was welcomed by Dr. B.E.F. Fender, Director of the ILL, who presented him with a model of the High Flux Reactor.

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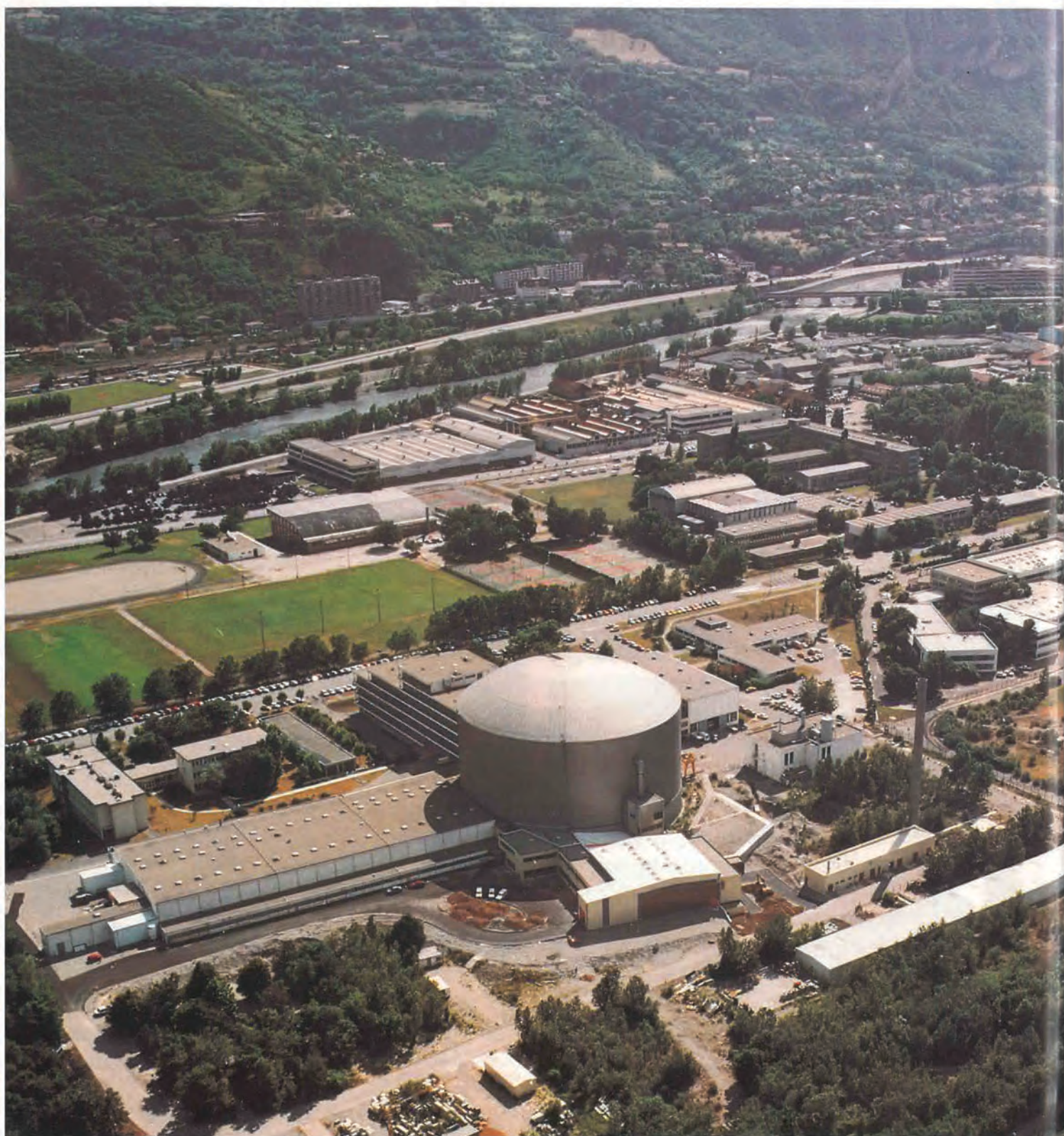
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The Institut Max von Laue - Paul Langevin

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.

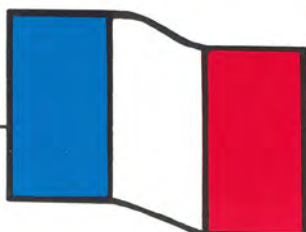
Designing and operating instruments and helping the visiting users to carry out their experiments is thus the principal task of the Institut's own scientists. The experimental use of the instruments by ILL staff is subject to the same approval system as their use by external teams.

External Organisation of the Institut Laue-Langevin 1984

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)
Ottewill (Univ. of Bristol)	Miquel (CNRS)	Simon (Max-Planck-Ges.)

Audit Commission

Pettet Millington	Polderman Racine	Binder Riess
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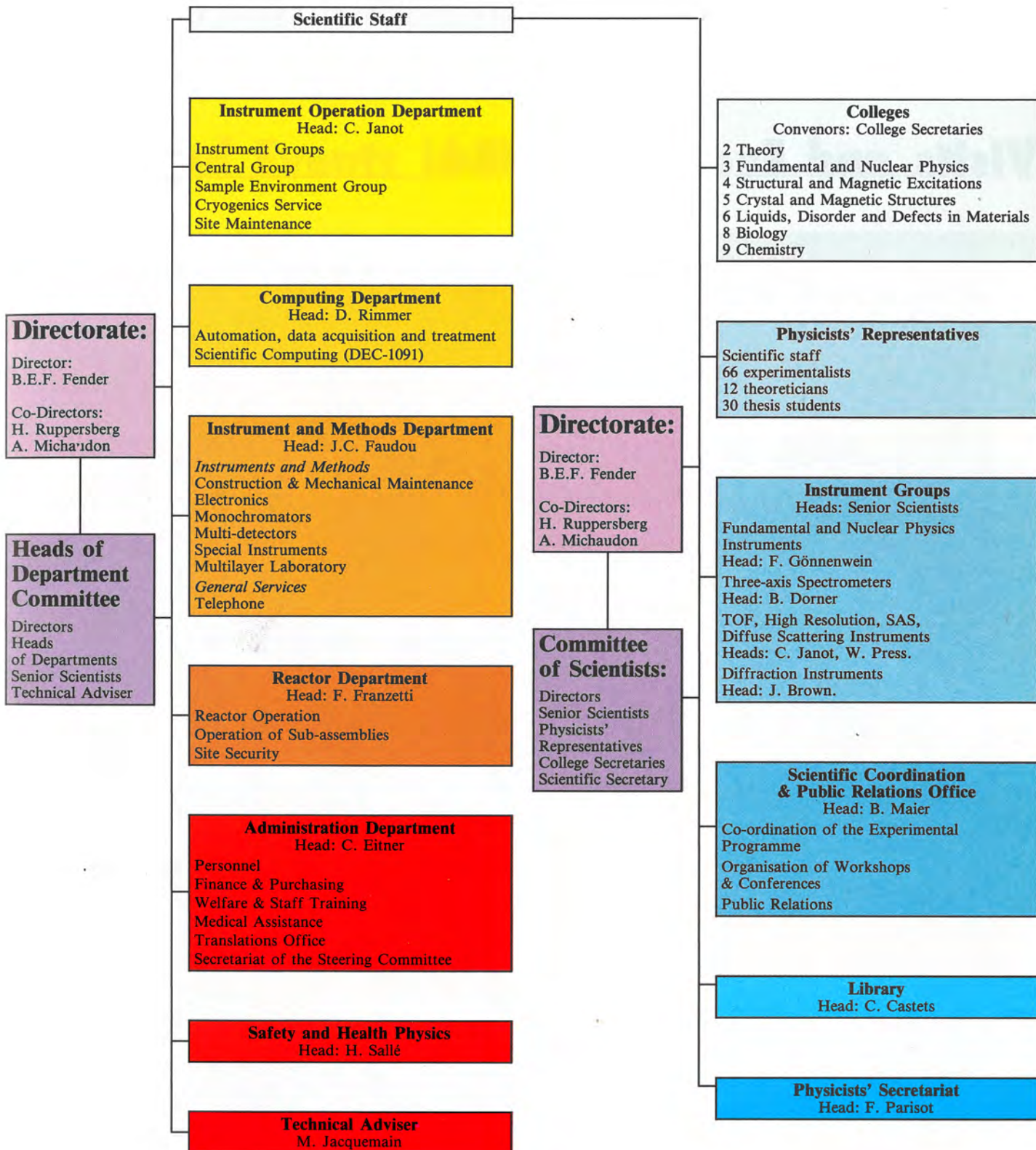
Scientific Council (at its last meeting)

Armbruster — GSI Darmstadt	Fender — ILL (Chairman)	Nierhaus — MPI Berlin
Bienfait — Univ. Marseille	Franck — Univ. Karlsruhe	Pendry — Imperial College
Blanquet — Ecole Polytech. Palaiseau	Gläser — TU München	Rainford — Univ. Southampton
Comes — Univ. Paris-Sud	Hahn — TH Aachen	Rossat-Mignod — CEN Grenoble
Cowley — Univ. Edinburgh	Horner — Univ. Heidelberg	— ILL
Dianoux — ILL	Joly — CEN Saclay	Schreckenbach — ILL
Drifford — CEN Saclay	Maier — ILL	Smith — Unilever Research
Eitner — ILL	Michaudon — ILL	
Enderby — Univ. Bristol	Miller — Univ. Edinburgh	

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 <i>Schult</i> Signarbieux Sinclair Specht Vinh Mau	Edwards Hanke Horner Hutchings Lajzerowicz Lambert Rainford Rossat-Mignod <i>Schmatz</i>	<i>Coles</i> Day Fuess Goodenough Plumier Prandl Souletie Zinn	Bronger Cheetham Fischer <i>Galy</i> Marezio Pouget Sim	Dupuy Durand Enderby Hensel Schilling <i>Schofield</i> Stewart Suck	Blundell Chabre <i>Fuller</i> Giège Janin Miller Nierhaus Saenger Schulz	Charvolin Cotton Hoffmann Kilian <i>Ottewill</i> Picot Richards	Clough Conard Ehrhardt Forstmann <i>Hüller</i> Lassègues Thomas	Alefeld Bergère Charpak Pépy Reichardt <i>Scherm</i> Stewart Steyerl Taylor Williams

General Organigramme



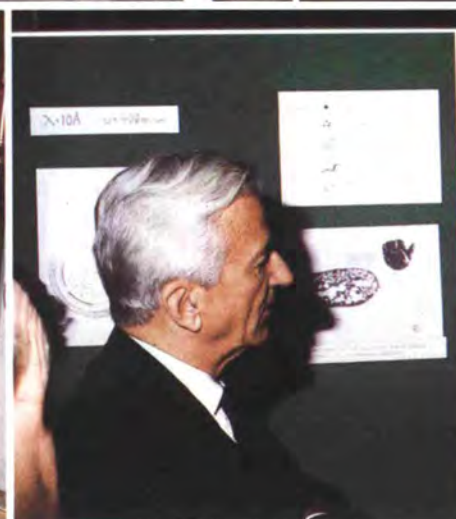
Visits and Events in 1984

The President of the Federal Republic of Germany, Dr. Richard von Weizsäcker visited the ILL on 7 November 1984.



1. The arrival of the President.

Visits and Events in 1984



2. The President replying to the Director's speech of welcome. In the picture from left to right: Dr. v. Weizsäcker, Dr. A. Michaudon, French Co-Director, Dr. B.E.F. Fender (Director), Professor H. Ruppertsberg, German Co-Director, Monsieur L. Mermaz, Président du Conseil Régional de l'Isère et Président de l'Assemblée Nationale, M. J.P. Pensa, Préfet de l'Isère.

3. Professor H. Maier-Leibnitz, Professor O. Schärpf (ILL) and Professor H. Ruppertsberg found time for talking science on the occasion of the presidential visit.

4. The German President visited part of the ILL's experimental areas. In the Guide Hall he listened to explanations from Dr. W. Press. In the picture from left to right: M. J.P. Pensa; Dr. B.E.F. Fender; Monsieur L. Mermaz, Président du Conseil Régional de l'Isère et Président de l'Assemblée Nationale, Dr. W. Press (ILL); Dr. R.v. Weizsäcker; Monsieur Carignon, Mayor of Grenoble and Professor H. Maier-Leibnitz, one of the founders of the ILL.

5. The President with Dr. W. Press.

Visits and Events in 1984



6. A delegation from the Chinese Academy of Sciences was received by the ILL on 6 November 1984. Dr. B.E.F. Fender guided the delegation and in the picture is seen explaining the instrument D7 to Professor Lu Jiaxi, President of the Chinese Academy of Sciences.

7. Dr. Probst, parlamentarischer Staatssekretär in the German Federal Ministry of Research and Technology visited the ILL on 29 March 1984. From left to right: Dr. Probst, Professor Ruppertsberg (ILL) and Dr. Dorner (ILL) during the visit to the reactor hall.

8. Monsieur L. Mermaz, Président du Conseil Régional de l'Isère and Président de l'Assemblée Nationale, visited the ILL on 28 June 1984. On this occasion he was briefed by the Director, Dr. B.E.F. Fender, on the ILL case for consideration as a site for the ESRF (European Synchrotron Radiation Facility).

9. Dr. J. Rembscher, Ministerialdirigent in the German Federal Ministry for Research and Technology visited the ILL on 30 October 1984. In the picture he is talking to Dr. E. Bauer from the ILL Reactor Department. He was guided on his tour by Professor H. Ruppertsberg (on the right), and Dr. B. Maier (Scientific Secretary).

Visits and Events in 1984

10a



10b



10c



10d



11



10. Pictures from the last meeting of the Steering Committee of December 1984 held at Grenoble showing part of the Committee (a) Chairman Dr. Atkinson (b) From left to right: Dr. Eitner, Professor Ruppertsberg, Dr. Michaudon, Dr. Fender, M. Auché-Fossié, Dr. Horowitz, (c) From left to right: Dr. Schildt, Dr. Hobbies, Professor Leadbetter, (d) From left to right: Professor Haensel, Dr. Wessels, Dr. Bläsing, Professor Klose.

11. On 16 July 1984 a delegation from the Daresbury Laboratory (UK) had a series of discussions with ILL experts on the Institut visitors programme and on the ILL's application as a synchrotron site. From left to right: M. J. Courteau (ILL), Dr. R. Williams, Chairman of the Daresbury Synchrotron Radiation Facility Committee, Dr. D. J. Thompson, Responsible for the Daresbury Synchrotron, Professor L. Green, Director of the Daresbury Laboratory, Dr. B.E.F. Fender (Director of the ILL).

Director's Report

I write this, my third and final report as Director, on yet another fine 1 January with sun and clouds chasing each other from the Belledonne to the Vercors, from time to time coquettishly revealing the sharp whiteness of early season snow. The town of Grenoble is on holiday, the Institut still, as it catches its breath for the last phase of the reactor renewal programme. The shift crew as always is on watch over the reactor and only a few scientists who have escaped the festivities to use the central computer can be seen.

Despite today's momentary calm, 1984 has been an excellent year for the Institut.

Scientific programme

A full scientific programme was carried out until October as visitors and in-house scientists sought to exploit every hour of the Institut's instruments before the shut-down. On the last day around 50 scheduled instruments, special beam instruments and test positions were operating. In total, 707 experiments approved by the Scientific subcommittees were completed in 1984.

As I have emphasized on many previous occasions, the information provided by neutron scattering is so direct, so relatively unambiguous, that almost every publication adds significantly to our understanding of condensed matter. In a similar way the data obtained from nuclei after neutron capture gives unique information about the structure of the nucleus and of fission while the properties of the neutron itself remain of great interest in terms of parity violation and unification theories. Out of 400 or so publications in 1984 arising from work at the ILL it remains as difficult as ever to select the "best" publications of the year. As usual, later in the report College Secretaries present some highlights, and following now customary practice there is a general review — this time on "Low Resolution Structures of Biological Complexes Studied by Neutron Scattering" by P. A. Timmins and G. Zaccai. The three ILL workshops published during the year are also recommended for those who wish to gauge the diversity of activities around the high flux reactor. They are: "Reactor-based Fundamental Physics", *J. de Physique*, C3, 1984; "Water", *J. de Physique*, C7, 1984; "Sample Environments in Neutron and X-ray Experiments", *Revue de Physique Appliquée* 19, 1984, p. 643-857.

Another way to understand the breadth of science using neutrons is to examine the publications of the last week or two. From this slice of activity we see that high neutron flux coupled with very precise and efficient Bragg crystal and pair spectrometers has opened up the possibility in light and medium-weight nuclei of following the γ -ray flux emitted by an excited nucleus all the way down to the ground state. These studies on the structure of low-lying nuclear states can be correlated

with models (e.g. the Fermi gas model) of nuclei at a few MeV excitation. In solid state physics we are reminded once again that our grasp of what happens near or at a phase transition is heavily dependent on neutron scattering results. Current interest continues to centre on incommensurably modulated solids and ThBr_4 is a particularly attractive model system because (i) the ionic displacements associated with the modulation remain small in amplitude and sinusoidal in character down to the lowest temperatures, and (ii) the displacive character is such that the phason branch can be identified by high resolution neutron inelastic scattering. Much of the ThBr_4 story is now complete although the possible role of impurities in influencing modulated structures points to a future participation by solid state chemists.

Magnetism is another area heavily dependent on neutron results although the magnetic properties themselves are often of secondary interest to the light they shed on electronic behaviour. In this respect f electron systems pose exacting questions. For example, in the anomalous (i.e. mixed valence) rare earth systems there is a debate as to whether the ions should be described as single particles or whether the ions couple with conduction electrons to form a coherent band. The latest results on YbAl_3 give the clearest evidence so far of the latter view. The 5 f electrons of the actinides are less tightly bound and even more sensitive to the environment as witnessed by the presence of a charge density wave in α uranium and five allotropic forms of plutonium metal. For obvious reasons, much of our present knowledge comes from uranium with the risk therefore of a one-sided understanding. In a recent experimental "tour de force" physicists from five laboratories and four countries have examined with polarised neutrons the magnetic form factor of a single crystal of PuSb . The results clearly show a $5f^5$ state and identify the ground state wave function.

In studying the structure of disordered systems, the special virtue of the neutron as a probe arises from the contrast effects which can be obtained by isotopic substitution. The technique, which has been particularly successful in the study of aqueous solutions, can clearly be extended to give details of the structure of amorphous metals as a recent examination of $(\text{Fe}_{1-x}\text{Mn}_x)_{75}\text{P}_{15}\text{C}_{10}$ shows. Here the manganese plays the role of an isotope of iron and its negative scattering length gives the necessary scattering contrast.

Classical structural studies on a wide range of interesting materials also feature among the latest publications; these include the changes of site occupation of benzene observed in a zeolite and the modelling of nucleation and growth processes in a glass ceramic using data derived from small angle scattering data.

Some of the most significant recent publications however are in physical chemistry where cold neutron techniques are particularly well matched to studies of colloids and micelles. Thus

small angle scattering measurements, allied with both selective deuteration and explicit computation of interference effects between particles, show how a small molecule (pentanol) is incorporated into a micelle (sodium octanoate) and how this varies with concentration. Selective deuteration or strictly selective protonation can be used to pick out the dynamics of a particular component by following the quasielastic scattering. This has been reported through a progression of phase changes from the micelle to oil in water and water in oil micro-emulsions. These neutron scattering studies on concentrated micellar and colloid systems, like earlier studies on concentrated polymer systems, are likely to stimulate general interest in a very important field.

Reactor renewal programme

The goals of this last and most extensive stage of the present reactor renewal programme are simple. They are (i) to replace all the parts at the heart of the reactor (i.e. inside the reflector tank) which have received the heaviest radiation doses; (ii) to definitively repair the damaged heavy water collector; and (iii) to replace the existing vertical cold source with a new source of improved design. The biggest single operations are the replacement of the H1/H2 beam tube which serves the cold and thermal guides; the replacement of the H6/H7 through beam tube, and an electro-erosion intervention on the heavy water collector. At this time the removal of the various components is almost complete. That this complex and difficult work is entirely on schedule is a tribute to the superb planning and execution of the Reactor Department assisted at all times by the Radioprotection Service.

Instruments & Methods, Instrument Operation and Computing Departments

Although the spotlight at the end of the year is on the Reactor Department, other departments have also carried out sterling work during the year. I note in particular the special efforts of EDEX in supporting first an experimental programme which ran from 8 August 1983 to 2 October 1984 with only short breaks between cycles and then the major tasks associated with the shut-down itself. The Department of Computing, apart from its customary support of scientific experiments, has improved the Institut network particularly with respect to the flow of data from instruments to the central computer. It has been involved with extensive programming for VAX computers which are now needed for the high data rate instruments and in the development of money-saving administrative computing. The Department of Instruments and Methods remains crucial for the long-term success of the Institut. I quote from the recent American Academy of Science Commission on Major

Facilities for Materials Research and Related Disciplines (the Seitz Report): "The consequences of this investment gap (in new spectrometer development and construction) over the past decade between European and U.S. research reactors were being felt increasingly in our (U.S.) inability to compete in new areas of science involving such techniques as high resolution neutron spectroscopy, small and medium-angle diffraction and diffuse scattering". As was clear from elsewhere in the report the commission was referring notably to the ILL, and to underline that point, in the weeks before the shut-down three major new instruments went through their first tests. They were IN20 (the triple axis spectrometer equipped for full polarisation analysis), DB21 (the biological diffractometer built in collaboration with EMBL and designed to look at very large unit cells), and D2B (the improved powder diffractometer replacement for D1A).

Improvements in basic techniques are just as important as completed instruments because they can improve the performance of several instruments. In this respect the optimum definition of the incoming neutron beam (e.g. with a monochromator) and the detection of scattered neutrons are paramount. Although a number of new ideas for better position sensitive detectors have been explored, the most promising development of 1984 was the production of mixed Si-Ge crystals of very high quality. The immediate effect is to enhance the capability of the high resolution back-scattering instrument IN10 but the long-range prospects if fulfilled could improve many instruments.

Administration, manpower and the budget

In a fully active research institute, where there are always more ideas than money to implement them, there will always be strong pressure on the administration. Add to that, the fact that the Steering Committee has asked for a 3 1/2 % reduction in the total number of employees by 1987, take into account that governments of whatever political complexion examine ever closer the detailed workings of every organisation and you have a hard-pressed administration. The ILL is well served by its Department of Administration. The Department is small in proportion to many national laboratories or universities, even before considering the ILL's international character and its enormous flow of visitors. Alas the prospect is for fewer rather than additional posts, and some (but I hope not serious) reductions in service.

I am pleased to report it will be possible to gradually increase the proportion of permanent scientists at the Institut, which will enable us to make the maximum use of our excellent facilities. The priority will be to make appointments which assure the continuity of major instruments and to provide expertise in domains more recently studied by neutrons.

The 1985 budget will allow all the main instrument projects

Director's Report

to proceed at rates only a little slower than optimum, but given the need to be able to plan these developments well ahead, we hope the Associates will soon be able to give a clear indication as to the level of the post-modernisation programme budget.

Personnel and Visitors

Among many visitors to the ILL the outstanding event was the very successful visit of Richard von Weizsäcker, the President of the German Federal Republic. Our congratulations go in particular to P. Nozières who has been awarded the 1985 Wolf prize for Physics and also to Pierre Becker who from January 1985 is to become Professor of Physics at the University of Grenoble, and a recent visitor to the Theory College, Sigfried Hess, has become a full Professor at the Technical University in Berlin. Not all ILL scientists follow conventional routes: Otto Schärpf, who has made D7 such an outstanding instrument, was preparing to take a day or two off to perform the wedding service in Austria of his instrument co-responsible Willi Just!

As usual, a feature of ILL life is the positive attitude of all staff towards the tasks at hand, whether this be expressed informally or through the formal procedures of the Works Committee.

1985 and beyond

I ended my report last year with the dream of closer links between the ILL and the European X-ray synchrotron source. During the year the Institut formally presented its arguments and the dream became closer to reality with the announcement in October that France and Germany would propose Grenoble as their chosen site. Some of the vision which launched the ILL will still be necessary if the project is to get solidly under way in 1986. The ESRF ought to be broadly European from the start but in the meantime aspirations for a wider membership of the ILL slowly transform into an expectation. I retain also the hope that the ILL will see its first direct users from industry in 1985.

A last word

As I come to the end of this report I find it is snowing heavily. That is appropriate enough, for like any other limited contract scientist, I will be sad to leave the ILL, although again like others I plan to return as a user. I thank all sections of the Institut, but my co-directors Henner Ruppertsberg and André Michaudon in particular, for much help and assistance.

B.E.F. Fender

Bericht des Direktors

Auch diesen dritten und letzten "Bericht des Direktors" schreibe ich an einem herrlichen Neujahrstag bei eitlem Sonnenschein, wobei Wolken von der Belledonnekette zum Vercors jagen und von Zeit zu Zeit den Blick auf das strahlende Weiss von frisch gefallenem Schnee freigeben. Die Bewohner der Stadt Grenoble sind in Ferien und auch das Institut ist ruhig, so als wolle es Atem holen für die letzte Phase der Modernisierung des Reaktors. Die Reaktorbetriebsmannschaft ist wie immer auf ihrem Posten und nur einige Wissenschaftler, die offenbar der Hektik der Festtage entronnen sind, arbeiten am Zentralrechner. Diese kurzfristige Ruhe ist jedoch trügerisch, denn sie lässt kaum vermuten, dass 1984 für das Institut ein ausgezeichnetes Jahr war.

Wissenschaftliches Programm

Das wissenschaftliche Programm lief planmässig und ohne Einschränkungen bis Oktober und die Wissenschaftler und Gastforscher nutzten jede Minute bis zum Abschalten des Reaktors. Noch am letzten Tag waren etwa 50 Instrumente mit geplantem Experimentierprogramm sowie spezielle Instrumente und Versuchsaufbauten in Betrieb. Insgesamt wurden 707 vom wissenschaftlichen Rat beilligte Experimente durchgeführt.

Wie bereits bei früheren Anlässen betont, sind die durch Neutronen gelieferten Informationen derart unmittelbar und eindeutig, dass fast jede daraus entstehende Veröffentlichung wesentlich zu unserem Verständnis der kondensierten Materie beiträgt. In ähnlicher Weise geben die Daten von Atomkernen beim Neutroneneinfang in einzigartiger Weise Aufschluss über Kernstruktur und Spaltprozesse. Die Eigenschaften des Neutrons selbst, vor allem in Hinblick auf Paritätsverletzung und "unification theories", bleiben weiterhin von grossem Interesse.

Es ist wie eh und jeh schwierig, aus den etwa 400 aus ILL-Arbeiten hervorgegangenen Veröffentlichungen des letzten Jahres die "besten" auszuwählen. Wie gewohnt werden weiter unten in diesem Jahresbericht die Kollegiumssekretäre einige herausragende Resultate präsentieren; ausserdem wird, einem neuen Brauch folgend, wieder ein Übersichtsartikel gebracht, diesmal über "Strukturuntersuchungen von biologischen Komplexen mittels schwachauflösender Neutronenstreuung" (von P.A. Timmins und G. Zaccari). Die Veröffentlichungen der Beiträge zu drei vom ILL organisierten Workshops sind im Laufe des Jahres erschienen und seien all denjenigen zur Lektüre empfohlen, die sich einen Begriff von der Vielfalt der ILL-Aktivitäten machen wollen. Sie behandeln die folgenden Themen: "Grundlagenphysik an Reaktoren (J. Physique, C3, 1984); "Wasser" (J. Physique, C7, 1984) und "Probenumgebungen bei Neutronen- und Röntgenstrahlexperimenten" (Revue de Physique Appliquée 19, 1984, p. 643-687).

Eine andere Methode, die Breite der mit Neutronen zugänglichen Wissenschaft zu analysieren ist die Heranziehung der Veröffentlichungen der letzten ein oder zwei Wochen. Diese "Scheibe" der wissenschaftlichen Arbeiten zeigt uns, wie es mit Hilfe des hohen HFR- Neutronenflusses in Verbindung mit äusserst genauen Kristall- und Paarspektrometern von hohem Wirkungsgrad möglich ist, in leichten und mittelschweren Atomkernen die vom angeregten Kern ausgesandte Gammastrahlung bis tief hinunter zum Grundzustand zu verfolgen. Diese Untersuchungen über die Struktur tiefliegender Kernzustände kann mit Kernmodellen (z.B. Fermigas-Modell) bei Anregungen von einigen MeV korreliert werden. In der Festkörperphysik werden wir wieder einmal daran erinnert, dass unser Verständnis von Phänomenen nahe beim oder am Phasenübergang stark von den Ergebnissen der Neutronenstreuung abhängt. Das gegenwärtige Interesse konzentriert sich weiterhin auf inkommensurabel modulierte Festkörper; ThBr_4 ist ein besonders attraktives Modell, da i) die Amplituden der mit der Modulation verbundenen Ionenverschiebungen bis hinunter zu tiefsten Temperaturen klein und sinusförmig bleiben und; ii) der Verschiebungscharakter dergestalt ist, dass der Phasonenzweig durch hochauflösende inelastische Neutronenstreuung identifiziert werden kann.

Der Grossteil des Problemkreises um ThBr_4 scheint jetzt weitgehend geklärt zu sein, obwohl der mögliche Einfluss von Verunreinigungen auf modulierte Strukturen auf eine zukünftige Beteiligung von Festkörperchemikern hindeutet.

Auch Magnetismus ist ein Gebiet, welches stark von den Ergebnissen der Neutronenstreuung abhängt, obgleich die magnetischen Eigenschaften selbst oft von zweitrangigem Interesse sind verglichen mit der Aufhellung des elektronischen Verhaltens. In dieser Hinsicht werfen f-Elektronensysteme schwierige Fragen auf. Zum Beispiel in anomalen Systemen seltener Erden (d.h. mit gemischten Valenzen) ist eine Debatte darüber entfacht, ob die Ionen als Einzelteilchen beschrieben werden sollen, oder ob diese mit Leitungselektronen ein kohärentes Band bilden. Die jüngsten Resultate an YbAl_3 liefern ziemlich deutlich den Beweis für die letztere Annahme. Die 5f-Elektronen der Aktiniden sind weniger stark gebunden und reagieren sogar empfindlicher auf ihre Umgebung, was durch das Auftreten einer Ladungsdichtenwelle in α -Uran und fünf allotropischen Formen von Plutonium-Metall bezeugt wird. Aus offensichtlichen Gründen stützt sich der Grossteil unseres gegenwärtigen Verständnisses auf Uran, was natürlich das Risiko einer einseitigen Auslegung nach sich zieht. In einem kürzlich von Physikern von 5 Instituten aus 4 Ländern durchgeführten « tour de force » Experiment, wurde der magnetische Formfaktor eines Einkristalls von PuSb mit polarisierten Neutronen untersucht. Die Ergebnisse zeigen deutlich einen 5f⁵-Zustand und identifizieren die Wellenfunktion des Grundzustands.

Bericht des Direktors

Bei der Untersuchung von ungeordneten Systemen mit Neutronen als Sonden besticht der Kontrasteffekt, der durch Isotopensubstitution erzielt werden kann. Diese Technik, die ganz besonders bei wässrigen Lösungen erfolgreich ist, kann natürlich auch auf die Aufklärung von Strukturdetails in amorphen Metallen ausgedehnt werden, wie ein noch nicht lange zurückliegendes Experiment an $(\text{Fe}_{1-x}\text{Mn}_x)_{75}\text{P}_{15}\text{C}_{10}$ zeigt. Hier spielt das Mangan die Rolle eines Eisenisotops, wobei seine negative Streulänge den nötigen Streukontrast liefert.

Unter den jüngsten Veröffentlichungen finden sich klassische Strukturuntersuchungen an einer breiten Skala von interessanten Stoffen; so behandeln sie zum Beispiel die Änderung der Platzbesetzung von Benzol in Zeoliten ebenso wie die Modell-Darstellung der Kernbildungs- und Wachstumsprozesse in einer Glas-Keramik. Alle diese Daten wurden mit Hilfe der Kleinwinkelstreuung erzielt.

Einige der bedeutungsvollsten Arbeiten jüngsten Datums wurden jedoch auf dem Gebiet der physikalischen Chemie veröffentlicht, wo die Technik kalter Neutronen ganz besonders für die Untersuchung von Kolloiden und Mizellen geeignet ist. Hier zeigen Kleinwinkelmessungen zusammen mit selektiver Deuterierung und expliziter Berechnung von Interferenzeffekten zwischen Teilchen, wie ein kleines Molekül (Pentanol) in ein Mizell (Natriumoktanoat) eingebaut ist, und wie dieses sich mit der Konzentration ändert. Selektive Deuterierung oder strikt selektive Protonierung in Verbindung mit quasielastischer Streuung kann dazu dienen, die Dynamik einer speziellen Komponente zu analysieren. Dies wurde von Experimenten bestätigt, bei denen der Phasenübergang verfolgt wurde, indem man schrittweise vom Mizell bis zu "Öl in Wasser" und "Wasser in öligen Mikroemulsionen" ging. Diese Neutronenstreuexperimente an konzentrierten Mizellen und Kolloidsystemen ähnlich wie weiter zurückliegende Untersuchungen an konzentrierten Polymersystemen werden wahrscheinlich das allgemeine Interesse an diesem sehr wichtigen Gebiet wecken.

Erneuerungsprogramm des Reaktors

Die Ziele dieser letzten und teuersten Phase des gegenwärtig laufenden HFR-Erneuerungsprogramms liegen auf der Hand: (1) Der Ersatz aller, radioaktiver Strahlung am stärksten ausgesetzten, Strahlrohreinheiten im Innern des Reaktors, d.h. innerhalb des Schwerwassertanks, (2) die endgültige Reparatur des beschädigten Schwerwasseransaugstutzens und (3) die Auswechslung der bestehenden vertikalen kalten Quelle durch eine neue von höherer Effizienz. Die aufwendigsten Eingriffe stellen der Ersatz des H1/H2-Einschubs (der die kalten und thermischen Neutronenleiter versorgt), des durchgehenden Strahlrohrs H6/H7 und die Intervention mittels Elektroerosion am Schwerwasseransaugstutzen dar. Zum Zeitpunkt dieses Berichts war ein Grossteil dieser Reaktorkomponenten bereits ausgebaut. Dass dieses komplexe und schwierige Un-

terfangen bisher planmässig verlief, ist das Verdienst der hervorragenden Planung und Durchführung durch die Reaktorabteilung, die bei ihrer Arbeit ständig von der Abteilung für Strahlenschutz unterstützt wird.

Abteilungen "Instrumente & Methoden", "Instrumentierbetrieb" und Rechenabteilung

Obwohl am Jahresende vor allem die Reaktorabteilung im Rampenlicht stand, haben auch andere Abteilungen während des Jahres gediegene Arbeit geleistet. Zu erwähnen ist vor allem die grosse Anstrengung von EDEX, zuerst das Experimentierprogramm zu unterstützen, das vom 8. August 1983 bis zum 2. Oktober 1984 mit nur kurzen Unterbrechungen (zwischen den Zyklen) abrollte, und anschliessend die grossen Aufgaben in Verbindung mit dem Reaktorhalt zu bewältigen. Die Rechenabteilung, abgesehen von ihrer gewohnten Unterstützung der wissenschaftlichen Experimente, tat sich durch eine Verbesserung des Datennetzes hervor, ganz besonders was den Datenfluss von den Instrumenten zum Zentralrechner anlangt. Es war ausserdem mit sehr ausgedehnten Programmieraufgaben für VAX-Rechner beschäftigt, die für Instrumente mit grossem Datenausstoss und für geldsparende, administrative Rechenarbeiten nötig wurden. Die Abteilung "Instrumente & Methoden" bleibt ein entscheidender Faktor des Langzeiterfolgs des ILL. Ich zitiere aus dem jüngsten Bericht der "American Academy of Science Commission" über *Grossforschungseinrichtungen für Materialforschung und verwandte Gebiete* (Seitz-Bericht):

"Die Folgen dieser Investitionslücke (bei der Entwicklung und dem Bau neuer Spektrometer) im Laufe der letzten 10 Jahre, die sich zwischen europäischen und amerikanischen Forschungsreaktoren aufgetan hat, bringen uns immer mehr unsere (US) Unfähigkeit zum Bewusstsein, den Wettbewerb in neuen Wissenschaftsgebieten aufzunehmen, welche von Techniken wie der hochauflösenden Neutronenspektroskopie, Klein- und Mittelwinkelstreuung und diffuser Streuung Gebrauch machen".

An anderer Stelle wurde ganz ausdrücklich auf das ILL Bezug genommen. Um diesen Punkt noch zu unterstreichen, sollte nicht unerwähnt bleiben, dass drei neue wichtige ILL-Instrumente noch vor dem Abschalten des Reaktors ihre Tests bestanden. Es handelt sich dabei um IN20 (3-Achsen-Spektrometer mit voller Polarisationsanalyse), DB21 (das in Zusammenarbeit mit EMBL gebaute biologische Diffraktometer für sehr grosse Einheitszellen) und D2B (das verbesserte Modell des Pulverdiffraktometers D1A).

Verbesserungen grundlegender Messtechniken sind von ebenso grosser Bedeutung wie fertiggestellte Instrumente, da jene die Leistung von gleich mehreren Geräten erhöhen. In dieser Beziehung sind die optimale Definition des einfallenden Neutronenstrahls (z.B. mit Hilfe eines Monochromators) und

der Nachweis der gestreuten Neutronen von erstrangiger Bedeutung. Eine Reihe neuer Ideen für bessere ortsempfindliche Detektoren (PSD) wurde verfolgt ; unter ihnen war die vielversprechendste Entwicklung des vergangenen Jahres die Herstellung von gemischten Si-Ge-Kristallen von sehr hoher Qualität. Ein auf der Hand liegender Effekt ist die Erhöhung des Wirkungsgrads des Rückstreu-spektrometers IN10 ; auf lange Sicht könnten davon jedoch noch viele andere Instrumente profitieren, sofern sich diese Technik bewährt.

Administration, Arbeitspotential und Budget

In einem auf vollen Touren laufenden Forschungsinstitut gibt es immer mehr Ideen als Geld zu deren Finanzierung, was notgedrungen seine Verwaltung unter starken Druck hält. Hinzu kommt die Forderung des Lenkungsausschusses, das Personal bis 1987 um 3,5% zu reduzieren und die Tatsache, dass heutzutage Regierungen, ganz gleich welcher politischen Richtung, Betriebsdetails jeder Organisation einer immer intensiveren Kontrolle unterwerfen. Das ILL wird von seiner im Vergleich zu anderen nationalen Laboratorien und Universitäten kleinen Administration gut bedient (auch wenn man den internationalen Charakter und den enormen Besucherstrom nicht in Rechnung setzt). Leider wird das ILL in der Zukunft eher weniger als mehr Stellen zur Verfügung haben, was eine gewisse, wenn auch hoffentlich nicht schwerwiegende Dienstleistungsverminderung nach sich ziehen wird.

Mit Freude vermerke ich die mögliche schrittweise Erhöhung des Anteils permanenter Wissenschaftlerstellen. Dies wird uns gestatten, unsere ausgezeichneten Geräte maximal zu nutzen. Die Priorität bei der Vergabe von Dauerverträgen wird so gesetzt werden, dass die Kontinuität des Betriebs der wichtigsten Instrumente sowie die Bereitstellung von Erfahrung auf neuen Gebieten der Neutronenforschung gewährleistet sind. Das Budget 1985 wird es gestatten, alle wesentlichen Instrumentprojekte wenn auch im Vergleich zur optimalen Planung mit etwas geringerem Tempo durchzuziehen. Diese Entwicklungen müssen genügend weit vorausgeplant werden und deshalb hoffen wir auf die baldige Bereitschaft der Gesellschafter zu einer klaren Stellungnahme zum Budgetrahmen für die Zeit nach dem Modernisierungsprogramm.

Personal und Besucher

Unter den vielen Besuchern des ILL war der prominenteste Gast der Präsident der Bundesrepublik Deutschland, Richard von Weizsäcker. Unsere Glückwünsche gehen im besonderen an P. Nozières, der mit dem Wolf-Preis 1985 für Physik ausgezeichnet wurde, sowie an Pierre Becker, der ab 1. Januar 1985 Physikprofessor an der Universität Grenoble wurde, und an Siegfried Hess, einem Besucher des Theoriekollegiums, der

zum ordentlichen Professor an der Technischen Universität Berlin ernannt wurde. Nicht alle ILL-Wissenschaftler gehen konventionelle Wege : Otto Schärpf, der aus D7 ein überragendes Gerät machte, nahm sich ein paar Tage frei, um die kirchliche Trauung seines Kollegen Willi Just in Österreich vorzunehmen.

Ich möchte auch diesmal wieder die positive Einstellung aller Mitarbeiter zu ihrer Arbeit erwähnen, sei es dass dies informell seinen Ausdruck fand, oder formell über den Betriebsrat bekundet wurde.

1985 und darüber hinaus

Ich schloss meinen Bericht vom vergangenen Jahr mit dem Traum von engeren Beziehungen zwischen dem ILL und der europäischen Synchrotronstrahlungsquelle (ESRF). Das ILL hatte im Frühjahr 1984 formell seine Argumente hierfür dargelegt und im Oktober näherte sich dieser Traum ein wenig der Wirklichkeit, als Frankreich und Deutschland Grenoble als Standort für diese Quelle ankündigten. Ein Teil der vom ILL entwickelten Begeisterung wird sicher noch nötig sein, wenn das Projekt 1986 mit gehörigem Elan starten soll. Es wird erwartet, dass die ESRF von Beginn eine breitangelegte europäische Basis haben wird.

Die Bemühungen des ILL um eine breitere Mitgliedschaft sind in der Zwischenzeit langsam einer Erwartung gewichen. Ich hoffe darüberhinaus, dass das ILL im kommenden Jahr die ersten Besucher aus der Industrie willkommen heißen kann.

Nachwort

Während ich mit meinem Bericht zum Ende komme, beginnt es draussen kräftig zu schneien. Dies ist angemessen, denn wie jeder Wissenschaftler mit befristetem Vertrag, werde auch ich dem ILL nachtrauern, obgleich ich wie so manch anderer als Benutzer zurückkehren möchte. Ich danke allen Abteilungen des Instituts, vor allem aber meinen Kodirektoren H. Ruppertsberg und A. Michaudon für ihre grosse Hilfe und Unterstützung.

B.E.F. Fender

Rapport du directeur

J' écris ce troisième et dernier rapport en tant que Directeur, et encore une fois par un beau Jour de l'An ; le soleil et les nuages se pourchassent de la Chaîne de Belledonne au Vercors, découvrant de temps en temps de façon provocante la blancheur éblouissante de la neige de ce début de saison.

La ville de Grenoble est en vacances, l'Institut est calme et se prépare pour la dernière phase du programme de renouvellement du réacteur. L'équipe de quart surveille le réacteur comme toujours et seulement quelques scientifiques sont visibles, qui ont échappé aux festivités afin d'utiliser l'ordinateur central.

Malgré la tranquillité momentanée de ce jour, l'année 1984 a été excellente pour l'Institut.

Programme scientifique

Un programme scientifique complet a été exécuté jusqu'en octobre, les chercheurs invités et les physiciens de l'ILL essayant d'exploiter chaque heure de mesure sur les dispositifs expérimentaux de l'Institut avant l'arrêt. Le dernier jour, environ 50 instruments programmés, instrument « S » et positions « test » fonctionnaient. En tout 707 expériences approuvées par le Conseil Scientifique ont été achevées en 1984.

Comme je l'ai plusieurs fois déjà souligné, les informations fournies par la diffusion neutronique sont si directes, si relativement précises que presque chaque publication ajoute de façon significative à notre compréhension de la matière condensée. De même, les données obtenues des noyaux après la capture de neutrons donnent des renseignements uniques au sujet de la structure du noyau ainsi que de la fission, tandis que les propriétés du neutron même restent d'un grand intérêt en ce qui concerne les théories de la violation de parité et de l'unification. Sur 400 publications environ en 1984, qui découlent des travaux à l'ILL, il est comme toujours difficile de choisir les « meilleures » publications de l'année. Comme d'habitude, dans la suite de ce rapport, les secrétaires de collège présentent quelques résultats exceptionnels ; selon la pratique, il y a maintenant une revue générale — cette fois au sujet des « structures des complexes biologiques étudiés par la diffusion neutronique à faible résolution » par P.A. Timmins et G. Zaccai. Les trois workshops à l'ILL publiés pendant l'année sont également recommandés pour ceux qui veulent évaluer la large gamme d'activités autour du réacteur à haut flux. Il s'agit de "Reactor based fundamental physics" (J. de Physique, C3, 1984) ; "Water" (J. de Physique, C7, 1984) ; "Sample Environments in Neutron and X-ray Experiments" (Revue de Physique Appliquée 19, 1984, p. 643-857). Une autre façon de comprendre le vaste domaine de la science utilisant les neutrons est de revoir les publications des dernières semaines. A

partir de cette tranche d'activités on voit que le haut flux des neutrons alliés aux spectromètres à cristal très précis et efficaces ainsi qu'aux spectromètres pairs, a ouvert la possibilité dans les noyaux légers et moyens de suivre jusqu'à l'état fondamental les transitions gamma émises par un noyau excité. Ces études des structures des états nucléaires bas peuvent être mises en corrélation avec des modèles (par exemple le modèle du gaz de Fermi) des noyaux à une excitation de quelques MeV. Dans la physique de l'état solide, il nous est rappelé encore une fois que notre compréhension de ce qui se passe à ou près d'une transition de phase dépend fortement des résultats de la diffusion neutronique. L'intérêt actuel continue d'être centré sur des solides modulés de façon incommensurable, et le Th Br₄ représente un système particulièrement séduisant parce que : 1) les déplacements ioniques associés à la modulation restent de petite amplitude et sont de caractère sinusoïde jusqu'aux températures les plus basses, et 2) le caractère mobile est tel que la branche phason peut être identifiée par la diffusion neutronique inélastique à haute résolution. Une grande partie de l'histoire du ThBr₄ est maintenant connue, bien que le rôle éventuel d'impuretés influençant les structures modulées indique une participation future des spécialistes de la chimie de l'état solide.

Le magnétisme est un autre domaine qui dépend beaucoup des résultats neutroniques, bien que les caractéristiques magnétiques elles-mêmes soient souvent d'intérêt secondaire par rapport à l'information qu'ils donnent sur le comportement électronique. Dans ce contexte les systèmes d'électrons f posent des questions astreignantes. Par exemple, dans les systèmes de terres rares anormaux (c'est-à-dire de valence mixte) il y a controverse si les ions sont à décrire comme des particules indépendantes ou si les ions se raccordent avec des électrons de conduction pour former une bande cohérente.

Les derniers résultats pour Yb Al₃ donnent les évidences les plus claires jusqu'à présent de cette dernière interprétation. Les électrons 5f des actinides sont moins étroitement liés et encore plus sensibles à l'environnement, comme en témoigne la présence d'une onde de densité de charge dans l'uranium α et dans cinq formes allotropiques du plutonium métallique. Pour des raisons évidentes, une grande partie de nos connaissances actuelles se base sur l'uranium, ce qui entraîne le risque d'une compréhension partielle. Par un tour de force expérimental récent, des physiciens de cinq laboratoires et de quatre pays ont examiné avec des neutrons polarisés le facteur de forme magnétique d'un cristal simple de PuSb. Les résultats montrent clairement un état 5 f⁵ et précisent la fonction d'onde de l'état fondamental.

Pour l'étude des systèmes désordonnés la qualité particulière du neutron comme sonde est mise en évidence par l'effet de contraste qui peut être obtenu par la substitution isotopique. La technique qui a été particulièrement efficace pour l'étude des solutions aqueuses peut évidemment être étendue pour

fournir des détails de la structure des métaux, comme l'a montré une étude récente de $(\text{Fe}_{1-2}\text{Mn}_x)_{75}\text{P}_{15}\text{C}_{10}$. Dans ce cas le manganèse joue le rôle d'un isotope de fer et sa longueur négative de diffusion donne le contraste de diffusion nécessaire.

Des études classiques structurales d'une gamme étendue de matériaux intéressants apparaissent également dans les dernières publications ; on y trouve par exemple les changements d'occupation de site du benzène observés dans un zéolite et la modélisation des procédés de nucléation et croissance dans une céramique de verre utilisant des données obtenues à partir de données de diffusion à petits angles.

Quelques-unes des publications récentes les plus significatives sont dans le domaine de la chimie physique, où les techniques des neutrons froids sont particulièrement appropriées à des études des colloïdes et des micelles. Ainsi les mesures de diffusion à petits angles associées à la deutération sélective et au calcul explicite des effets d'interférence entre les particules montrent comment une petite molécule (pentanol) s'incorpore dans une micelle (octonoate de sodium) et comment ceci varie avec la concentration. La deutération sélective ou la protonation strictement sélective, en liaison avec la diffusion quasi-élastique, peut être utilisée afin de démontrer la dynamique d'un composant particulier. Les rapports ont suivi une série de transitions de phase de la micelle en passant par l'huile dans l'eau jusqu'à l'eau dans des microémulsions huileuses. Ces études de diffusion neutronique sur les micelles concentrées et les systèmes de colloïdes, tout comme les études antérieures des systèmes de polymères concentrés, vont probablement stimuler l'intérêt général pour un domaine très important.

Programme de renouvellement du réacteur

Les buts de cette dernière et très grande phase du programme de renouvellement du Réacteur sont simples. Ce sont 1) le remplacement de toutes les parties du cœur du réacteur (c'est-à-dire à l'intérieur du bidon réflecteur) qui ont été soumises à des doses de radiation les plus importantes, 2) la réparation définitive du collecteur de reprise d'eau lourde endommagé et 3) le remplacement de la source froide verticale existante par une nouvelle source de modèle amélioré.

Les opérations simples les plus importantes sont le remplacement des canaux H1/H2 qui desservent les guides froids et thermiques ; le remplacement du canal traversier H6/7 ainsi qu'une intervention d'électroérosion sur le collecteur de reprise. Jusqu'à présent le démontage des différents organes est presque terminé. Le fait que ce travail complexe et difficile soit entièrement sur plan rend hommage aux excellentes prévisions et à l'exécution du Département Réacteur assisté à tout moment par le Service Radioprotection.

Départements Instruments & Méthodes, Exploitation des Instruments et Informatique

Bien qu'à la fin de l'année on ait mis en valeur le travail du Département Réacteur, d'autres départements ont également réalisé un excellent travail durant l'année. Je note en particulier les gros efforts d'EDEX qui a soutenu tout d'abord un programme expérimental s'étalant du 8 août 1983 au 2 octobre 1984 avec seulement de courtes interruptions entre les cycles, puis les principales tâches liées à l'arrêt lui-même. Le Département Informatique, indépendamment de son soutien habituel d'expériences scientifiques, a amélioré le réseau d'ordinateurs de l'Institut, particulièrement en ce qui concerne le transfert de données des instruments au calculateur central. Cela a nécessité une vaste programmation pour les ordinateurs VAX dont on a besoin maintenant pour les instruments à taux élevé de données, ainsi que pour le développement de l'informatique administrative dans le but de réaliser des économies. Le travail du Département Instrument & Méthodes reste crucial pour le succès à long terme de l'Institut. Je cite le rapport récent de la Commission de l'Académie des Sciences Américaine au sujet de "Major Facilities for Materials Research and Related Disciplines (rapport Seitz)" s'y rapportant. Les conséquences de cet écart d'investissement (dans le développement et la construction de nouveaux spectromètres) sur la dernière décennie entre les réacteurs de recherche européens et américains se font sentir de plus en plus dans notre incapacité (Etats-Unis) de faire concurrence dans les nouveaux domaines de la Science utilisant des techniques telles que la spectroscopie de neutrons à haute résolution, diffraction de petits et moyens angles et diffusion diffuse ; par ailleurs, il était clair dans le rapport que la commission se référait notamment à l'ILL et comme pour souligner ce point, dans les semaines précédant le grand arrêt, trois nouveaux instruments importants ont subi leurs premiers tests. Ce sont IN20 (le spectromètre 3 axes équipé pour l'analyse complète de la polarisation), DB21 (le diffractomètre pour la biologie construit en collaboration avec EMBL et conçu pour étudier de très grandes cellules élémentaires) et D2B (le remplacement amélioré du diffractomètre à poudre de D1A).

Les améliorations des techniques de base sont tout aussi importantes que les instruments entiers parce qu'elles peuvent améliorer les performances de plusieurs instruments. A cet égard la définition optimale du faisceau incidant de neutrons (par exemple avec un monochromateur) et la détection des neutrons diffusés est essentielle. Bien qu'un grand nombre de nouvelles idées pour des détecteurs localisants améliorés ait été exploré, le développement le plus prometteur de 1984 a été la production de cristaux mixtes Si-Ge de très haute qualité. L'effet immédiat est de mettre en valeur la faculté de l'instrument IN10 de rétro-diffusion à haute résolution mais les perspectives à longue portée, si elles se réalisent, pourraient améliorer beaucoup d'instruments.

Rapport du directeur

Administration, main d'œuvre et budget

Dans un institut de recherche pleinement actif où l'on trouve toujours beaucoup plus d'idées que d'argent pour les réaliser, il y aura toujours une forte pression sur l'administration. Ajouter à cela le fait que le Comité de Direction a demandé une réduction de 3,5% de l'effectif total du personnel pour 1987 ; tenir compte du fait que les gouvernements de quelque caractère que ce soit examinent de près les travaux détaillés de chaque organisation et vous avez ainsi une administration sous pression. L'ILL est bien servi à cet égard par son Département Administratif. Celui-ci est petit par rapport à beaucoup de laboratoires nationaux ou universités, même en ne tenant pas compte du caractère international de l'ILL et de son énorme flot de visiteurs.

La perspective est pour moins plutôt que davantage de postes et quelques réductions de prestations de service pas trop sérieuses, je l'espère.

Je suis heureux de pouvoir dire qu'il sera possible d'augmenter peu à peu la proportion de scientifiques permanents de l'Institut, ce qui nous permettra d'utiliser au maximum nos excellentes installations. La priorité sera de recruter des candidats qui permettront d'avoir une continuité des instruments importants et de fournir des connaissances techniques dans les domaines plus récemment étudiés par neutrons.

Le budget 1985 permettra à tous les principaux projets d'instruments de poursuivre à une allure seulement un peu plus lente que la vitesse optimale mais, étant donné le besoin de pouvoir projeter ces améliorations bien à l'avant, nous espérons qu'il sera bientôt possible aux associés de donner des éléments assez clairs en ce qui concerne le niveau du budget de l'après-programme de modernisation.

Personnel et visiteurs

Parmi les nombreuses visites à l'ILL, l'événement le plus marquant a été la visite très réussie de Richard von Weizsäcker, Président de la République Fédérale d'Allemagne. Toutes nos félicitations à P. Nozières qui a reçu le prix Wolf 1985 de Physique, à Pierre Becker qui, à partir de janvier 1985, devient Professeur de Physique à l'Université de Grenoble, ainsi qu'à Siegfried Hess, visiteur récent dans le Collège Théorie, qui est également nommé Professeur à l'Université Technique de Berlin. Tous les scientifiques de l'ILL ne suivent pas une voie classique, Otto Schärpf qui a fait de D7 un aussi performant instrument et qui s'apprête à prendre un ou deux jours pour célébrer le mariage en Autriche de son co-responsable d'instrument Willi Just !

Comme d'habitude, un trait de la vie à l'ILL est l'attitude positive de tous les collaborateurs envers les tâches confiées, que cela soit exprimé d'une manière informelle ou par les procédures formelles du Comité d'Entreprise.

1985 et au-delà

L'an dernier, je terminais mon rapport en rêvant de liens plus étroits entre l'ILL et la source européenne Synchrotron à rayons X. Pendant toute l'année, l'Institut a exposé de manière formelle ses arguments et ainsi le rêve s'est un peu rapproché de la réalité avec l'annonce en octobre que la France et l'Allemagne proposeraient Grenoble comme site de leur choix. Un brin de l'imagination qui a lancé l'ILL sera encore nécessaire si l'on veut que le projet démarre bien en 1986.

La Source Européenne à Rayonnement Synchrotron devrait être largement européenne dès le début. Entre-temps, les aspirations de l'ILL d'obtenir une adhésion plus large se sont lentement transformées en attente. Il faut aussi mentionner qu'il y a maintenant l'espoir que l'ILL voie ses premiers utilisateurs industriels directs en 1985.

Un dernier mot

J'arrive à la fin de mon rapport et je trouve qu'il neige de plus en plus fort. C'est tout à fait approprié, car comme tout autre scientifique à contrat à durée limitée, je suis triste de quitter l'ILL, bien que comme les autres, je prévoie de revenir comme utilisateur. Je remercie tous les services de l'Institut mais en particulier mes directeurs-adjoints Henner Ruppertsberg et André Michaudon, pour m'avoir si souvent aidé et assisté.

B.E.F. Fender



A fish's-eye view of the ILL's reactor and main building.

1

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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

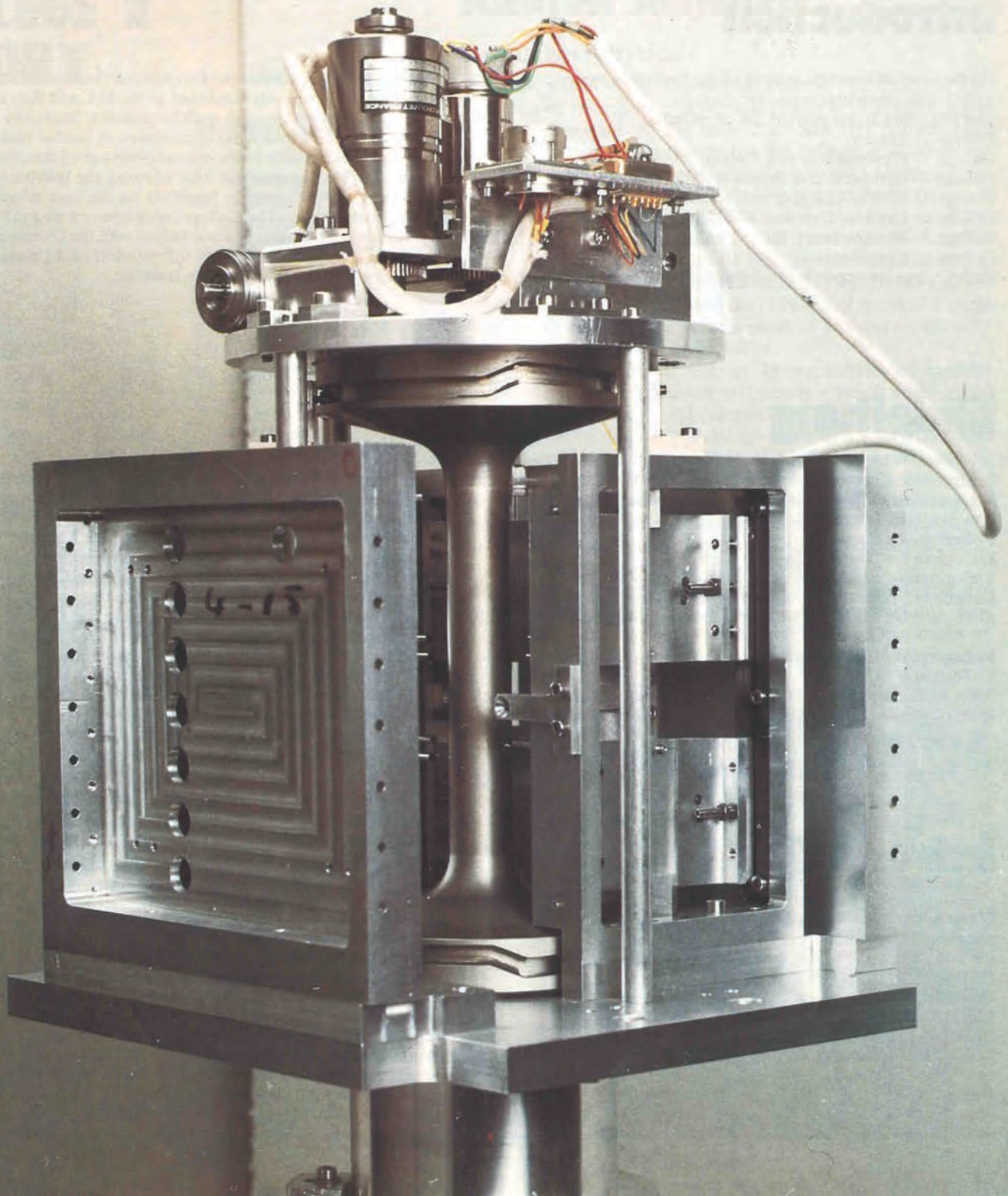
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COLLEGE 9

Chemistry

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COLLEGES



1

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.

COLLEGE 2 THEORY

Members

Ph. Nozières
P. Becker
T. Burkhardt
B. Desplanques
U. Felderhof
G. Ford
D. Gempel
R. Hasse
F. Hirshfeld
D. Quemada
J.M. Richard
H.J. Schulz
M. Uwaha
T. Ziman

Medium term visitors:

A. Andreev (USSR)
T. Eisenriegler (FRG)
G. Gehring (UK)
I. Guim (USA)
H. Fogedby (Denmark)
K. Ishikawa (Japan)
J. Jensen (Denmark)
J. Keating (UK)
S. Noguera (Spain)
U. Stroth (FRG)
V. Symons (UK)

INTRODUCTION

In addition to furthering their individual research programs which covered most subjects of interest at the ILL, the members of the Theory college contributed to the general scientific life of the ILL. As is usual the weekly general colloquium was organized within the college, first by Ziman and then by Gempel. Gempel and Nozières also arranged the theory seminar, held weekly in conjunction with other Grenoble Laboratories. Nozières delivered two series of lectures for the Collège de France : one in Paris on crystal morphology, the other in Grenoble on the subject of itinerant magnetism. In March Hasse organized a Workshop on "Semiclassical Methods in Nuclear Physics". Becker and Hirshfeld have, with J. Brown of College V, arranged a workshop on the "Interpretation and Uses of Electronic Distributions" for March 1985. Becker's appointment to a chair at the University of Grenoble should help maintain the links between the ILL and the local scientific community.

P. Nozières has been awarded jointly with C. Herring, the Wolf Prize for Physics for 1985. This prize will be presented to him by the Israeli parliament to honour his outstanding contributions to physics of condensed matter.

SCIENTIFIC ACTIVITY

1. Surface physics

Nozières and Uwaha developed theories to describe the dynamics of interfaces and the kinetics of crystal growth for the particular case of the quantum solid ^4He . In addition Nozières constructed a theory for the influence of finite inclination on the roughening transition in order to interpret experiments carried out at the Ecole Normale in Paris. Gempel worked with J. Villain of the CENG on the theory of roughening and stability of high index crystal faces with the specific end of calculating the Debye-Waller factors for diffraction from copper crystals as measured by J. Lapujoularde and his group at Saclay. Schulz studied the problem of the equilibrium shape of crystals, and delivered a series of lectures on the subject at a workshop at Les Houches.

Burkhardt continues his activity in the subject of surface critical phenomena: effects at surfaces in systems undergoing a bulk phase transition. He calculated effects due to spatially inhomogeneous magnetic exchange close to the interface and also showed how the hypothesis of conformal invariance of critical correlations can be exploited to calculate exactly order parameter profiles in confined geometries. This last work, apart from its direct experimental consequences, is important for the theoretical question of the effects of boundary conditions on finite size scaling calculations.

Ford brought to the ILL a long-standing interest and experience in the calculation of electromagnetic interactions close to metal surfaces, as regards in particular the phenomena of molecular fluorescence and surface enhanced Raman scattering.



Professor P. Nozières, the animator and head of the ILL theory group.

Magnetism

Ziman and Schulz continued studies of the zero temperature correlations in one-dimensional magnetic insulators. While directed primarily at determining the ground state correlations by reliable calculation of the critical exponent in the massless phase of axially symmetric models, the methods have led to the possibility of calculating a renormalized excitation spectrum which should be valuable in interpreting dynamic measurements of the CsNiF_3 family of compounds in terms of microscopic Hamiltonians.

Nozières revived a continued interest in magnetic alloys to extend the current understanding of the single impurity Kondo problem to more concentrated alloys, exploring the possible hierarchy of crossovers between regimes of complete or partial screening and magnetic order.

Becker and Hirshfeld worked closely with C. Cohen-Addad (CNRS) and M.S. Lehmann (ILL) to calculate charge and spin densities in crystals with sulphur-oxygen bonding. Becker directed a thesis project at Saclay on the experiment and theory of magnetism in solid oxygen crystals.

3. Modulated and disordered solids

Becker worked with M. Bonnet (ILL) and F. Vigneron (CNRS) on modelling the modulated magnetic phases of rare earth beryllium compounds and CeSb , as have been observed at the ILL. He is also involved, with P. Coppens (Buffalo N.Y.) in the problem of refinement of crystallographic studies of structurally modulated crystals performed at the Cornell Synchrotron.

Ziman pursued, with P.A. Lindgård of Risø, his development of a theory for the dynamic structure factor of modulated magnetic structures, in particular the rare earths neodymium and praseodymium. With summer stagiaire Keating he extended the work to the spin wave dynamics of the helical phase with the inclusion of anisotropy-induced "bunching" as has been seen in static studies of Holmium.

Grepel worked on the closely related theoretical problem of localization in almost periodic Hamiltonians, extending previous work to calculate the frequency dependent conductivity, with results that differ interestingly from those of disordered systems.

Felderhof and Ford are advancing the use of cluster expansion techniques for wave propagation and radiation transfer in disordered media with inclusion of effects of multiple scattering and localization. They have made practical application to the transport properties of electrons in liquid metals and of solutions of electrolytes.

Ziman worked on a scaling analysis of the low frequency spin-wave dynamics of dilute Heisenberg antiferromagnets near the percolation threshold at which effective medium theories break

down. With the help of the summer stagiaire V. Symons he developed computational means to estimate the critical behaviour of the coefficients of a "hydrodynamic" description near percolation.

4. Stochastic processes

Both Ford and Grepel have been studying the delicate question of introducing quantum mechanical interference effects to the classical description of stochasticity. Ford has formulated and applied a procedure for calculating the Stark effect in the presence of black-body radiation.

5. Physics of fluids

Hess left the ILL in April after a fruitful collaboration with experimental groups in simulating and calculating the structure of simple fluids and colloids under stress. Quemada's arrival maintains the College's strength in the field, however, bringing as he does a wide experience in rheological modelling of concentrated dispersions applied to a variety of industrial and vital fluids ranging from crude oil emulsions to bronchial mucus. Since his arrival, he and Nozières have constructed a theory of flow stability of suspensions which may become a theory of sedimentation.

6. Theoretical nuclear and particle physics

Hasse devoted part of his effort to semi-classical methods of scattering and calculating optical potentials, level densities and response functions. His work on nuclear fission and the cold fragmentation of actinides was in close collaboration with members of College 3, and is directed at providing a detailed quantum-mechanical calculation of such processes. He also developed the theory of nuclear matter in terms of collisionally damped Landau equations.

Desplanques who, while at the ILL, worked with Noguera on the non-conservation of parity in nuclei, returned to Orsay. Richard has recently arrived in the group: his expertise is represented by recent work in the fields of neutron anti-neutron oscillations, nucleon anti-nucleon annihilation and the quark model of hadronic spectroscopy.

Secretary: T. Ziman

COLLEGE 3

Members of the College

I. Internal Members

H.G. Börner
 F. Blönnigen
 J.P. Bocquet
 R. Brissot
 G. Colvin
 H.R. Faust
 I. Förster
 P. Geltenbort
 F. Gönnewein
 H. Hanewinkel
 F. Hoyer
 C. Jewell
 S.A. Kerr
 W. Mampe
 P. Miranda
 B. More
 J. Pannicke
 B. Pfeiffer
 K. Schreckenbach
 U. Stöhlker
 H. Weikard

II. Long-term Visitors

R. Deslattes (NBS)
 W. Gelletly (Manchester)
 G. Greene (NBS)
 E. Krüger
 (PTB Braunschweig)
 P. Liaud (Chambéry)
 N. McLeish (Manchester)
 W. Nistler
 (PTB Braunschweig)
 W. Weirauch
 (PTB Braunschweig)
 D. White
 (Monmouth Oregon)

Collaboration of College 3 with Institutes and Universities in 1984

Argonne	Köln
Belgrade	Lancaster
Bochum	Leningrad
Bordeaux	Livermore LL
Braunschweig PTB	Lyon
Braunschweig University	Mainz
Brookhaven National	Manchester
Laboratory	Mol
Darmstadt GSI	München TU
Darmstadt TH	München University
Fribourg	Münster
Geel JRC	Nice
Giessen	Ottawa NRC
Grenoble CEN	Rutherford Laboratory
Grenoble ISN	Seattle
Grenoble University	Surrey
Harvard	Sussex
Heidelberg	Tübingen
Jülich KFA	Washington NBS

GENERAL SUMMARY

In view of the long reactor shutdown 84/85, College 3 activity was concentrated on very intense experimental activity on all instruments. The widespread scientific interests covered by College 3 become evident from the following summary of the main fields:

1. Nuclear Structure Studies were performed using the PN2 electron spectrometer (BILL), the curved crystal spectrometers PN3 (GAMS), the PN4-pair spectrometer, the PN6 on-line mass separator (OSTIS) and the γ - γ angular correlation facility at H22F.

The high flux at the in-pile targets of BILL, GAMS and PN4 and the high resolution of these instruments have enabled the study of nuclei produced by double neutron capture as well as the measurement of very weak transitions and multipole mixing ratios. The information gathered in these experiments is essential to test theoretical predictions as for example the interacting boson approximation and to search for the possible realization of supersymmetries in nuclei (see box). The con-



The platform of SN5 is a very busy and rapidly changing experimental area. P. Ageron and W. Mampe (on the right), are two ILL experts in the cold neutron domain. On the extreme right of the picture is a test set-up (collaboration ILL/J.C. Bates; Risley, UK) for a feasibility study of neutron life-time measurements using stored neutrons in bottles with low loss liquid surfaces. On the left is an apparatus for measuring surface reflectivities as a function of neutron wavelengths aiming at the improvement of neutron guides.

struction of complete level schemes up to high excitation energies offers an additional possibility to probe the statistical properties of nuclear excitations. The systematic study of actinide nuclei is important for the understanding of fission, nuclear shapes and stability. The new high temperature source at PN6 opened up a new region of neutron rich isotopes in the vicinity of the double magic nucleus ^{132}Sn . From the life time measurement of excited nuclear states (H22F) absolute electromagnetic transition probabilities can be deduced. As these quantities depend on details of the nuclear wavefunction they provide a sensitive test to any nuclear model.

2. In the **Fission** domain the energy-time-of-flight spectrometer PN8 (COSI FAN TUTTE) moved into routine operation with studies of thermal neutron induced fission on ^{229}Th , ^{235}U and ^{249}Cf . Light particle accompanied fission of ^{245}Cm was studied at PN8, and at the double torus ionization chamber DIOGENES (H22E). The experiment on ternary fission in ^{242}Pu was completed. The high flux at the PN1 (LOHENGRIN) target enabled the study of thermal neutron induced fission on ^{238}Np ($T_{1/2} = 2.1$ days) bred from the neutron capture in ^{237}Np to be carried out. The new ionization chamber at PN1 offered the possibility of investigating the process of cold fragmentation (see box 1983) on ^{239}Pu and the isotopic yield distribution of fission fragments after cold fragmentation of ^{233}U . The tripartition process was studied using solid state detectors and a ΔE proportional chamber and the isotopic yields of elements up to oxygen were measured. In this experiment a search for ^{10}He was undertaken. The systematic determination of nuclear masses in the fission fragment region by measuring Q_{β} values was continued on both PN1 and PN6.

3. In **Fundamental Physics** UCN storage times up to 600 sec were obtained in a Foublin oil coated glass bottle. This enabled a feasibility study of a neutron lifetime measurement using two different bottle volumes, which led to a preliminary result of $\tau_n = 850 \pm 60$ s. The focussing characteristics of the neutron microscope was studied by measuring the image of line sources. The EDM experiment has been transferred to the UCN source and will be continued with higher UCN density and under improved conditions. The neutron half life experiment S35, in which α -events of the ^3He (n, α) reaction determine the neutron density and the electron emission rate yields the neutron decay probability, is still in a test phase at position T16. The β -decay of polarized neutrons has been measured with the superconducting spectrometer PERKEO at the SN7 position. For the first time the energy dependence of the β -decay asymmetry was determined and from the absolute value of the asymmetry the ratio of weak coupling constants g_A/g_V was obtained. The measurement of the cumulated β -spectrum of ^{235}U and ^{239}Pu at PN2 (BILL) will significantly aid those groups studying neutrino oscillations at power reactors in the interpretation of their data.

SCIENTIFIC TRENDS AND HIGHLIGHTS IN 1984

Nuclear structure

Work has concentrated in four main areas:

i) Tests of the Interacting Boson Approximation (IBA) model including supersymmetries, ii) Measurement of electric-monopole (E0) transitions and their spectroscopic interpretations, iii) Actinide spectroscopy and iv) Construction of extensive level schemes.

Tests of the IBA and related topics have taken the lions share of the beam time on BILL, GAMS and PN4. Supersymmetries have been tested by a variety of reactions such as $^{194}\text{Pt}(n, e^-)$ on BILL and $^{191,193}\text{Ir}(2n, e^-)$ and $^{191,193}\text{Ir}(2n, \gamma)$ on BILL and GAMS. For the former reaction, particular attention was paid to the E0 transitions and M1/E2 mixing ratios in ^{195}Pt in order to more clearly determine a possible alternative group decomposition for the U(6/12) multi-j supersymmetry. E0 transitions were chosen because in the low energy region they are forbidden in one group decomposition scheme, whilst in a second scheme, certain E0 strengths are expected. Even though the cross section of ^{194}Pt is only of the order of 1 barn good sensitivity was achieved by multi-scanning small regions of interest and summing together the resulting electron spectra. Studies of the applicability of supersymmetry in $^{193,195}\text{Ir}$ have been conducted by double neutron capture in $^{191,193}\text{Ir}$. This type of reaction is achievable at the BILL and GAMS spectrometers due to the high neutron fluxes available. Time variations in intensities were used to select double capture events. These experiments have shown that this technique is well adapted to the study of extremely complex spectra showing up in these measurements (note that the intermediate $^{192,194}\text{Ir}$ are odd-odd nuclei and cross-sections are of the order of 10^3 barns). This is almost entirely due to the outstanding resolution of these two instruments.

Further tests of the IBA were performed by electron measurements in ^{102}Ru and ^{78}Se . In the latter case, attention was again focussed on E0 transitions, as these have a characteristic pattern in the IBA wave functions, particularly near the O(6) limit. The nucleus ^{156}Gd has been studied in the search for transitions which differentiate the IBA from the geometrical model (Fig. 1). The measured branching ratio of the $2^+_{\gamma} \rightarrow 0^+_{\beta}$ and the $2^+_{\gamma} \rightarrow 0^+_{\text{g}}$ transition, $B(E2, 2^+_{\gamma} \rightarrow 0^+_{\beta}) / B(E2, 2^+_{\gamma} \rightarrow 0^+_{\text{g}}) = 0.97$ (50) is in good agreement with the prediction of the IBA. To measure this ratio a sensitivity of $3 \cdot 10^{-6}$ γ -quanta per captured neutron at 100 keV γ energy had to be achieved.

A careful study of selected transitions in ^{168}Er has been completed in order to compare experimental and theoretical E2/M1 mixing ratios. Results show that IBA - 1 calculations (no dif-

ferentiation between neutron and proton bosons) for these ratios are on average a factor of two higher than the measured values. In this case $\Delta K = 1$ mixing with higher lying states could explain the enhanced M1 component. Recent discovery of a collective $K^\pi = 1^+$ antisymmetric state at about 3 MeV excitation energy in ^{156}Gd , ^{168}Er and ^{174}Yb , supports the idea of $\Delta K = 1$ mixing.

Work has continued on systematic studies of actinide nuclei. The year 1984 saw the measurement of ^{241}Pu at BILL and GAMS (Fig. 2) and ^{232}Pa on BILL. Recent completion of data analysis for ^{231}Th has yielded an extensive knowledge of the single particle and vibrational structure of this odd-neutron nucleus. Large admixtures of E0 strength are observed in ten transitions, and eight of these have been placed in the level-scheme, depopulating four bands containing $K = 0^+$ vibrational amplitudes. Previously, evidence for E0 admixtures in de-exciting transitions have already been observed in other odd neutron actinides. Most of these states are interpreted as $K = 0^+$ vibrational components coupled to low lying single particle states, namely $1/2$ [631], $5/2$ [622] and $5/2$ [752]. These investigations have also shown evidence for $K^\pi = 2^+$ and $K^\pi = 0^-$ phonons coupled to quasiparticle excitations involving states such as $1/2$ [631], $3/2$ [631], $5/2$ [622] and $7/2$ [743]. A comparison between theory and experiment shows that many of the experimental features in the actinide region cannot be reproduced by the calculations.

Studies of the thermal neutron capture reaction in light nuclei using the pairspectrometer PN4 and GAMS were continued with the interpretation of the level scheme deduced for ^{42}K . The construction of complete level schemes for these nuclei plays an important role in the discussion of new theoretical approaches to the understanding of the nucleus. It has been shown for instance, that the knowledge of many individual levels leads to a deeper understanding of the statistical properties of nuclei and enables the identification of special structures in nuclear excitations.

The γ -spectroscopic work at PN6 (OSTIS) was centred on the determination of spins and parities of even-even isotopes of Zr, Sn and Te by $\gamma\gamma$ -angular correlation measurements using 3 and 4 detector arrangements. The band head of the β -band in ^{100}Zr was found at 830 keV. $^{94,96}\text{Zr}$ have been measured for the first time. The largely extended running times of the high temperature ion sources opened a new region of neutron rich isotopes in the vicinity of the double magic nucleus ^{132}Sn to be studied at OSTIS. In 1984 first angular correlation measurements were performed in the mass chains 128 and 130. The systematic Q_β -measurements continued on neutron rich Ba and La isotopes with mass numbers 146 and 147. These nuclei with neutron numbers around $N = 90$ are situated at the transition from spherical to deformed nuclear shapes and already a preliminary data evaluation shows deviations from the predicted Q_β -values based on the assumption of spherical

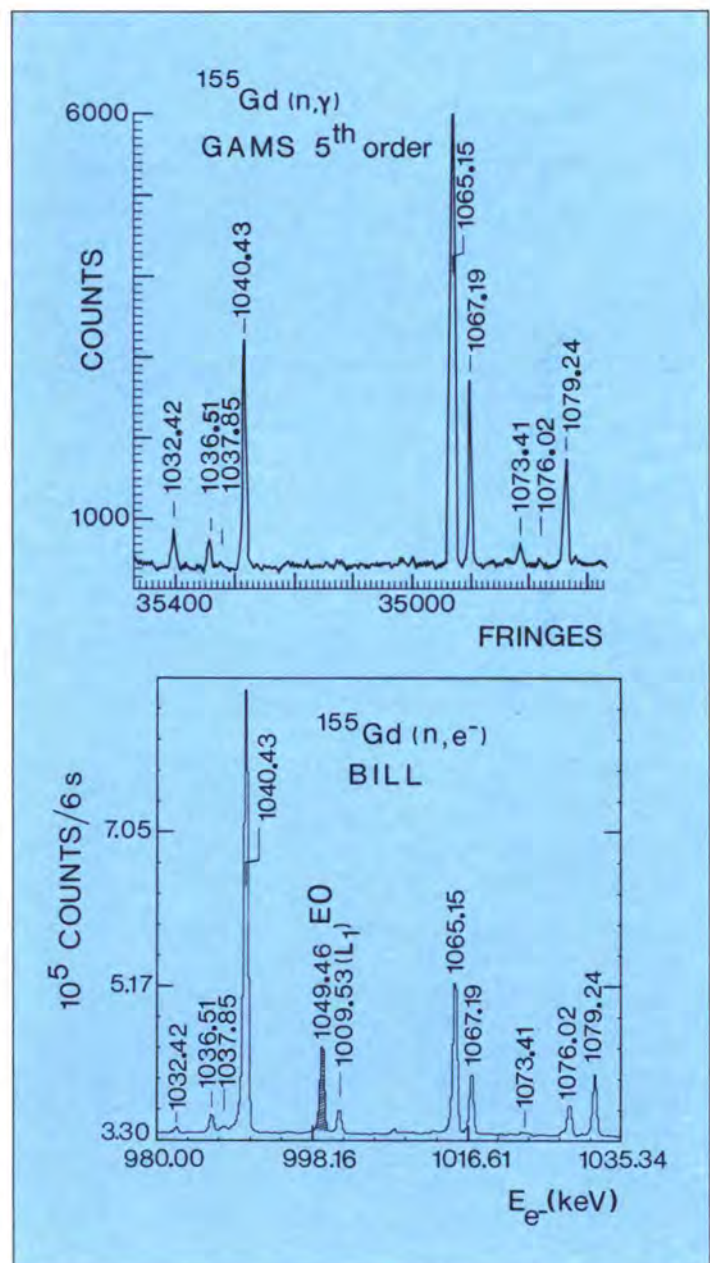


Figure 1: Comparison of a γ -ray spectrum measured with GAMS and a conversion electron spectrum measured with BILL. The relative intensities differ in the two spectra since the conversion coefficients depend on the multipolarity of the transition. The absence of the 1049.5 keV line in the γ -spectrum proves the E0-character of this transition.

shapes. High precision measurements were performed on the mass chains $A = 95 - 99$. By a careful choice of irradiation and cooling cycles or β - γ coincidence techniques, all β -decays in an isobaric mass chain were determined under equal condi-

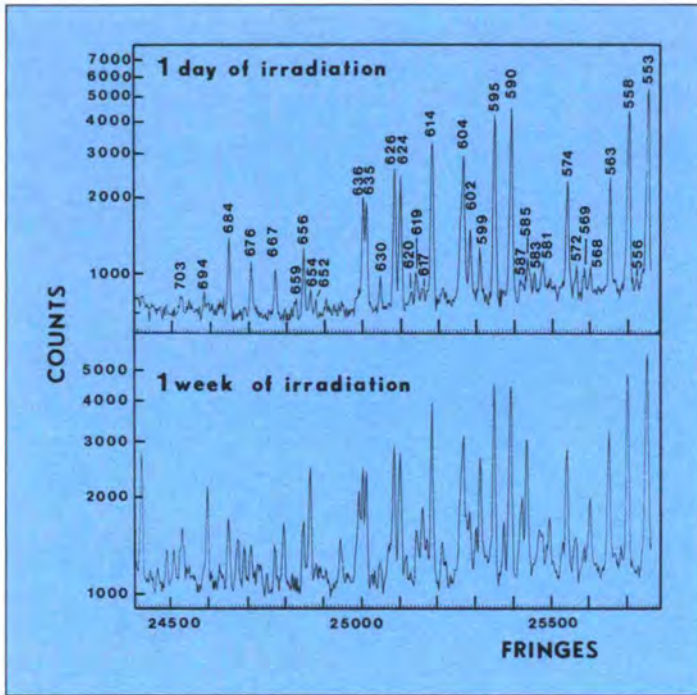


Figure 2: Part of the γ -spectrum of the $^{240}\text{Pu}(n,\gamma)$ reaction measured with GAMS 2. After one week of irradiation the growth of new lines stemming from fission products and double neutron capture can clearly be seen.

tions. Summing up all Q_{β} -values of the chain, mass excesses for $^{95-99}\text{Rb}$ are obtained with errors being small and comparable to direct mass measurements. As these are independent methods, inherent systematic errors may be detected by their comparison enforcing the confidence in the obtained results.

The new β -del-n- γ coincidence technique reported last year was used to determine the neutron feeding of excited states in heavy Ba isotopes. To reach good resolution for delayed neutron spectra below 100 keV by time-of-flight large surface Li-glass detectors were used.

Additionally, a careful study was undertaken to determine the applicability of on-line mass separators, equipped with ion sources for one specific element, to measure relative isotopic fission yields by β -counting techniques. Special care was taken to monitor the isotopic composition of the ion beam by γ -spectra techniques. First measurements were performed on $^{75-82}\text{Ga}$ and $^{119-133}\text{In}$.

Fission

A considerable part of the beam time on PN1 (LOHENGRIN) was devoted to continuation of long term research program-

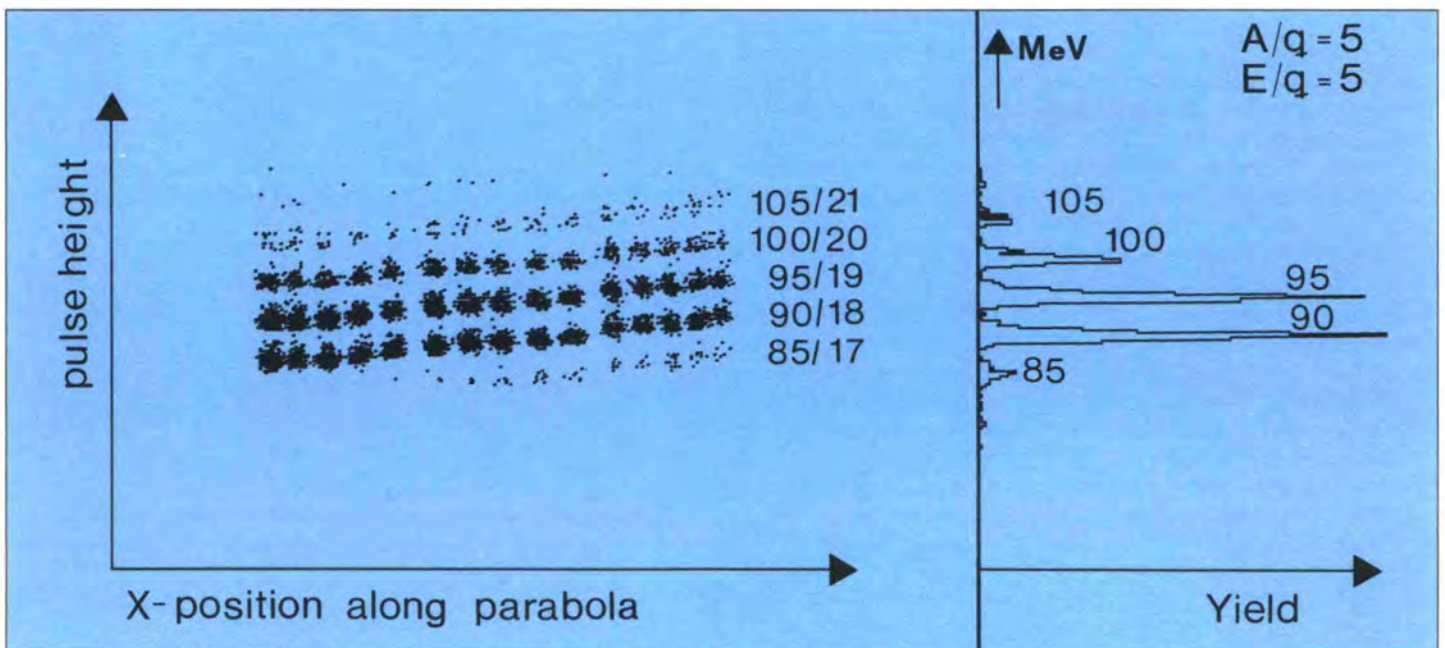


Figure 3: Bidimensional fission spectrum taken with the new big ionization chamber at Lohengrin. The length of the entrance window covers 45 cm of the focal plane of the spectrometer. For calibration purposes a grid was positioned before the entrance window which gives rise to the intensity pattern in the X-position. The spectrometer was set to select a mass over ionic charge ratio $A/q=5$ and a kinetic energy over ionic charge ratio $E/q=5$. The 45 cm of the focal plane cover an energy variation of about 6%, this is why the mass lines are inclined in the pulse height direction. To demonstrate the energy resolution of the chamber the intensity at a given X-position is projected on the energy axis.

mes, such as the determination of masses in the fission fragment region by measuring Q_{β} -values and the determination of isotopic yields and isomer ratios in the heavy fragment group. The measurement of Q_{β} -values is a longstanding effort. One has first to reach a complete set of Q_{β} 's, ranging from the very neutron rich fission fragments down to the valley of β -stable nuclei with masses known from standard mass-spectroscopy, before one is in a position to infer the masses of a whole mass chain. The experimental findings will have to be compared to the masses as predicted by the many semi-empirical mass formulas. This allows calculations of reliable Q -values of fission reactions and gives more confidence into the extrapolation of mass formulas into regions of the nuclide chart which are so far not accessible to experiments. However, these nuclei play an important role in the process of nucleosynthesis in stars.

The investigation of cold fragmentation of ^{239}Pu and the measurement of isotopic yields in the cold fragmentation regime in ^{233}U fission became feasible by the installation of the new big ionization chamber (Fig. 3). With the same set-up the mass distribution of $^{238}\text{Np}(n,f)$ fission, which was bred from ^{237}Np in the target position of PN1, was completed. The isotopic yield for the most probable kinetic energies of the ^{239}Np compound nucleus was also measured. The ^{237}Np -target on Lohengrin is the first of a series, where one exploits the high neutron flux at the in-pile target position to first breed a nucleus by neutron capture and which then is fissile with thermal neutrons. The nuclei in question are the heavy odd Z actinides ^{231}Pa , ^{237}Np , ^{241}Am and ^{243}Am . The fission characteristics of these nuclei at low excitation energies are only poorly known.

A detector arrangement with solid state detectors and a ΔE proportional chamber was used to investigate the yields and energy spectra of light particles from ternary fission. The isotopic yields of elements up to oxygen were measured and, more specifically, a search for ^{10}He was undertaken.

Making use of the mass- and energy separated fission fragment beam available on Lohengrin, a calibration scheme for ionization chambers to be used in fission studies was set up. The measurements show that the response function of ionization chambers are linear in mass and energy of the incoming heavy ions. However, even for chambers with the highest energy resolution ever observed (less than 270 keV for the light fragment group) there is a non-negligible pulse height defect. On the same chamber, the specific ionization of fission fragments being slowed down in the counter gas, was further investigated. Their Bragg curves are obtained on an event-by-event basis by a sampling technique. A striking result is the irregular shape of the Bragg curves for individual events. The behaviour becomes more pronounced the heavier the fragments and the heavier the counter gas. It was verified experimentally that the large fluctuations of the Bragg curves are due to atomic collisions (Fig. 4).

In 1984 the energy-time-of-flight spectrometer "Cosi fan tutte" (PN8) for fission fragments was commissioned and put into routine operation. Generally speaking, it was experienced that the instrument is working properly, under the condition, however, that sufficient time is foreseen for the turnaround from one experiment to another. This is due to the fact that the ultimate performance of the detectors is only reached after a few days of operation, allowing for the temperature, the composition of the counter gas in the ionization chambers, the high voltage stability of secondary electron detectors (channel plates of the time pick-off system) etc to reach stable values.

The first fission reaction to be studied — with a special view to "cold fragmentation" — was $^{235}\text{U}(n,f)$. Different configurations of detectors, both for the energy and the time-of-flight, were tested. The allocated beam time and the difficulties mentioned above did not allow the experiment to be finished. The next fissile targets proposed for analysis were rather exotic: ^{229}Th , ^{245}Cm and ^{249}Cf . Besides the mass and energy distributions of the fission fragments it was also aimed to gain information on the nuclear charges for a given mass and kinetic energy. In the case of $^{245}\text{Cm}(n,f)$ a set of surface barrier detectors placed close to the target intercepted in addition the light particles from ternary fission in coincidence with the fission fragments.

Fundamental physics

The neutron microscope profited from the restoration of the UCN flux by new liners inserted into the in-pile guide. The

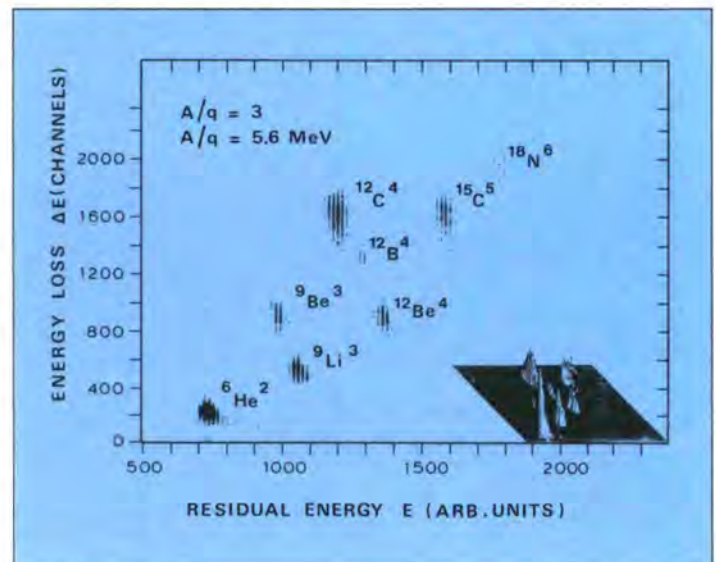


Figure 4: Spectrum of light particles generated in thermal neutron induced fission of ^{235}U . The particles have been detected at the exit slit on Lohengrin with a $E-\Delta E$ telescope. The setting of the electric and magnetic field corresponds to a value mass / ionic charge = 3 and kinetic energy / ionic charge = 5.6 MeV. The particles in the $E\Delta E$ -plane are labelled by their mass and ionic charge.

focussing characteristics of the microscope were studied by measuring the image of a line source well above the background.

It was shown unambiguously for the first time that in a Beryllium coated bottle the UCN reflection losses decrease with temperature to the theoretical expected value.

The neutron electric dipole moment experiment has been transferred to the UCN He source and will be continued with a higher UCN density and under improved conditions. UCN life-times as high as 600 sec were obtained in a Foulin oil coated glass bottle and a feasibility study of a neutron life-time measurement using two different bottle volumes gave a preliminary result of $\tau_n = 850 \pm 60$ sec. An improved version of the experiment is in preparation.

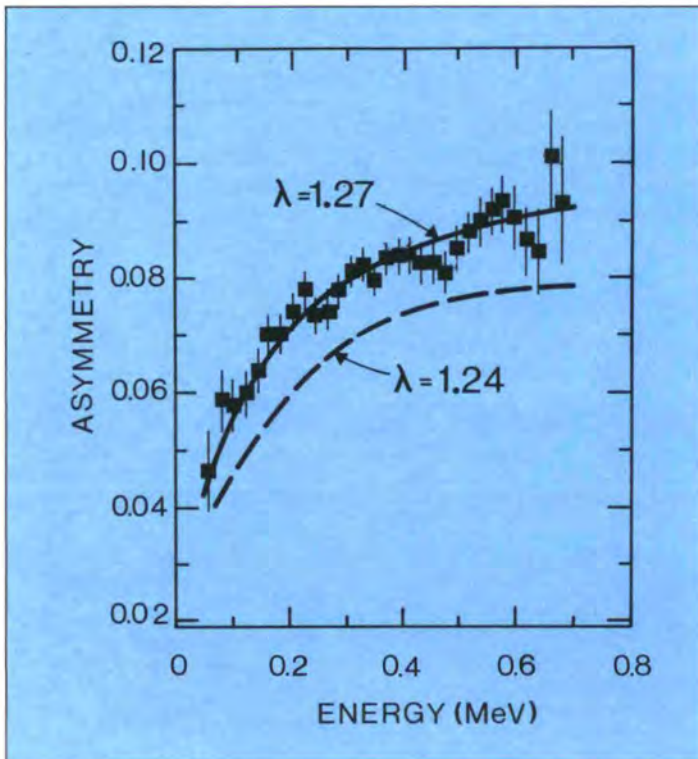


Figure 5: Experimental β -ray asymmetry from one run as a function of β -energy. The curves are expectations for two values of λ .

The ^4He drift chamber for the neutron life-time experiment S52 was tested in the monochromatic neutron beam at T16. It is planned to measure in a first stage the neutron life-time by filling the counter with natural He. A throughgoing neutron beam will induce $^3\text{He}(n,\alpha)$ events and produce electrons from the neutron beta decays. These two types of events can be well discriminated in the detector and their relative rates will determine the neutron life-time, since the (n,α) reaction monitors the neutron density and the electron emission rate measures the neutron decay probability.

The β -decay of polarized neutrons has been measured with the superconducting spectrometer PERKEO at the SN7 position.



Removal of the storage bottle and shield for the EDM experiment from the platform of SN5 and transfer to the H17 guide.

From the absolute value of the asymmetry the ratio of the weak coupling constants $\lambda = |g_A/g_V|$ was found to be 1.270(9).

From this ratio a new value for the neutron life-time of $\tau_n = (890 \pm 10)$ s can be deduced. The recommended value of $\tau_n = (925 \pm 11)$ s leads to a ratio $\lambda = 1.24$. Figure 5 shows that this value is in disagreement with the experimental data by more than 2 standard deviations.

A measurement of the cumulated β -spectrum of ^{235}U and ^{239}Pu fission was completed in 1984. Those groups studying neutrino oscillations have shown that an improved knowledge of both the high energy (7–10 MeV) and the absolute rates of the reactor source spectrum would significantly aid in the interpretation of their data. In order to achieve a precision of the order of 4%, this measurement was performed at a reduced reactor power (4 MW). This low power relaxes the target mass restrictions due to fission self-heating and thus improves the signal to background ratio. The following absolute calibrations were performed at full reactor power. The result of these experiments are in the process of being analysed but promise to yield a considerable improvement (about a factor of 10 in sensitivity), over previous measurements.

Special beam experiments

At the H22F neutron guide two prompt gamma activation experiments were performed to investigate the fundamental aspects and best configuration for future work. Results show good correlations for Sm and Gd but there are still some problems concerning the analysis of B, F and Cl. Studies of rocks of $1.8 \cdot 10^9$ years from the Canadian shield, rocks of deep mantle origin from North Morocco and intrusive rocks from the Skye tertiary igneous centre searching for rare earth and trace elements, have been undertaken at the instrumental activation analysis facility.

First measurements of lifetimes of nuclear levels excited by the (n,γ) reaction using the $\gamma\gamma$ -delayed coincidence method proved that lifetimes in the sub-nanosecond region can be extracted.

At the double torus ionization chamber DIOGENES at H22E the experiment on ternary fission in ^{242}Pu was completed.

The facility H22D continued to be very useful to determine neutron cross sections under experimentally clean conditions. Two examples may highlight this. On the one hand, the fission cross section for thermal neutron induced fission of ^{238}U was reliably measured to be (11 ± 2) μbarns . On the other hand, the (n,p) reaction on the exotic target nucleus ^{26}Al was studied. This reaction is of interest in astrophysics. Several proton lines leading to excited states in ^{26}Mg were identified and cross sections assessed.



A view of the Cosi Fan Tutte spectrometer before removal (due to the replacement of the inclined beam-tube IH1).

SEMINARS

In 1984, 28 seminars dealing with theoretical and experimental problems in nuclear and fundamental physics were held.

Secretary: F. Hoyler

Symmetries in nuclear physics - The interacting boson approximation as a challenge in nuclear spectroscopy

A primary research area of physics is the study of the structure of atomic nuclei. As a quantum mechanical system the nucleus is characterized by excited states of well determined energies, angular momenta, parities and interlevel transitions.

Nuclei consist of a limited number of neutrons and protons, fermions, which interact strongly. To tackle the many-body problem of nuclear structure from first principles is a formidable task. In fact, the difficulty in trying to understand the structure of nuclei is that the exact form of the force governing the motion of these particles is not known and that the system is finite. Therefore, the development of models, such as the nuclear shellmodel⁽¹⁾, (which emphasizes single particle aspects and which is well adapted to interpret lighter nuclei) has been necessary to attempt an understanding of the observed nuclear structure.

Much of the structure of medium and heavy mass nuclei (with mass number $A \gtrsim 80$) appears to be of a predominantly collective nature, in which many particles must be participating. Until recently the most successful approach to understand these collective properties of nuclei was in terms of the geometrical model of Bohr and Mottelson⁽²⁾, where low-lying excitations of medium and heavy mass nuclei would correspond to vibrations and rotations of a nucleus characterized by a specific shape (e.g. spherical, deformed, etc.).

Since the beginning of nuclear structure studies the interpretation of nuclear states has always focussed on the search for states which are simply related. Such simple relationships are brought about by the invariance properties of the Hamiltonian. For instance the invariance under rotations of an even-even deformed axially symmetric nucleus leads to the well-known spin sequence $0^+, 2^+, 4^+, \dots$ of a rotational band. We know from the famous example in elementary particle physics that invariance principles have been treated very successfully by applying the ideas of group theory. States of elementary particles classified into sub-sets, provided insight into the underlying elementary structures.

During the past 10 years a new nuclear model, the Interacting Boson Model⁽³⁾ (IBM) has been developed following similar ideas. It attempts to describe the collective excitations of heavy nuclei in terms of group structures.

In a first step the IBM was limited to the description of even-even nuclei. The basic assumption was that the even-even (even number of protons, even number of neutrons) nucleus consists of an inert core plus some valence particles (protons or neutrons, outside the major closed shells at Z or $N = 50, 82, 126$) and that the valence particles pair together in states with angular momentum $L = 0$ (s-bosons) and $L = 2$ (d-bosons). This idea is similar to the building blocks for superconductivity, the Cooper pairs, but in nuclei there is considerable evidence for collective quadrupole excitations and, hence, the need for d bosons. In this simplest form there is an interaction among the bosons, but no distinction is made between neutron bosons and proton bosons. The number of bosons, N_B , is

just determined by the number of valence proton pairs, N_{π} , plus the number of valence neutron pairs, N_{ν} . The Hamiltonian is constructed by assuming that at most pairwise interactions between the bosons can take place. In general the Hamiltonian must be solved numerically by diagonalization. However, in certain special cases it is possible to solve it analytically by taking advantage of the group structure of this problem: given the five d bosons ($L = 2, \mu = 0, \pm 1, \pm 2$) and the single s boson ($L = 0, \mu = 0$), the group structure is that of $U(6)$ (for a fixed N_B). For certain values of the parameters in the Hamiltonian it can be solved analytically by forming the three possible chains of subgroups of $U(6)$: $U(5)$, $SU(3)$ or $O(6)$. The first two solutions resemble the well established geometrical pictures of the nucleus: An anharmonic vibrator ($U(5)$) and a specific type of a deformed, axially symmetric rotor ($SU(3)$). Examples of nuclei close to these types of nuclear structures have been known for a long time⁽²⁾. The most striking prediction of the IBM was that of a third, new symmetry, the $O(6)$ limit. Its empirical discovery⁽⁴⁾ in ^{196}Pt (BNL-ILL-collaboration) gave substantial confirmation to the ideas behind the IBM. A comparison between the empirical and $O(6)$ limit predicted level schemes for ^{196}Pt is shown in Fig. 6.

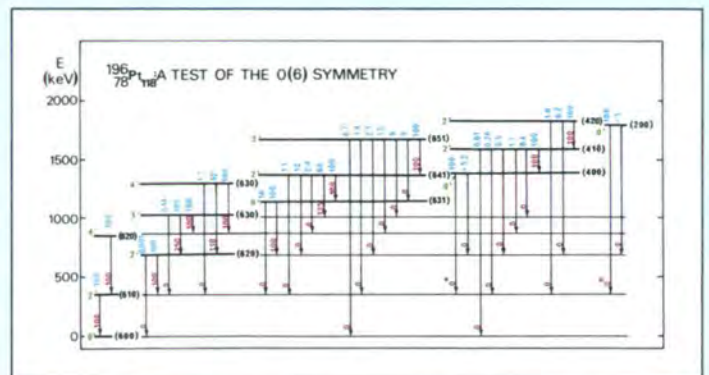


Figure 6: Positive-parity levels and branching ratios in $^{196}\text{Pt}(N_B = 6)$. The numbers in parentheses are the $O(6)$ quantum numbers (*orv*). The blue (red) number on the transition arrow is the measured⁽⁴⁾ (predicted⁽³⁾) relative $B(E2)$ value. x indicates transitions which are forbidden in $O(6)$ but whose branching becomes dominant whenever a small perturbation is present⁽³⁾.

Following the success of the IBM in describing the structure of even-even nuclei, the model was extended to odd-even and even-odd nuclei. In its most general form the Hamiltonian of the Interacting Boson Fermion Model (IBFM) is very complicated, but in the past

4 years considerable effort has been applied to establish analytical solutions by making use of *supergroup structures*, because now both bosons and fermions and interactions between these are important. The general supergroup has a structure $U(6/m)$, 6 dimensions for the bosons, m dimensions for the fermion, determined by the number and angular momenta of the orbitals the fermion can occupy. One such dynamical supersymmetry is $U(6/12)$ where the fermion can occupy $j=1/2, 3/2, 5/2$ single particle orbitals. The Hamiltonian can be solved analytically when a chain of subgroups can be identified in which at some step the boson group and fermion group have the same structure.

One of the most promising applications⁽⁵⁾ of the supersymmetry idea was to the structure of ^{195}Pt (BNL-ILL collaboration), a nucleus which could not be understood in the earlier geometrical framework. A comparison between experimental and $U(6/12)$ supersymmetry predicted level schemes is shown in Fig. 7.

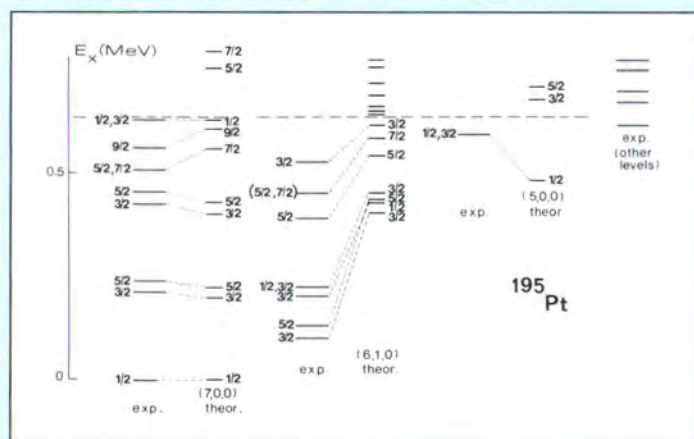


Figure 7: Comparison of observed negative parity levels in ^{195}Pt with the predictions of IBFM multi-j supersymmetry. The levels are grouped by the quantum numbers $(\sigma_1, \sigma_2, \sigma_3)$ of the model. The dashed line at ~ 600 keV indicates the limit of excitation energy up to which a one to one correspondence had been suggested between theoretical and experimental levels. The level scheme⁽⁵⁾ was deduced from a combination of (n,γ) -measurements at GAMS and average resonance neutron capture studies at BNL.

Although the most striking feature of the IBM-IBFM model is the simple level structure predicted in the limiting cases of one dominant symmetry, the entire Hamiltonian can be diagonalized numerically in a straightforward manner to facilitate the study of nuclei with structure intermediate between two limits. It has been found that the structure of $^{190,192}\text{Os}$ (near $O(6)$) and ^{168}Er (near $SU(3)$) can be understood as simple perturbations of limiting symmetries.

In fact, one of the very attractive aspects of the model is, that it is able to treat these complex transition regions, $U(5) \rightarrow SU(3)$ or $O(6) \rightarrow SU(3)$ in an extremely simple fashion. This is illustrated in Fig. 8 where the structures of transition regions are depicted in terms of a symmetry triangle (lower right) which in turn is color coded so that each nucleus in the accompanying chart of the nuclides can be given a color qualitatively describing its symmetry or transitional structure.

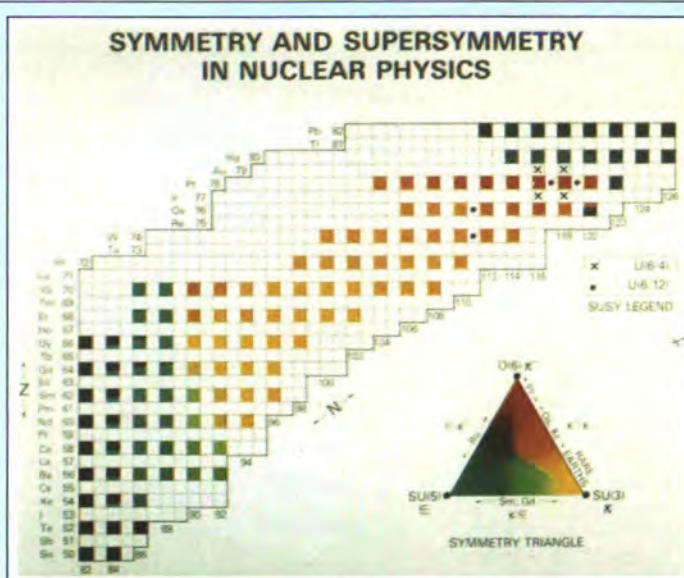


Figure 8: Symmetries and supersymmetries in Nuclear Physics. The colours give a qualitative picture of different transition regions as described in the text. A similar drawing was shown in an article by R.F. Casten and D.H. Feng in the November 1984 issue of *Physics Today*.

Refinements of the model to include neutron proton degrees of freedom and excitations outside of the s - d boson space are also quite straightforward and have been applied successfully. Current and future studies are concentrating on the establishment of supersymmetries, both theoretically and experimentally and are probing the limits of the simple IBM description.

The Interacting Boson Model has provided renewed interest in nuclear spectroscopy by demonstrating that the spectra of medium and heavy mass nuclei can be interpreted in terms of dynamical symmetries, which play also a crucial role in many other fields of physics. The basic model is certainly not able to describe, in a simple way, all properties in the large variety of nuclei. But, in studying the systematics of the few parameters needed, one is able to predict regions of nuclei where structures close so that of the limiting symmetries should occur. In other words, the models provide an ordering aspect in nuclear structure in form of symmetries which currently are supposed to be the essential finding in physics. Together with the *experimental* observation of these symmetries the models provide another excellent example and a thorough test of the use of group theory in the study of physical properties.

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COLLEGE 4

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II. External Members

C. Filippini

GENERAL SUMMARY

The scientific activity of College 4 members covers an extremely wide range in solid state physics. Excitations in various types of materials, including phase transitions can be investigated by making use of the energy- and Q-resolutions available on different instruments.

Most experiments are carried out on triple axis spectrometers (IN1, IN2, IN3, IN8 and IN12) of the three-axis group but time-of-flight instruments (IN4, IN5, IN6 and D7) and diffractometers (D5, D10) are also used.

As the College activity was curtailed by the reactor shut-down many members took that opportunity to carry out experiments at other research centres. However, many exciting results were obtained due to improvements of existing instruments as well as the use of inelastic polarized neutron scattering and it is also noteworthy that the demand for extreme sample environments is still increasing, as emphasized during the ILL Workshop on Sample Environment. Progress is being made in temperature control at very low and very high temperatures, as well as in cryomagnets and pressure techniques.

SCIENTIFIC TRENDS AND HIGHLIGHTS IN 1984

There has been a large increase in the study of magnetic systems which was motivated by the interest focused on topics such as itinerant magnetism, mixed valent and actinide compounds. The determination of lattice excitation spectra (phonons, phasons...) is of importance when investigating incommensurably modulated solids.

Incommensurate dielectrics

High resolution studies of low-frequency excitations in displacively-modulated dielectrics were effected, using the cold source 3-axis spectrometer IN12 and the thermal neutron spectrometer IN3. Two systems were investigated.

In $ThBr_4$, both the phase- and amplitude-mode dispersion branches have been previously identified⁽¹⁾. Recent intensity measurements⁽²⁾ near a strong satellite reflection, revealed an antisymmetric variation of the mode-structure factors, i.e. of the mode-eigenvectors, as a function of wavevector.

This behaviour is associated with the presence of odd order terms in the expansion of the soft-mode frequency about its dispersion minimum, in the undistorted phase ($T > T_i = 95$ K). Previous results⁽³⁾ on the phase-mode dispersion in K_2SeO_4 were confirmed and extended to several temperatures in the incommensurate ($T_L < T < T_i$) and commensurate ($T < T_L$) regimes ($T_i = 129$ K; $T_L = 94$ K)⁴. The high damping of the soft branch precludes the direct determination of the mode-eigenfrequencies from the experimental spectra, and systematic damped harmonic oscillator fits have been used. The results of the fitting procedure show a temperature independent gap of ≈ 80 GHz in the incommensurate phase-mode spectrum, which widens further below T_L . Although the physical origin of the gap is not fully understood, the neutron results are consistent with recent Raman⁵ and microwave data.

Aslanyan and Levanyuk attributed the existence of the INC phase of *Quartz* to a coupling of the soft mode to a transverse acoustic mode propagating along the [100] direction. Neutron TAS measurements were performed on IN3 to study the validity of these ideas⁶. The experiment has revealed a strong anisotropy in the (00 ℓ) plane between the transverse acoustic modes travelling in the [100] and [110] directions for phonon momenta roughly smaller than 0.1 \AA^{-1} .

A few degrees above T_i , the transition temperature from the high temperature β phase to the INC phase, the transverse mode along [110] is undisturbed whereas the one along [100] vanishes around $q \approx 0.05 a^*$ indicating the presence of a coupling phenomenon as foreseen by the theory. The soft mode of the transition which is overdamped at small q ($q < 0.1 a^*$) and temperatures below $T_i + 50$ K, if observed above this

temperature clearly shows an interaction mechanism with the TA mode of the classical anticrossing type as observed in perovskites for examples. This leads to pretransitional quasielastic scattering at the reciprocal positions at which satellites are observed for $T < T_i$.

High Energy Excitations

The magnetism of 3d metals is still the subject of many investigations. In Nickel it is difficult to understand whether magnetism is localized or itinerant. A measurement of the complete spin wave spectra provides detailed information that serves as an excellent test of any theoretical calculation made in the hopes of understanding the magnetic interactions in a material. Measuring the spin wave spectra for nickel is a very difficult neutron scattering experiment since the spin wave energies are much larger than the energies of thermal neutrons. Taking advantage of the recent improvements of the IN1 hot source triple-axis spectrometer, incident neutron energies of 250 THz were used in order to investigate excitations up to 60 THz with a reasonably small value of the momentum transfer (⁷).

The biggest improvement stems from the very large monochromator and analyzer assemblies made from an array of large copper crystals that can be adjusted continuously in vertical curvature for maximum neutron intensity. The sample was a high quality 400 g ⁶⁰Ni crystal which gave clean scattering results free from incoherent scattering effects and highly reduced contributions from phonon scattering. Fig. 9 shows the dispersion along much of the [111] direction at $T = 300$ K. It is seen that Stoner modes do not completely damp out the spin wave mode and that the spin wave continues to propagate in the Stoner continuum, but with a much reduced intensity. The spin wave broadens as it extends into the Stoner continuum at high energies. The inset in Fig. 9 shows three constant Q scans made near the top of the [111] dispersion curve.

This is the first direct measurement of the spin wave broadening as the spin wave encounters a dense region of Stoner excitations. This behaviour is in agreement with recent band calculations (⁸).

Along the [100] direction, unusual features are observed (Fig. 10). The dispersion curve is split into two parts in qualitative agreement with calculations (⁸) which predict the existence of an optical spin wave crossing the main spin wave branch. However, the experimental results show notable deviations from theoretical predictions.

Studies using polarization analysis

Polarized neutron scattering techniques are used either to single out purely magnetic scattering contributions or to distinguish

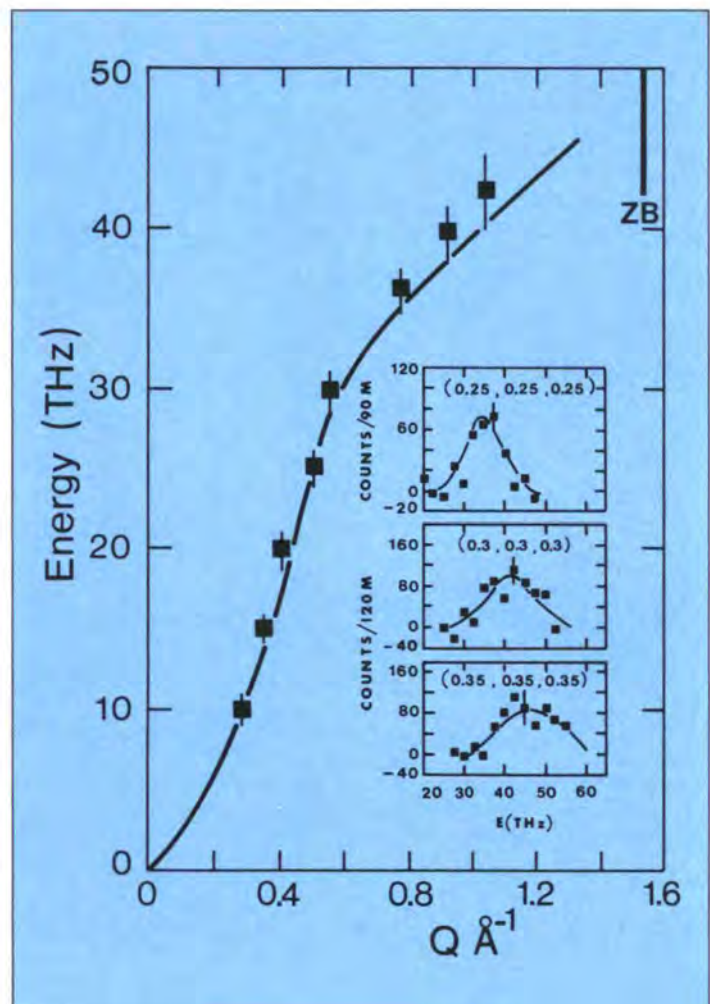


Figure 9: Spin wave dispersion curve for the [111] direction in Nickel. The solid line is from the calculation in Ref. 5. The inset shows the broadening of the spin wave when it extends at higher energies into the Stoner continuum.

between longitudinal and transverse components. The IN12 spectrometer has been already equipped with complete neutron polarization analysis and in the near future the new thermal neutron triple-axis spectrometer IN20 will be available for polarization analysis experiments. A feasibility study (⁹) on IN20 has indicated the existence in the weak ferromagnet-Ni3Al just above the Curie temperature of magnetic fluctuations at small q of detectable intensity, resolvable above the background. The possibility of determining the lineshape of the magnetic fluctuations with polarized inelastic neutron scattering is now established and will be the basis of future experiments.

Measurements of the longitudinal susceptibility of an isotropic ferromagnet (¹⁰), palladium 10% iron, were carried out on the



The new IN20 triple-axis spectrometer with polarization analysis and spin-echo option has been moved to its final position on the beam-hole H13. The picture was taken in October 1984.

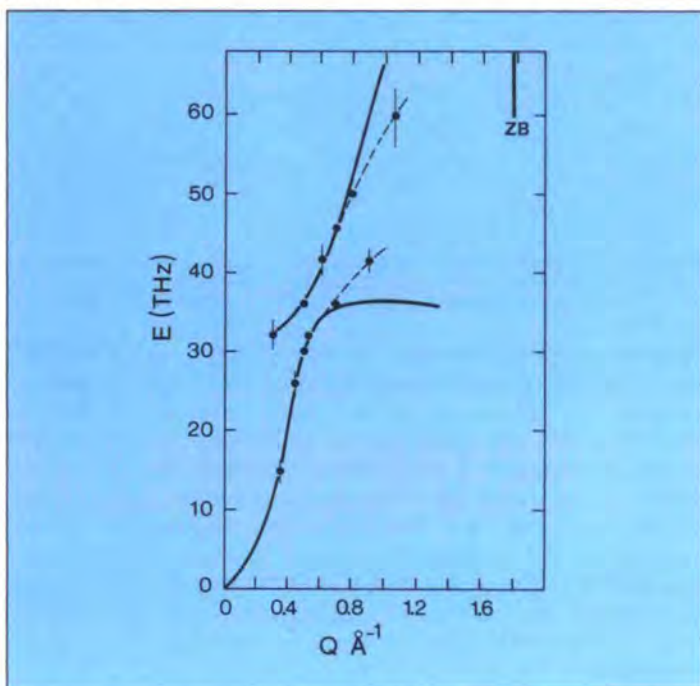


Figure 10: Spin wave dispersion curve for the (100) direction in Nickel. The solid line is from the calculation in Ref. 5.

cold source triple-axis spectrometer, IN12. The properties of the longitudinal susceptibility of isotropic ferromagnets have attracted a great deal of theoretical activity, but the results are controversial.

It was established that the longitudinal susceptibility diverges below T_c as the applied field, $H^{-1/2}$, and as $1/q$ in zero field, but the frequency dependence is still unclear. Predictions range from a three peak structure with inelastic peaks at spin wave frequencies as well as a central peak to a quasi-elastic peak structure which diverges as $(1/\omega)^{1/2}$.

Experimentally, the longitudinal fluctuation scattering may be distinguished from the transverse fluctuation (spin waves) scattering by its polarization dependence, from the magnetic Bragg scattering by its wavevector dependence, and from the nuclear incoherent elastic scattering by its frequency and temperature dependence. Above T_c , transverse and longitudinal fluctuations were found to be identical as expected. Below T_c , the spin-flip channel revealed two inelastic spin-wave peaks, whereas the non-spin-flip showed a broad quasi-elastic line which was identified as the longitudinal fluctuation scattering. In all experimental conditions, at which the longitudinal susceptibility could be measured, the corresponding neutron cross section was found to be quasi-elastic with no evidence for a structure with inelastic peaks. Unfortunately it was not possible to observe directly the predicted divergence of the susceptibility as a function of q and ω below T_c .

As mentioned earlier, the spin dynamics of 3d transition metals is a subject of considerable interest. Many studies have been made on materials with extremely steep spin-wave dispersion curves (Fe, Ni) which complicate the analysis and interpretation of conventional inelastic scattering measurements. In an attempt to alleviate such problems⁽¹¹⁾, a study was made of the ordered alloy Pt_3Mn which has a lower spin-wave stiffness constant and an easily attainable transition temperature of about 500 K. The D5 polarized neutron triple-axis spectrometer with both polarizing monochromator and analyser was used to measure the pure *magnetic* inelastic response near T_c . The spin-wave peak at the lowest temperature is seen to soften with increasing temperature, becomes overdamped near T_c and only a quasielastic response is observed above T_c . It appears that Pt_3Mn exhibits "normal" ferro-paramagnetic behavior, with no obvious sign of propagating magnetic modes above the transition.

Actinide compounds

Neutron inelastic scattering studies of a series of actinide (5f) compounds have greatly increased our knowledge of the electronic structure of these systems and, at the same time, have illustrated the complexity of the interactions in this part of the periodic table. All inelastic experiments have been performed on uranium compounds but a major interest has been in extending these measurements further into the actinide series,

despite formidable problems of sample handling. Large single crystals of $^{242}\text{PuSb}$ have been grown by the Transuranium Institute of Euratom at Karlsruhe. The first inelastic experiment ⁽¹²⁾ was carried out using the IN8 triple-axis spectrometer. Figure 11 shows representative spin-wave groups in monodomain PuSb , measured at low temperature at a number of different wavevectors in the Brillouin Zone. The intensity differences between, for example, (300) and (030), demonstrate the mono-domain nature of the sample, which enables one to determine unambiguously the polarization of the spin waves. The principal feature in the inelastic spectrum is the spin-wave branch at about 4 THz, which has little dispersion. Of particular interest, however, is the lower mode at (210) which is polarized *longitudinally* with respect to the propagation direction. Surprisingly, this mode has a minimum at the X-point and not at the zone-center which is where the usual frequency minimum is for a ferromagnet. This experiment is the first observation of excitations in transuranium material and clearly the fascination of actinide research extends beyond uranium!

Anomalous rare earth compounds

Neutron scattering experiments are extremely well suited for the study of rare earth compounds which show valence fluctuation properties. Ce and Yb compounds but also Sn, Eu, and Tm compounds may exhibit anomalous physical properties in relation to intermediate valence. In particular, phonon spectra may show degenerate longitudinal and transverse modes as in CeB_6 ⁽¹³⁾. But the unusual character of these compounds can be seen in the magnetic excitations spectrum.

In TmS , Tm ions are trivalent but strongly coupled to the conduction electrons. Although this compounds is not strongly mixed valent, anomalous features have been observed in the magnetic excitations ⁽¹⁴⁾. Experiments performed on a TmS single crystal using the triple axis spectrometer IN8 revealed broadened crystal field excitations with dispersion across the Brillouin zone. The minimum of the dispersion occurs at the L point in agreement with the almost type II antiferromagnetic ordering. Quasielastic scattering was observed in the magnetically ordered phase ($\Gamma/2 = 0.14$ THz at $T = 1.3$ K). The temperature dependence of the half width $\Gamma/2$ indicates that Γ remains finite even when $T = 0$ Kelvin. This indicates the existence of a degenerate ground state for the Tm ions. The origin of the large broadening of the inelastic crystal field transitions (full width at half maximum 0.7 THz) is not accounted for.

Considerable progress has been made in elucidating both the magnetic structure and excitations of the lanthanide element neodymium. Nd orders antiferromagnetically below $T_N = 19.9$ K to form a sequence of complicated modulated structures. The array of 12 satellite reflections observed between

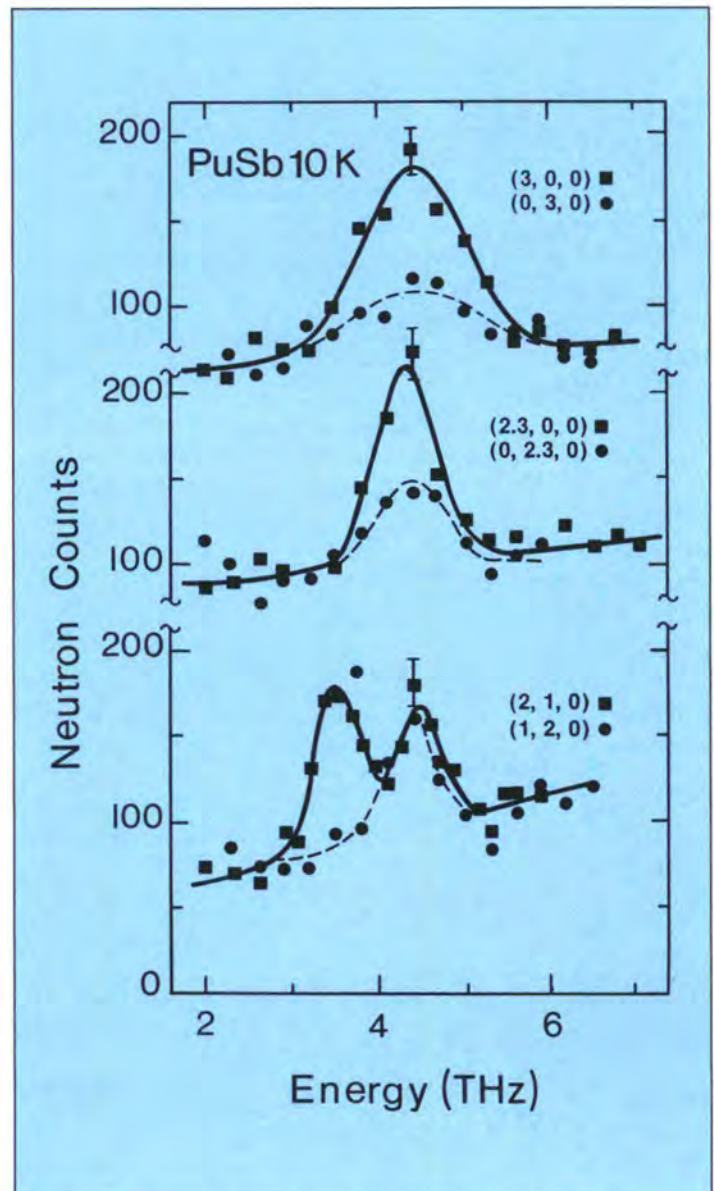


Figure 11: Examples of neutron groups observed with a monodomain single crystal sample of $^{242}\text{PuSb}$.

19 K and 8.5 K have been variously interpreted as arising from domains of single-q, double-q and triple-q structures. Recently, the application of an appropriate magnetic field was found to reduce the number of satellites to 4, consistent with the formation of a single-domain, double-q structure ⁽¹⁵⁾ (see

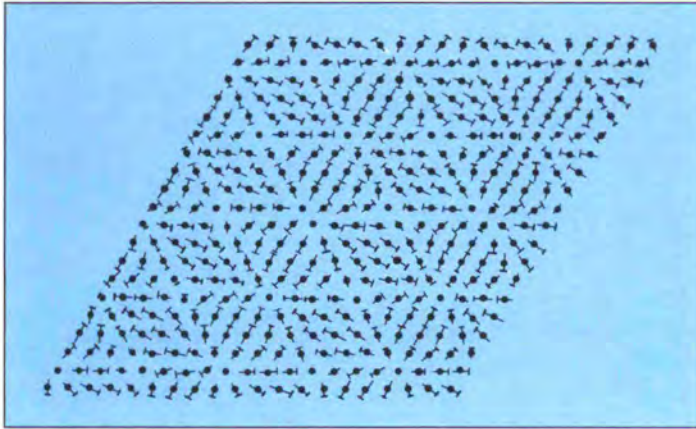


Figure 12: The double-q magnetic structure proposed for neodymium.

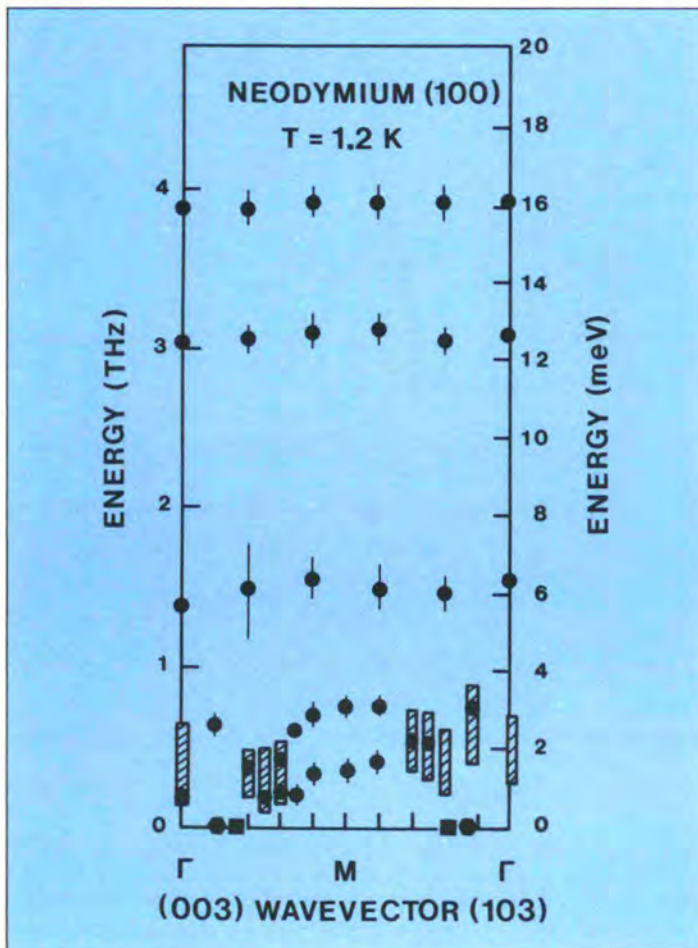


Figure 13: Dispersion of magnetic excitations propagating along the (100) direction (ΓM) in Nd at 1.2K. The shaded areas represent broad regions of inelastic scattering (see ref. 16).

Fig. 12). Higher fields induced a transition to a single-q state. An experiment on IN8 revealed three more branches of magnetic excitations⁽¹⁶⁾, additional to the two low energy branches observed earlier⁽¹⁷⁾ (see Fig. 13). These new modes exhibit rather little dispersion and are attributed to crystal-field-like excitations. The substantial linewidths of the low energy modes are a direct consequence of the incommensurable structure. These effects are also being studied theoretically⁽¹⁸⁾. At 1.2 K, the magnetic structure is exceedingly complex: 36 satellite reflections have now been observed around a reciprocal lattice point.

Other studies have been undertaken in order to evidence the existence of an hybridization in the f-band due to the coupling with conduction bands. Experiments on YbAl_3 were carried out on the time-of-flight spectrometer IN4¹⁹. The results showed a sharp increase in the paramagnetic spectral response around 8 THz at low temperature. With increasing temperature the step-like response broadens very rapidly and its energy is reduced. This effect is accounted for by assuming that the Fermi level is pinned close to one of the f-band gap edges which appear because of hybridization, leading to a sharp feature at low temperature. The step-like increase in the paramagnetic response results from the excitation of f-electrons across the hybridization gap when localized 4f electrons couple with the conduction bands. At higher temperatures, due to thermal smearing, this feature is expected to soften and broaden.

Secretary: C. Vettier

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COLLEGE 5 CRYSTAL AND MAGNETIC STRUCTURES

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G.A. Bentley	R. Müller
L. Bernard	A.P. Murani
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GENERAL SUMMARY

The experiments carried out in College V embrace a wide range of scientific interest which includes fundamental aspects of neutron diffraction and its application to problems in condensed matter physics, chemistry and biology. An increasing number of experiments concerned applied or industrial application of neutron scattering especially in the area of materials research. Owing to the impending long shut-down many experiments were concerned with finishing existing projects. The absence of both D8 and D2, for the latter part of 1984, curtailed experiments requiring a high neutron flux. However, the removal of these instruments enabled shielding of the new beam tube H11 to be tested and both D19 and D20 should be available for scheduling at the end of 1985.

Weekly seminars formed a focal point and encouraged an active exchange of ideas between visitors and College members. An international workshop organised in August 1984 assembled scientists based at steady state and pulsed neutron sources and provided a lively forum.

During 1984 J. Bouillot completed his two years as College Secretary and was replaced by W.F. Kuhs. Bouillot is currently spending a sabbatical year at N.B.S. in Washington and we would like to thank him for his exceptional work as College Secretary and wish him an interesting and profitable stay in the U.S.A.

WORKSHOP ON HIGH-RESOLUTION POWDER DIFFRACTION

This workshop was organised to mark the transition between the second generation of high resolution neutron powder diffractometers, and the new super machines now being built or planned on both reactor and pulsed sources. Representatives of most neutron scattering centres in Europe and overseas were among the 60 participants from 10 countries.

The performance of reactor and pulsed sources was extensively discussed, but no clear priorities were given, although both sides had some striking examples in favour of the one or the other. It was generally agreed that Rietveld's profile refinement method was responsible for the rapid progress obtained in the field. Other topics included applications of neutron powder diffraction in materials research (e.g. for designing strain free superconducting wires or testing pressure vessels) and the utility of reactor based time-of-flight techniques. The prospect of time-dependent powder diffraction was not forgotten, whilst all the medium flux reactors obviously still maintain their chance of doing interesting high-resolution powder diffraction work.

SCIENTIFIC TRENDS AND HIGHLIGHTS IN 1984

Structural Transitions

This domain has always been an important one in the College; better control of the sample environment now enables measurements to be made closer to the phase transitions both at high as well as at low temperatures. Further insight into the mechanism of phase transitions was obtained and further progress is expected in the future.

As a first example we present the study of thermal motions in AuCu₃ near the order-disorder phase transition ($T_c = 668$ K) performed on D9. The outstanding feature of the results is that

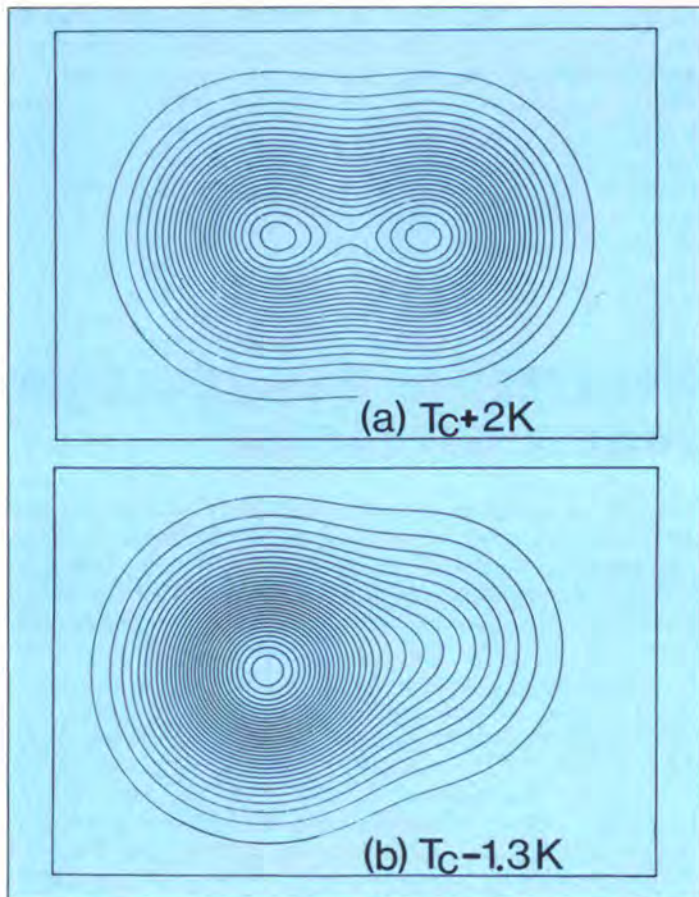


Figure 14: Proton distribution in KDP at T_c+2 and $T_c-1.3$ in the a - b plane.

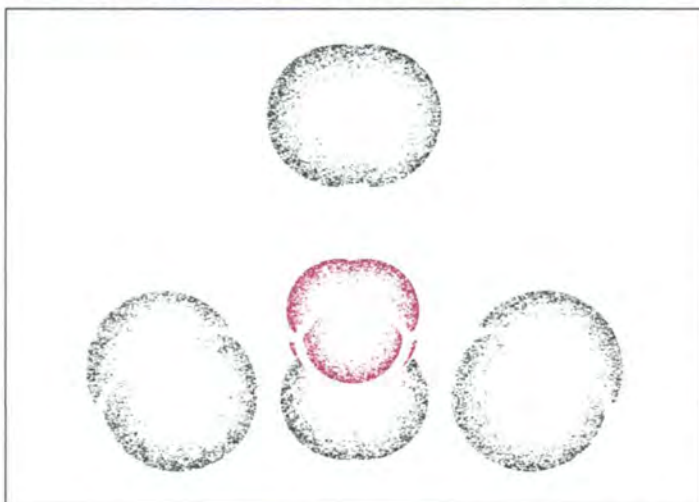


Figure 15: The plot is showing the atomic arrangement, i.e. the oxygen and proton disorder in ice Ih. (SCHAKAL computer graphics by E. Keller, Freiburg, FRG.).

whereas at low temperatures an anharmonic treatment of thermal motion is necessary to give an adequate account of the data, at T_c-4 thermal motions are harmonic with however strong anisotropy of the copper atoms; the amplitude is increased perpendicular to the plane of their four gold nearest neighbours. Such behaviour suggests that phonon anomalies may be responsible for the first order transition.

As a second example we chose a high-resolution study of KDP and its deuterated equivalent. Experiments on these materials have been going on for several years, but the latest experiments close to the ferro-electric phase transition have enabled a better understanding of the phase transition in these "classical" materials. D9 seems to be the best instrument for these kinds of studies. High-resolution diffraction data from monodomain crystals, obtained by applying an electric field, were collected at several temperatures in the ordering range below the tetragonal to orthorhombic phase transition. The results support a picture of the ferro-electric soft mode above T_c that includes local centre-of-mass fluctuations (freezing out below T_c) and show the spontaneous polarization, the proton ordering (see Fig. 14) and the heavy atom displacements below T_c , all have the same temperature dependence.

Structural Disorder

The study of structural disorder is a very heterogeneous field covering a whole variety of materials as well as instrumental techniques. High resolution powder diffraction has been proven to be a very powerful tool in studies of e.g. ionic conductors or disorder in molecular solids. Fine details of disordered systems have been obtained on high resolution single crystal diffractometers. Whilst other experimental techniques are certainly able to yield information on such systems, normally only crystallography gives the full three-dimensional picture of the disorder, very often being crucial for a better understanding of the physical properties.

Experimental work on hydrogen disorder in the high pressure phases of ice has been continued. Disordered ice VI has been studied on D1A at 1 GPa using the new maraging steel pressure cell; the data quality is much improved in this cell due to the much simpler diffraction pattern when compared to the alumina cell.

Studies on hexagonal ice have been performed with diluted samples (D_2O in H_2O) on D9. Together with the previous studies on the pure compounds, these experiments helped to establish the oxygen disorder in ice. There is direct crystallographic evidence for this disorder from structure refinements including anharmonic terms and together with information from IR- and Raman spectroscopy a firm picture of the structural disorder in ice was established (see Fig. 15). The anomalous long O-H distance, much discussed over the last years, can be explained as in part due to this oxygen disorder. The main contribution in the forelengthening is the cooperative nature of the hydrogen bonding.

Biological Crystallography

Although in part overlapping with work done by members of College 8, biological (mainly protein) crystallography has always been an important part of the College's activities. This activity, which includes studies of biological molecules at the atomic resolution level, is expected to increase with the scheduling of the new multidetector four-circle diffractometer D19. The first series of data collections on D19A has been successfully completed before the reactor shutdown.

However, excellent data have been obtainable in a reasonable time, using the single detector instrument D8 which enabled a study of ethanol-lysozyme interactions at the molecular level. The analysis was based on data at 2 Å resolution recorded in 9 days on a crystal of hen egg-white lysozyme solution of deuterated ethanol soaked in 25% ($\text{CD}_3\text{CD}_2\text{OH}$) in water. Because of the selective deuteration, ethanol should be very visible. Indeed it was possible to identify 13 ethanol sites with site occupancies of between 0.2 and 1.0. After structural refinements the crystallographic R-factor was as low as 0.097, and comparison with the non-alcoholic structure of lysozyme showed no significant change in the conformation. Likewise an analysis of the thermal motion parameters gave the same result for the flexibility. In this analysis it was necessary to include a correction for scattering from the solvent which contained disordered ethanol molecules. 70% of the interactions of the molecules were with hydrophobic parts of the surface, and typical interactions were with tryptophane, glycine, alanine and phenylalanine, but also the hydrophobic stems of lysine and arginine gave several contacts. Fig. 16 shows a stereo view of the location of one ethanol molecule in the active site of the protein.

Dynamical Diffraction and Basic Scattering

It should be remembered that a small group within the College is dealing with these subjects mainly using the neutron interferometer S18. Accurate determination of scattering lengths has become a routine operation for example. Another recent experiment on S18 confirmed nicely the dispersion law for thermal neutrons; the phase shift of the interference fringes was measured to an accuracy of 1.5% as a function of the wing velocity of the rotating phase shifter and found to be in excellent agreement with theory.

Another basic scattering experiment was performed to directly observe the thermal diffuse scattering (TDS) free from Bragg scattering. Measurement of the real space intensity distribution across the neutron beam diffracted off a perfect crystal in Bragg-case orientation allows the direct determination of the ratio of TDS intensity to Bragg diffracted intensity (see Fig. 17). The experiment was performed at different wave lengths in the region where the neutron speed is comparable



The new D2B diffractometer mounted on its test position at the H22 guide behind D1A/D1B.

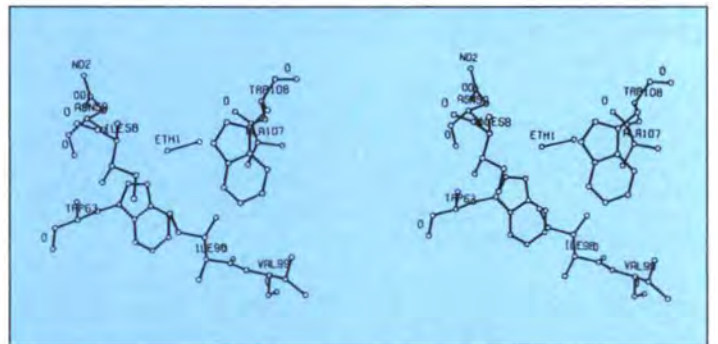


Figure 16: Location of an ethanol molecule in hen egg-white lysozyme obtained from single crystal study.

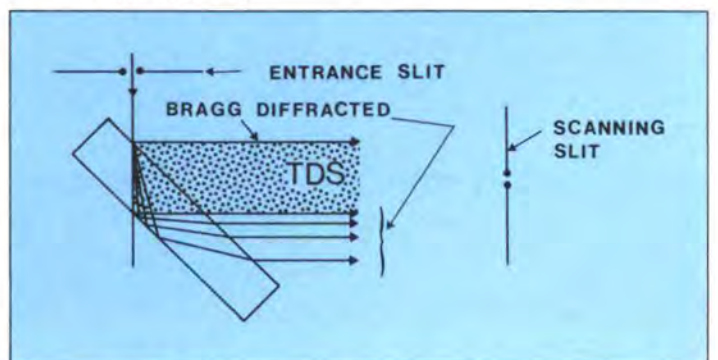


Figure 17: Principle of the observation of thermal diffuse scattering (TDS) free from Bragg scattering.

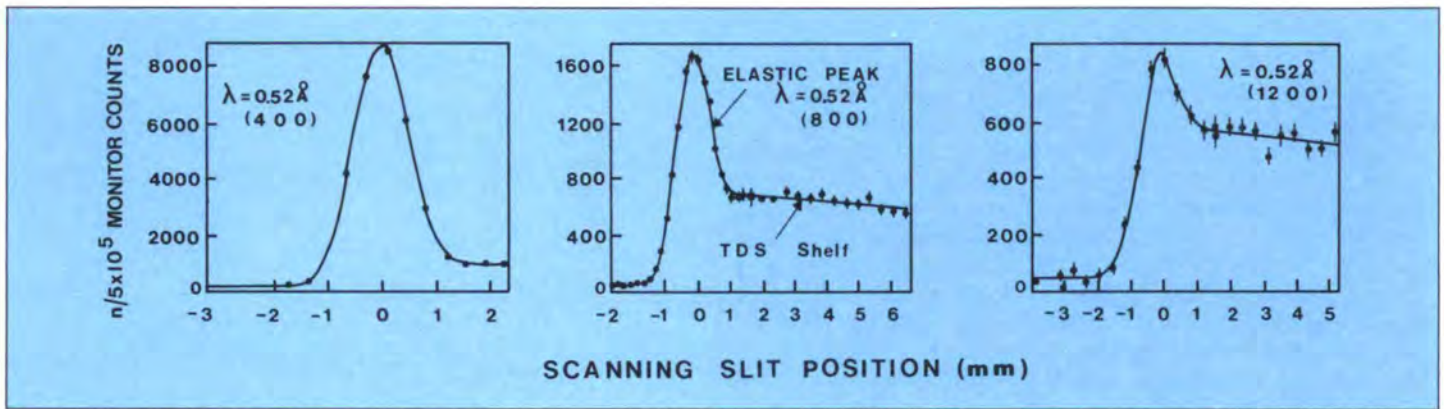


Figure 18: Characteristic results of the measurement of the distribution in real space of neutrons diffracted by a perfect crystal in on-Bragg orientation. The elastic Bragg peak and the TDS-shelf are clearly distinguishable.

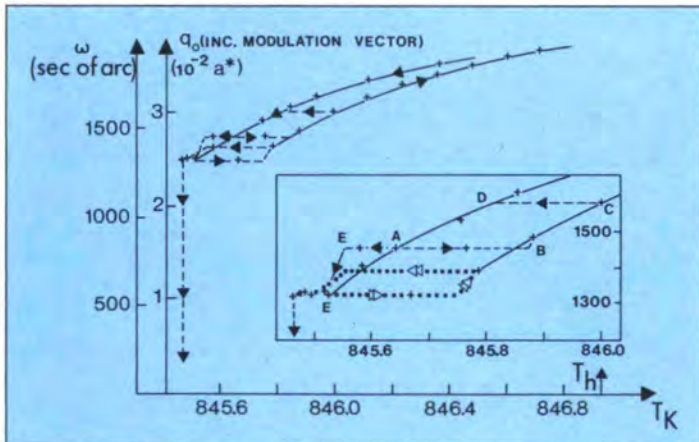


Figure 19: Global hysteresis of incommensurate Quartz.

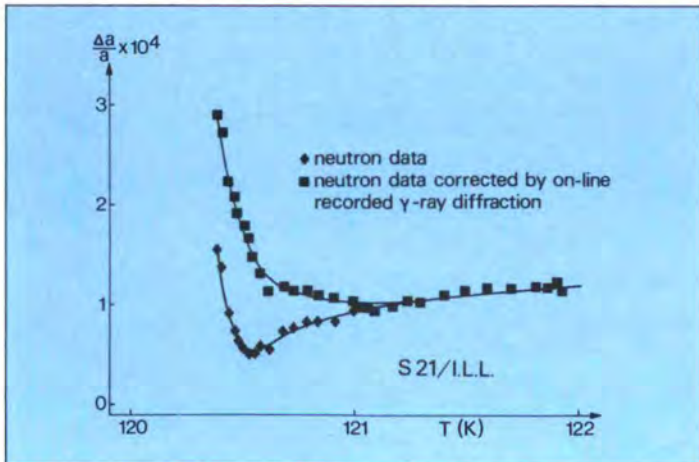


Figure 20: Relative lattice parameter variation $\frac{\Delta a}{a}$ of KDP under electric field showing the non negligible errors occurring if back-scattering neutron data is not corrected for by on-line γ -ray diffraction eliminating the effects of pure rotation of ferro-electric domains.

to the velocity of sound to determine this ratio in the transition region between elliptically and hyperbolically shaped scattering surfaces. The measurements confirmed directly that the ratio increased both with increasing scattering vector (see Fig. 18) and increasing neutron energy. Furthermore the width of the rocking curve through the TDS peak increases with increasing neutron energy which can be explained by flattening of the hyperbolic phonon scattering surface with increasing energy.

γ -Ray Diffraction

That the γ -ray laboratory at the ILL is much more than just an excellent facility for testing the quality of monochromator materials has been demonstrated quite often over the last years. As a recent example we present the study of the temperature variation of the incommensurate modulation vector of quartz between 845.4 and 846.8 K. Relatively large global hysteresis effects (see Fig. 19) were revealed for the first time in this extremely pure material and the coexistence state at the look-in transition to α -quartz could be studied in better detail than with neutron techniques. It is believed that the global hysteresis observed here may be at least partially due to the triple-q structure of incommensurate quartz as it costs more energy to change the size of a two dimensional triangular pattern.

Quite recently X-rays and neutrons got married on S21 (see instrument section) to make a very powerful instrument for extreme high-resolution studies. Using this combination of neutron backscattering and on-line γ -ray diffraction the lattice deformation under electric field was studied close to the ferroelectric phase transition of KDP. The (600) Bragg reflection was monitored with both techniques simultaneously and the results are given in Fig. 20. The pure neutron result, in agreement with earlier X-ray work exhibits a lattice deformation under an electric field which seemed difficult to understand. The truth is revealed when the on-line γ -ray correction

is applied (see Fig. 20). Physically this means that at the transition, lattice planes may rotate due to the appearance of spontaneous shear and thus backscattering results and the lattice parameters have to be corrected for the non negligible effects of pure rotation.

Materials Research

Neutron powder diffraction has been proven to be a very good tool to investigate technologically important materials, which very often are not available in form of single crystals. Zeolites and intercalates are good examples of these materials and structural studies on D1A have been carried out on these compounds repeatedly. The kinetic work on cements performed on D1B has been extended to silica-cement, and in addition the behaviour after addition of different growth inhibitors was studied. A study of the formation of gypsum showed that the hydration passes through the formation of a gel interphase. The measurement of residual stress in compounds is a problem of great technological importance. Neutron powder diffraction is a unique tool of getting the full three-dimensional information within a bulk specimen. Thick-walled steel tubes, in which beneficial residual compressive stresses have been introduced at the bore by autofrettage are used in many industrial applications where pulsating high pressure fluids have to be contained and failure could have catastrophic consequences. The traditional Sachs boring engineering method for determining the residual stress distributions in such tubing measures average stresses and is destructive. The high resolution characteristics of DIA have been employed to determine the residual stress distributions, non-destructively and locally, in a sample of autofrettaged tube by measuring the small Bragg peak shifts induced by stress. The neutron and traditional methods both gave results in satisfactory agreement, with good resolution. The neutron technique has the advantage of being able to determine asymmetrical stress distributions and revealed stress perturbations near the outside of the tube that had previously not been detected by the traditional method, and that had been induced by the manufacturing process (see Fig. 21).

The suitability of a multidetector four-circle diffractometer for more than just fast data collection on big molecules was demonstrated in an investigation of mechanically ordered pure trans-acetylene. The large area detector of the D19A multidetector permitted the rapid mapping of a two-dimensional section through reciprocal space, an undertaking which would have been prohibitively long with a single detector.

The last example is really on the border-line between College 5 and 6: the study of crystallization of amorphous alloys. These studies have a twofold interest; firstly, they are concerned with the problem of nucleation and growth in these materials and secondly, they help to understand the differences in free energy of amorphous and crystalline compounds. The kinetics of the

precipitation of crystallites of α -iron in an amorphous matrix of $\text{Fe}_{75}(\text{PC})_{25}$ has been studied in situ on D1B with different heating rates (see Fig. 22). Precipitation and crystallization temperature are shifted towards higher temperatures with

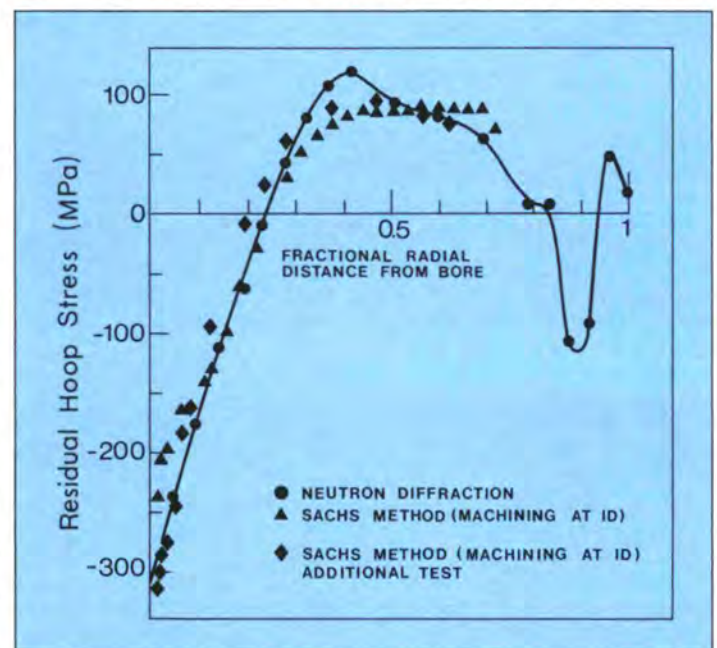


Figure 21: Comparison of residual hoop stresses, as a function of radial distance from the bore, determined by the neutron diffraction and Sachs boring methods for an autofrettaged ring sample.

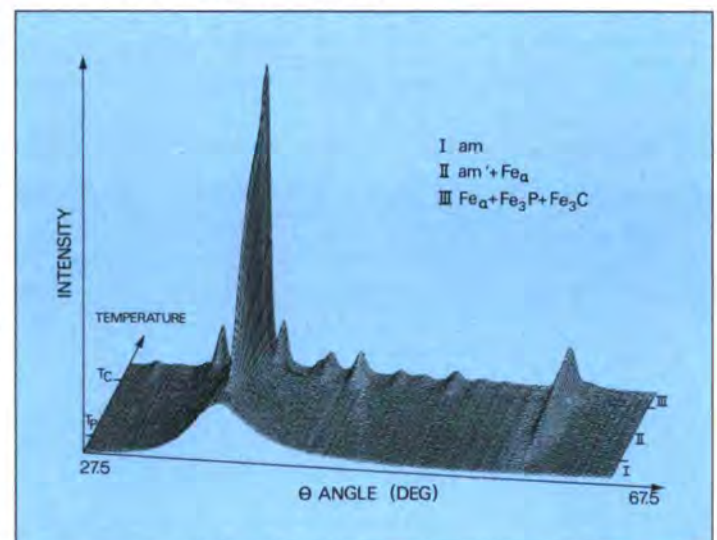


Figure 22: Evolution of the diffraction pattern during the crystallization of a $\text{Fe}_{80}\text{P}_{10}\text{C}_{10}$ amorphous alloy. Stage I, the alloy is still amorphous. Stage II corresponds to a primary crystallization. Stage III shows an eutectic crystallization.

increased heating rate, while the fraction of precipitated α -iron stays constant and is only a function of the alloy composition. The free energy diagram shown in Fig. 23 was constructed from these results.

Miscellanea

There is always room and interest for more exotic problems in the College. A nice example is the study of the Goldanskii-Karyagin effect in α -SnF₂. This effect manifests itself as the perturbation in the relative line intensities of the Mössbauer

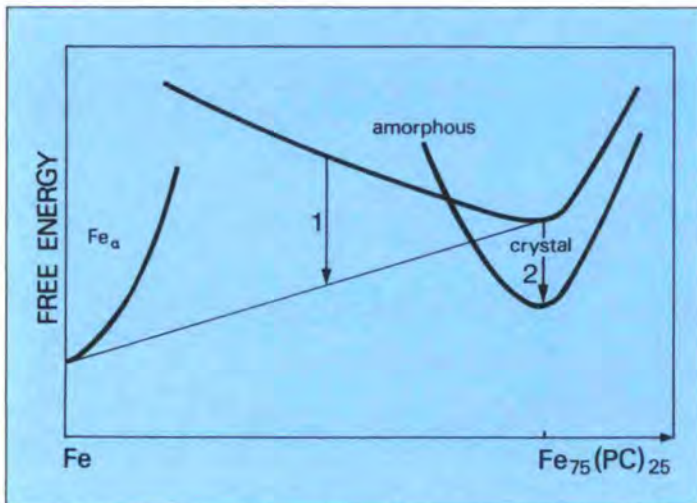


Figure 23: Schematic free energy diagram exhibiting a primary crystallization (1) and an eutectic crystallization (2).

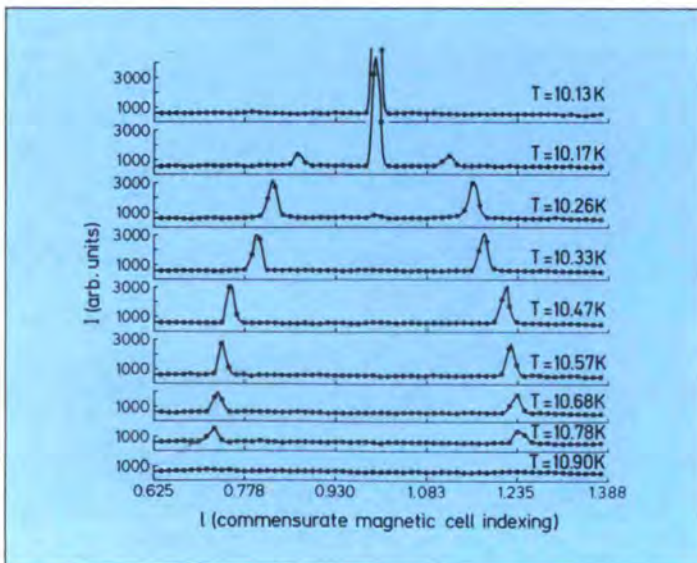


Figure 24: Temperature variation of the intensities of the $\bar{1}01$ magnetic reflexion and its satellites in EuAs_3 .

spectrum due to the anisotropy of the recoilless fraction. The best method to prove the existence of this effect is to calculate the expected perturbations from the anisotropic thermal vibration tensors and compare these with the Mössbauer data. The thermal parameters were refined using single crystal data collected on D8. The validity of Karyagin's theorem has been confirmed. The values of the anisotropy parameters obtained by both methods agree very well at high temperatures. At lower temperatures Mössbauer absorption yields a somewhat higher anisotropy, which might be due to the different probing of correlated atomic motions.

Magnetic Powder Diffraction

The absence of D2 for the latter half of the year substantially reduced the number of magnetic studies by powder diffraction. Measurements were primarily concerned with establishing magnetic phase diagrams in alloy systems such as Co-Mn, Fe-Al or CrSn. Other measurements were concerned with the magnetic structure of spinels or the change of crystal structure with the onset of magnetic order. In the intermetallic compound series $\text{Pd}_2\text{MnIn}_{1-x}\text{Sn}_x$ a variety of magnetic structures is observed ranging from fcc antiferromagnetic type 2 (AF2) to fcc antiferromagnetic type 3A (AF3A) to ferromagnetism as the electron concentration is changed by increasing x in the range 0 to 1. The high angle dispersion and resolution characteristics of D1A were employed to determine the tetragonal lattice distortion, induced in $\text{Pd}_2\text{MnIn}_{0.6}\text{Sn}_{0.4}$ by the onset of the AF3A magnetic structure, simultaneously with the ordered magnetic moment as a function of temperature. The data were combined to establish the essentially linear relationship between lattice distortion and the square of the moment, in agreement with theoretical predictions. In contrast, no measurable distortion was observed in Pd_2MnIn , which has the AF2 structure, due to cancellation of the magnetostrictive forces by the magnetic symmetry.

Single Crystal Diffraction

A large effort has been expended on experiments concerned with incommensurate magnetic structures using both classical four-circle and normal beam methods. Experiments of this kind very often need extremely well controlled sample environments since incommensurate phases often extend over a few tenths of a degree only. The Q resolution also has to be very good. D10 is probably the most suitable instrument but some work has been carried out on D9 and D15. A neutron diffraction study on EuAs_3 near the magnetic phase transition has been performed on D15 successfully. Below 10 K EuAs_3 is antiferromagnetically ordered. In the range between 10 and 11 K an incommensurate antiferromagnetic phase has been found whose periodicity changes continuously with temperature. Fig. 24 shows the intensity variation for the $(\bar{1}01)$ reflec-

tion along with its satellites. Since the satellites are observed only near magnetic reflections of the commensurate antiferromagnetic phase, the incommensurate phase is antiferromagnetic with a continuously changing propagation vector. The possibility of an incommensurate structure in the antiferromagnet YMn_2 has been investigated and further measurements have also been carried out on the Gd-Y system both at the Gd and Y rich end of the series (see Fig. 25). The magnetic structures of transition metal oxides have been extensively studied, but until recently the magnetic structure of CuO was unknown. Recent availability of mm sized single crystals allowed the detailed determination of the low temperature antiferromagnetic structure described in the 1982 Annual Report. In Figure 26 dependence of the intensity of the $(0.5, 0, -0.5)$ reflection given by this structure is plotted as a function of temperature. The intensity vanishes abruptly at $T_c = 213$ K, 17 degrees below the Neel temperature deduced from susceptibility measurements. We have found that in the region between 213 K and 230 K an incommensurate antiferromagnetic phase occurs which is characterised by a propagation vector $\tau: -0.506 a^* + 0.483 c^*$. This propagation does not change significantly in the temperature range 213 to 230 K. The intensities of the magnetic reflections lead to a model in which the couplings between moments within a unit cell are essentially the same as for the commensurate phase but in which the spin direction rotates in the $a-c$ plane so that the angle between spins separated by a vector τ is $2KT \cdot \tau$. The temperature dependence of the $(0.506, 0, -0.483)$ satellite intensity is also plotted in Figure 26. The intensity has been multiplied by a factor 2 to compensate for the $a-c$ phase orientation of the moment. The plotted intensities are therefore proportional to the mean square value of the moment on the same arbitrary scale for both phases.

A significant improvement in the study of incommensurate structures is provided by the two dimensional detector on the

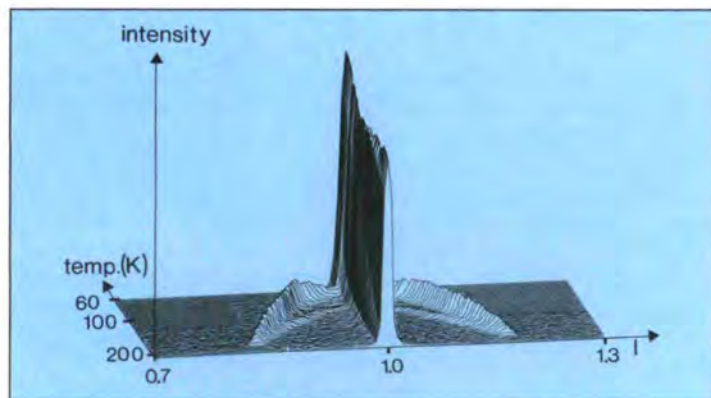


Figure 25: Diffracted intensity along the $10 l$ direction versus temperature for $\text{Gd}_{0.62}\text{Y}_{0.38}$. The outer pair of satellites is due to the inplane component of the basal-plane helix, the inner pair to an out-of-plane oscillation of the spin vector.

long wavelength diffractometer D16. This arrangement has been used to simultaneously record the magnetic intensity distribution in the basal planes of $\text{Ni}_{1-x}\text{Fe}_x\text{Br}_2$ (Fig. 27).

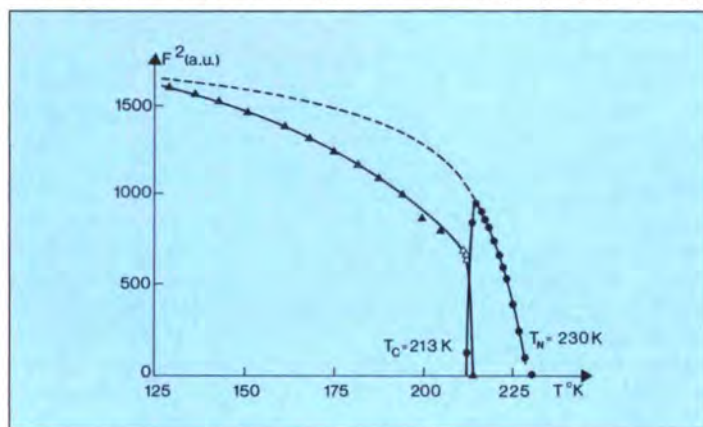


Figure 26: Temperature dependence of the magnetic scattering in CuO . The triangles represent measurements of the $(0.5, 0, -0.5)$ reflexion and the circles measurements of the $(0.506, 0, -0.483)$ reflexion on twice the relative scale.

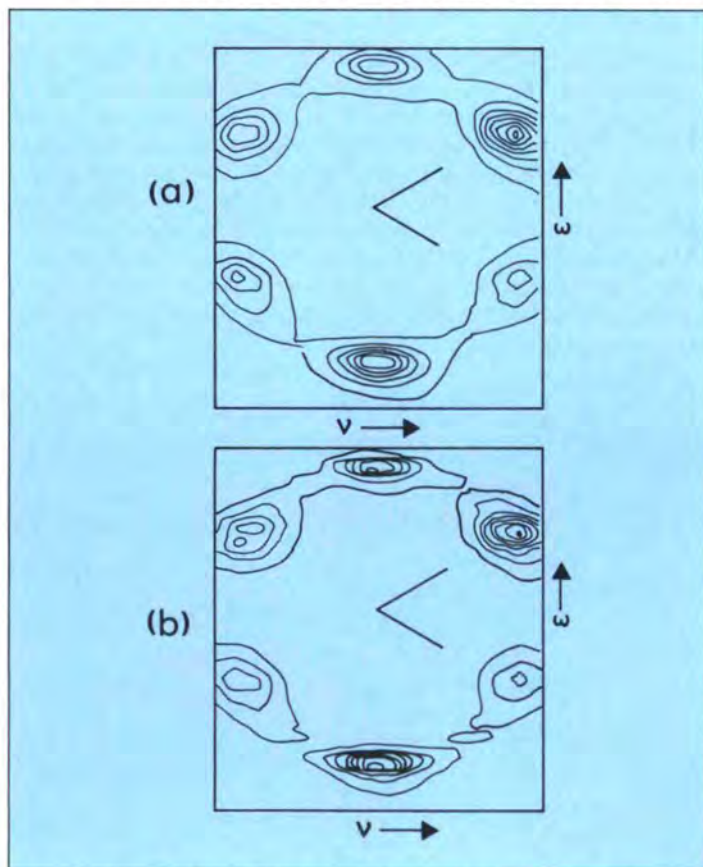


Figure 27: Observed (a) and calculated (b) intensity profiles of the magnetic satellites around 003_M in $\text{Ni}_{91}\text{Fe}_9\text{Br}_2$ at 4K (contours at 2300 count intervals).

The same technique was also used to establish the invariance of the magnetic moment in the incommensurate and spin flop phases of MnSi.

Conventional studies were concerned with establishing magnetic phase diagrams, for example in $\text{RbFeCl}_x\text{Br}_{3-x}$ or in preliminary structural determinations. In the latter category the measurements on $(\text{CH}_3)_4\text{N Mn Br}_3$ – TMMB and $(\text{CD}_3)_4\text{N Mn Br}_3$ – D12 TMMB are worthy of note. A first order reversible phase transition at 140 K substantially affects the physical properties at low temperatures. At 140 K the crystal transforms from a hexagonal phase at high temperature to a multidomain monoclinic phase. Below 2.28 K TMMB orders antiferromagnetically with the propagation vector along [110] with the spins rotated by 120° . The Néel temperature of the deuterated crystal D12 TMMB is 2.4 K and the propagation vector is along [100] (Fig. 28). The origin of the magnetic structure is believed to be a delicate balance between the dipolar anisotropy and the inter-chain super-exchange.

Polarization Analysis

Paramagnetic scattering measurements on iron and nickel were continued. A series of constant Q scans were performed up to 200 MeV using substantially improved instrumental resolution provided by a Fe Co monochromator and analyser. Comparative studies were also carried out on several transition metal compounds Pd_3Fe , Pd_3Mn , CrMn and YMn_2 . The technique of polarization analysis was increasingly applied to the problem of intermediate valence and heavy Fermion superconductors. In the case of intermediate valence, measurements on CeSn_3 and CePd_3 have established the singlet nature of the ground state. Furthermore the unique facility of D5 (located on the hot source) has enabled a magnetic excitation to be observed at ~ 50 THz [2400 K] in αCe . Indeed constant Q

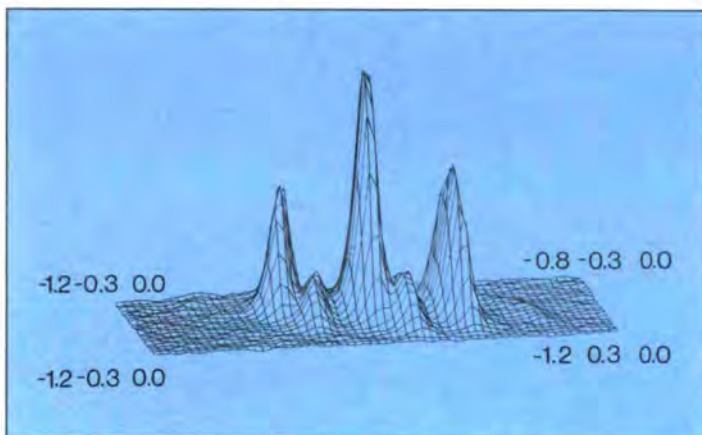


Figure 28: The formation of nuclear domains around the hexagonal 010 position at temperatures below $T_{ph} = 140$ K in TMMB.

scans were carried out up to ~ 75 THz [3600 K]. These results suggest that current models applied to I.V. require serious revision.

The paramagnetic response in CeCu_2Si_2 and UPt_3 was determined as a function of energy and wavevector both above and below the superconducting transition. These measurements provide detailed information regarding the existence of δ or P wave superconductivity.

Magnetization Density

The magnetization density distribution has been determined in a wide range of compounds. Although the majority of materials investigated contained either transition or rare earth elements an increasing demand was made for measurements on compounds containing actinide elements. Extensive results on compounds which exhibit intermediate valence behaviour e.g. CeSn_3 have established that the enhanced form factor observed below 40 K is not an intrinsic property of CeSn_3 but arises from clusters of free Ce atoms. The new results are of particular importance since the enhancement of the form factor had been taken as evidence for the polarization of the conduction band expected in a Kondo lattice description of intermediate valence. Measurements on transition metal compounds were primarily concerned with effects of co-valency. In the case of insulating compounds such as RbFeCl_3 the interest was primarily concerned with the relative importance of super-exchange in a pseudo singlet ground state system. In the 3d intermetallic compounds Pt_3Ti , Pt_3V and Au_4V the interest centred on the moment formation and the nature of any asymmetry. Measurements were made on both chemically ordered and disordered specimen such that the effects of a nearest neighbour transition metal environment could be quantified. Ternary intermetallic compounds at the stoichiometric composition X_2YZ (Heusler alloys) in which the magnetic moment is confined to the Y atoms, usually manganese, are ideal systems for studying local moment properties in 3d metals. The availability of reliable band structure calculations has stimulated considerable interest and measurements have been systematically extended to systems expected to have properties intermediate of local and itinerant behaviour, e.g. Fe_2MnSi and Co_2MnSi (Fig. 29), etc. Polarized neutron measurements have shown in Fe_2FeSi , Fe_4Si and Fe_2MnSi that the moment on the Y site, which has a transition metal nearest neighbour environment, has essentially e_g character as observed in αFe . In addition to these fundamental studies, Heusler alloys provide excellent neutron polarizing monochromators. The [111] reflection from the prototype Heusler Alloy, Cu_2MnAl is an established neutron polarizer. However the large lattice spacing gives rise to relaxed resolution similar to that obtained for the 002 reflection from pyrolytic graphite often used in conventional triple-axis measurements. Furthermore, the large structure factor of the [222] reflection in

Cu₂MnAl gives rise to serious problems with $\lambda/2$ contamination. Flipping ratio measurements using D3 indicate that several “alloys” in the related intermetallic compound series Pd_{2-x}MnSb, 0 < x < 1, give rise to minimal $\lambda/2$ contamination and have enhanced polarizing properties, particularly if cooled. Other Heusler alloys in the series Co₂MnZ, where Z is a group III or IV element, have also been shown to polarize well at ambient temperature on the [111], [002], [220] and some higher order reflections enabling higher “take-off” angles to be used with subsequent improvements in instrumental resolution.

Topography

Polarized neutron diffraction topography is the only technique available to observe some kinds of antiferromagnetic do-

main. As an example, domains differentiated by the sense of the rotation of the spiral “chirality domains” were observed on single crystal samples of MnP. The domains mainly occur as strips, about 150 μm in width and several mm in length, perpendicular to the axis of the helix (Fig. 30). A gross imbalance in the domain population (3 compared to 1) was observed and the domain pattern was found to be reproducible under thermal cycling. Polishing the sample, or applying an uniaxial stress, modifies the domain structure and size, as well as the ratio of the volumes occupied by the two types of domain. Similar observations were performed in Ho: domains having no crystallographic orientation (Fig. 31). This different behaviour is qualitatively explained when taking into account that in MnP the helical phase nucleates from a ferromagnetic one, while this is not the case for Ho.

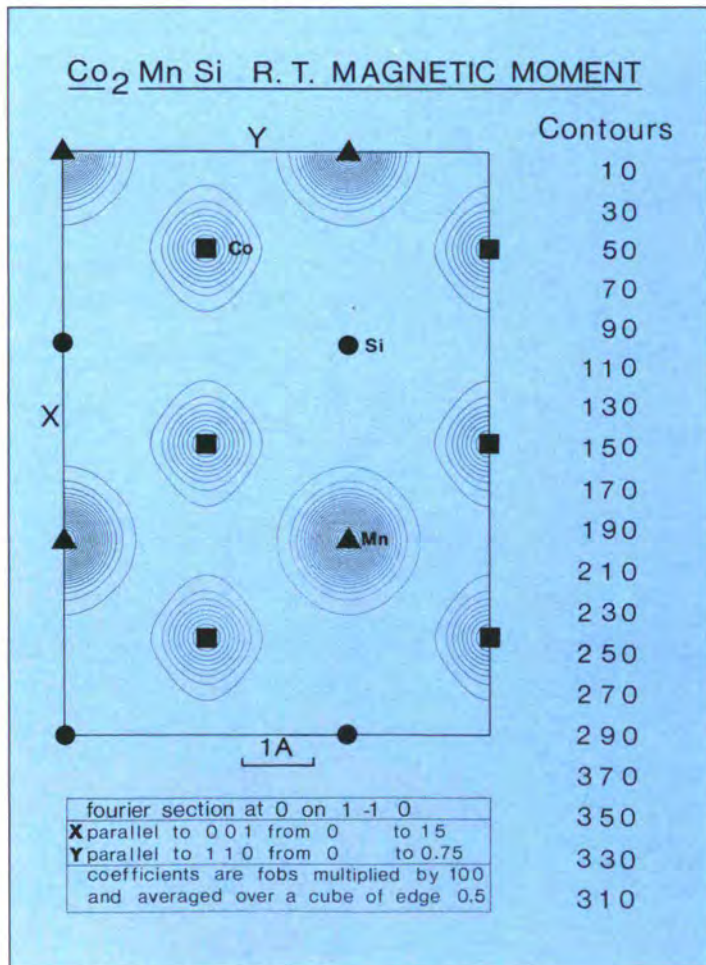


Figure 29: The magnetization density in the (110)(001) plane of Co₂MnSi at room temperature indicating the lack of spherical symmetry at both the Co and Mn sites.

Secretaries: W.F. Kuhs, K.R.A. Ziebeck

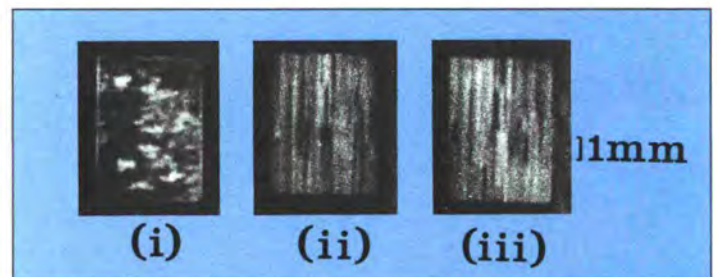


Figure 30: Chirality domains in the helimagnetic phase of MnP. i) 200 nuclear reflexion: only crystallographic defects are visible, ii) 200 magnetic satellite, “plus” neutron polarization and iii) 200+, “minus polarization”: domains are visible on the last topographs as stripes with reversing contrast.

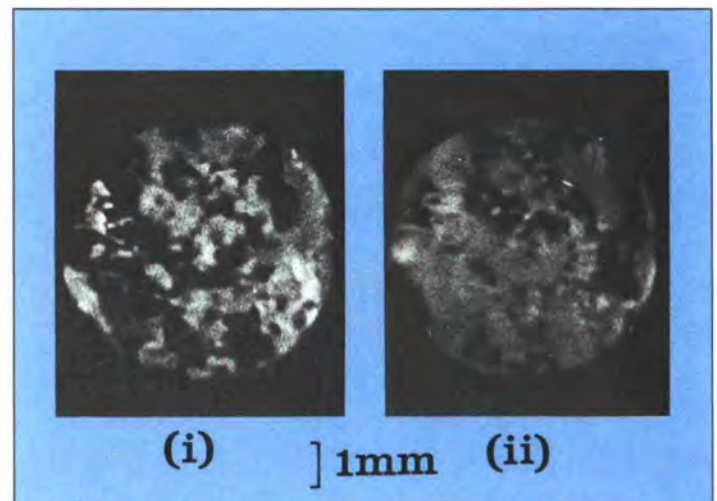


Figure 31: Chirality domains in the helimagnetic phase of holmium: walls have no simple crystallographic orientations.

Profile refinement

The name profile refinement is used to describe a particular technique for obtaining structural information from diffraction measurements on polycrystalline samples. The straightforward analysis of a powder diffraction pattern consists in associating individual peaks with particular Bragg reflections (indexing the pattern) and evaluating a diffracted intensity for each reflection by integrating the area under the peak in a plot of intensity versus scattering angle. Intensities thus obtained can be used in the usual way for crystallographic structure determination. A problem arises when the resolution of the pattern is not fine enough to completely resolve all the Bragg peaks. In this case a "conventional" analysis requires that some arbitrary division be made of the intensity in overlapping peaks between the component Bragg reflections. The profile refinement technique which was originated by Rietveld ⁽¹⁾ and is sometimes known by his name, addresses this problem by including each measured point of the diffraction pattern as an observation in a least squares fitting procedure. The parameters included in the fit then include ones which define the peak shapes and positions in addition to the crystallographic structural and thermal parameters. The "profile refinement technique" has been extremely successful in extending the range of materials for which structure refinements from powder diffraction can be made. The method is particularly well adapted to neutron powder diffraction because the diffraction profiles are well described by Gaussian envelopes and the scattering extends to high momentum transfers. Profile refinement has wide application in the study of structural phase transitions as a function of temperature and pressure, and enables the small structural distortions and atomic displacements associated with such transitions to be determined. The method has been extended to allow refinement of multiphase systems and the figure shows a point by point fit to the diffraction pattern of the proton (deuteron) conductor $\text{DUO}_2 \cdot \text{AsO}_4 \cdot 4\text{D}_2\text{O}$ (D U P) with ice at 4 K (Fig. 32).

Reference

1 H.M. Rietveld (1969) *J. Appl. Cryst.* 2, 65-71.

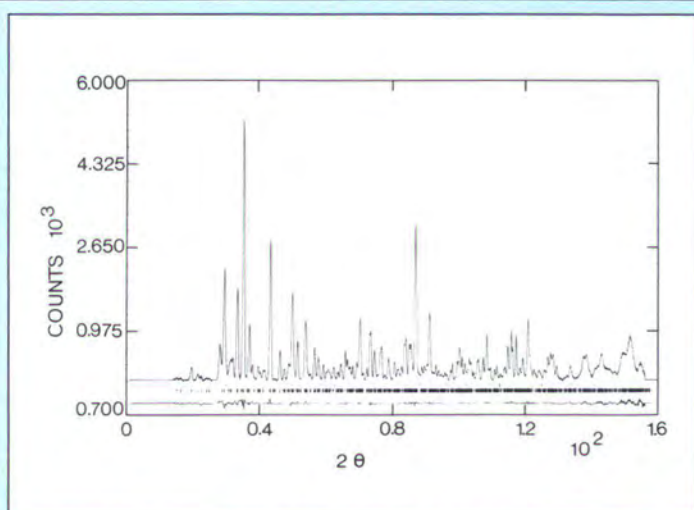


Figure 32: Diffraction pattern of $\text{DU}_{0.2}\text{AsO}_4 \cdot 4\text{D}_2\text{O}$ with ice at 4K. The upper curve gives the observed diffraction pattern as points and the fitted profile as a full curve. The two sets of vertical lines below mark the positions of the Bragg peaks for the two components. The lower plotted curve shows the difference between the observed and calculated patterns.

COLLEGE 6 LIQUIDS, DISORDER AND DEFECTS IN MATERIALS

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GENERAL SUMMARY

As in the past College VI has been active in a very broad scientific field. Both structural and dynamical aspects in systems as widespread as e.g. simple liquids and quantum liquids are

studied. The great diversity of problems is also reflected by the wide range of instruments used by the College. In this context the availability of the improved instruments D4, D7 and IN1B was much appreciated.

The scientific activity has been stimulated by a number of seminars, some of them organized together with College IX. Recently their number has been increased and for the future it is planned to have lectures on a fortnightly basis.

SCIENTIFIC TRENDS AND HIGHLIGHTS IN 1984

Amorphous Structures

Complete sets of partial structure factors $I_{ij}(Q)$ of quenched $Ni_{33}Y_{67}$ and $Cu_{33}Y_{67}$ were obtained (Exp. 6-08-126). For $Ni_{33}Y_{67}$ three neutron diffraction patterns ($Ni_{33}^{nat}Y_{67}$, $Ni_{33}^{60}Y_{67}$, $Ni_{33}^{38}Y_{67}$) and for $Cu_{33}Y_{67}$ two neutron patterns ($Cu_{33}^{nat}Y_{67}$, $Cu_{33}^{65}Y_{67}$) and one X-ray pattern ($Cu_{33}^{nat}Y_{67}$) were taken (Fig. 33). The partial radial distribution functions obtained by Fourier transformation of the $I_{ij}(Q)$ revealed that the Ni-Ni correlations differ greatly from the Cu-Cu correlations,

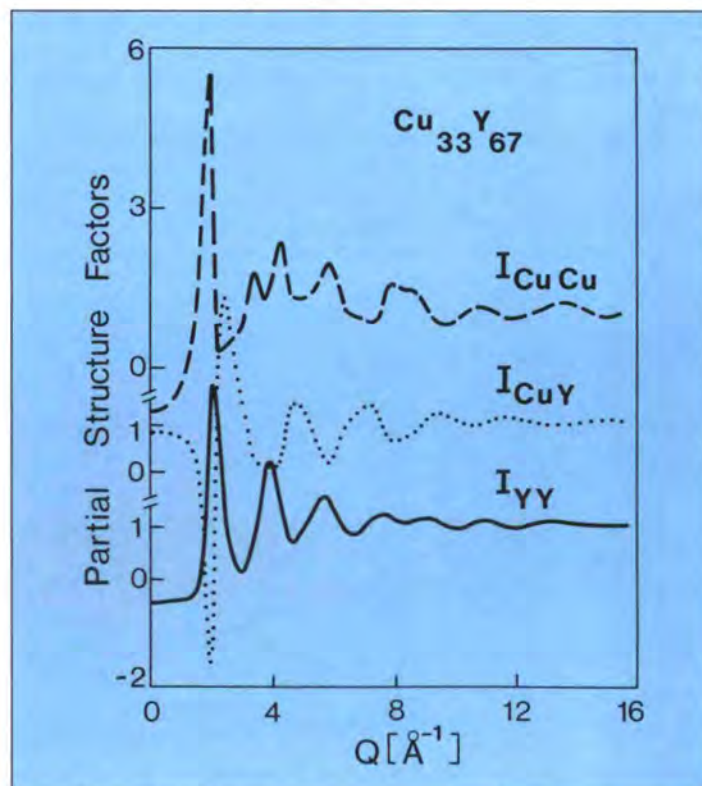


Figure 33: Partial structure factors $I_{ij}(Q)$ of as quenched $Cu_{33}Y_{67}$ amorphous metal.

whereas the Y-Y and Y-Mt (Mt = Cu, Ni) correlations are similar. Indeed interesting resemblances of the short range order in the amorphous state and in the stable crystalline state (Y_3Ni_2 , YCu) are found. The crystallisation processes were followed in situ on the D1B spectrometer. $Ni_{33}Y_{67}$ crystallizes in a single step with the occurrence of $\langle Y_3Ni \rangle$ and $\langle Y_3Ni_2 \rangle$, while $Cu_{33}Y_{67}$ crystallizes in two steps with an intermediate phase change at higher temperature into the cubic $\langle YCu \rangle$ phase and pure $\langle Y \rangle$.

Diffraction studies were also performed on the amorphous alloys $(Fe_{1-x}Mn_x)_{75}P_{15}C_{10}$ with $x=0, 0.29, 0.70, 0.84$ corresponding to:

- alloy without neutron contrast between metal site and metalloid site ($x=0.29$)
- alloy with zero scattering length for metal site ($x=0.70$)
- alloy with zero scattering length ($x=0.84$).

X-ray diffraction has shown that all these alloys are amorphous and that Mn and Fe are isomorphically substituting each other. The partial structure factors can therefore be determined by neutron diffraction (Exp. 6-08-110). Complementary magnetization measurements on the alloy with $x=0.29$ revealed two magnetic phase transitions. At $T_c = 172.5$ K the alloy becomes ferromagnetically ordered. The second transition is observed near 30 K corresponding to a reentrant spin glass behaviour. The total scattering intensity in the small angle regime shows a cusp at T_c and a further pronounced increase is found at lower temperatures towards the spin glass state providing evidence for a cluster model (Fig. 34).

SANS has also been performed on amorphous $Fe_{70}Cr_5P_{15}C_{10}$ with and without an external magnetic field and/or immersion of the sample in a deuterated liquid in order to separate scattering originating from magnetic heterogeneities, from surface imperfections and from bulk properties. The experiment

(Exp. 6-12-46) showed that about 95% of the SANS signal is due to magnetic inhomogeneities, 4.9% of the scattering is due to surface imperfections and a mere 0.1% fraction, hardly emerging from the background, can be attributed to bulk non-magnetic properties.

Dynamics in Amorphous Materials

The vibrational excitations in vitreous silica above 150 GHz were investigated at 50, 100 and 290 K by inelastic neutron scattering (IN6). A detailed study of the frequency and wavevector dependence showed that even at the lowest frequencies only a small part of the scattering is due to acoustic phonons. The type of motion of the dominating additional low-frequency modes is identified as a coupled rotation of SiO_4 tetrahedra thus providing new arguments for the discussion of the low temperature anomalies commonly observed in glasses.

Diffusive motions in amorphous $AgI-AgPO_3$ (1:1) have also been studied in the temperature range from -143° C to $+95^\circ$ C (Exp. 6-14-19). The high diffusion coefficient and the low activation energy (~ 9 kJ mol $^{-1}$) found for the Ag^+ ions suggest a liquid-type motion similar to the superionic conductor $\alpha-AgI$ rather than a jump diffusion mechanism.

As an alternative technique SANS has been applied to measure the diffusion constant in contrast-modulated samples (Exp. 6-14-43). Successive films of amorphous Si and Ge have been evaporated onto a glass substrate. The thickness of each layer was 100 Å and there were 100 layers in a sample. Using D17 at a wavelength of 10 Å it has been possible to observe a satellite peak at $\theta = 1^\circ 20'$. Following thermal treatment, the contrast distribution was modified by atom migration. From the variation of the intensity of the satellite peak it was possible to measure a diffusion constant for the amorphous Si-Ge system as small as 10^{-23} cm 2 s $^{-1}$ at 300° C.

Diffusion in Liquids

The study of diffusive motions in the liquid state ranging from simple atomic liquids to complex ionic solutions remained a central point in the activities of College VI.

The first experiment on D7 this year with polarization analysis was on the dynamics of the simple liquid sodium (Exp. 6-02-61). With this technique coherent and incoherent scattering can be separated. The data were corrected by Monte Carlo techniques for multiple scattering with and without spinflip and both scattering contributions are shown individually in Fig. 35. Because of the extended wavevector range of this experiment (incident wavelength 3.1 Å), it was also possible to study the interesting region where the transition from a liquid-type to a gas-type diffusion takes place.

Extensive and high quality quasi-elastic incoherent data were also collected on molecular liquids such as water over a temperature range from $+20^\circ$ C down to -20° C in the

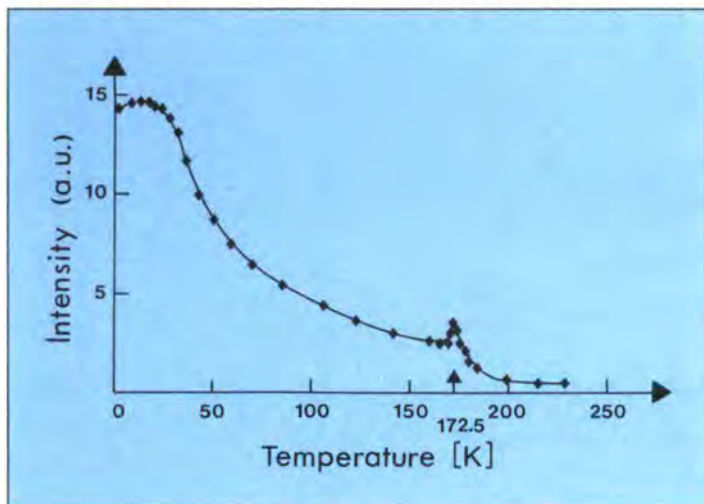


Figure 34: Temperature dependence of the total small angle intensity of $(Fe_{29}Mn_{71})_{75}P_{15}C_{10}$.

supercooled state (Exp. 6-05-60). Three new results were obtained: i) two relaxation times are clearly identified at all temperatures in relation to the short time and intermediate time diffusion of water molecules; ii) one of these relaxation times is associated with the jump diffusion of the protons and the temperature dependence of the jump length was qualitatively determined; iii) the Q-dependence of the scattered intensity integrated over the quasi-elastic region follows a Debye-Waller factor which is temperature independent. Some results are shown in Fig. 36.

A comparative study of the diffusive motions of protons in pure water and in an ionic solution such as $ZnCl_2/H_2O$ (Exp. 6-07-78) emphasized the importance of the rotational motion of the water molecules. The observed Q-dependence of the translational linewidth follows the random jump diffusion model with about the same jump length for pure water and for the saturated solution. It is also close to the distance between the protons in the water molecule. Complementary investigations by Raman, Rayleigh wing and inelastic neutron scattering were performed on the same system. The results confirm that it is best viewed as a locally amorphous solid. The locally ordered, dynamically correlated patches are strongly influenced by the solute — in particular by its action on the water hydrogen bond.

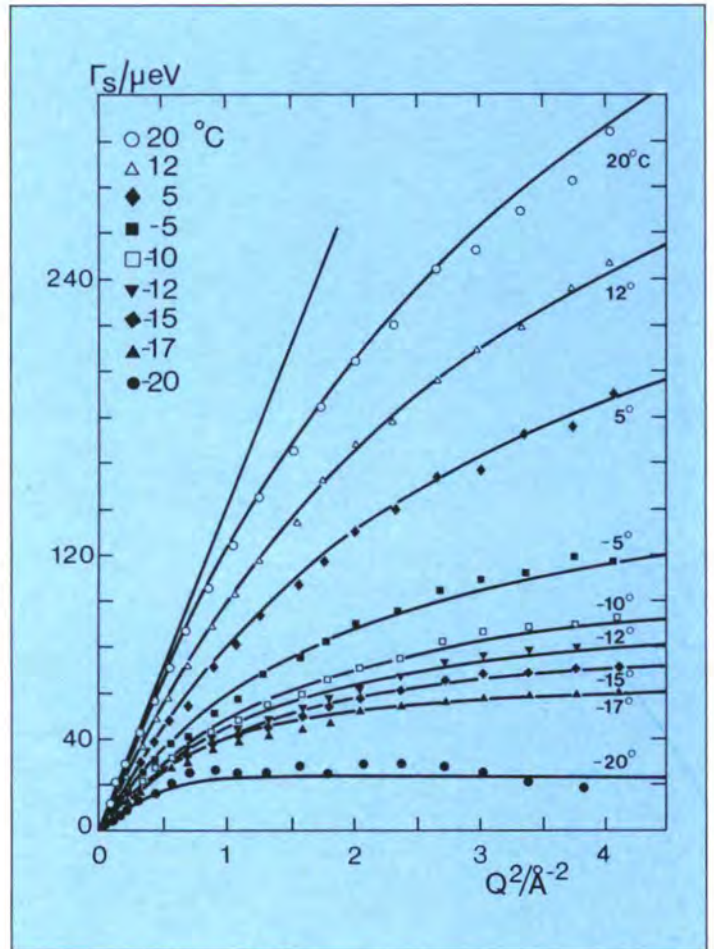


Figure 36: Quasi-elastic linewidth Γ from the translational motion in water versus Q^2 . The straight line gives the self diffusion constant at $20^\circ C$.

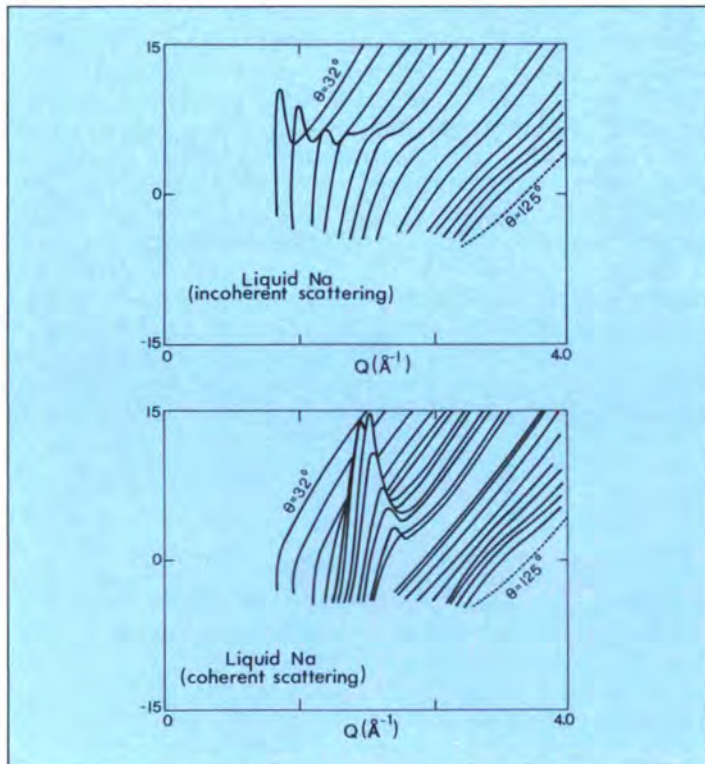


Figure 35: Incoherent (a) and coherent (b) quasi-elastic scattering from liquid sodium. Spectra were obtained on D7 with polarisation analysis.

Hydrogen in Metals

In the field of metal-hydrogen systems there is a continuing demand for beam time to study dynamical aspects such as high frequency optic/local modes or hydrogen diffusion. In recent applications there is a tendency to move away from simple host metals to more complicated systems like amorphous metals or systems with multiple site occupation. Also the study on the hydrogen delocalisation over equivalent sites is a Nb host metal revealed very remarkable results.

The Yttrium-hydrogen system (Exp. 6-14-66) has recently become a point of interest since the hexagonal α -phase solution allows one to study a complex system with possibly octahedral (O) and tetrahedral (T) site occupation in a pure metal where single crystals are available. Quasi-elastic measurements showed i) a major occupation of T sites, ii) a rapid local mo-

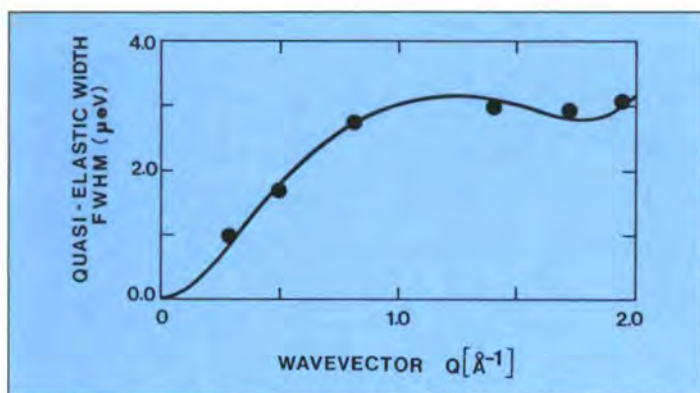


Figure 37: Fit of a multiple sublattice jump model to quasi-elastic data taken on IN10 for $\text{YH}_{0.15}$ single crystal at 695 K.

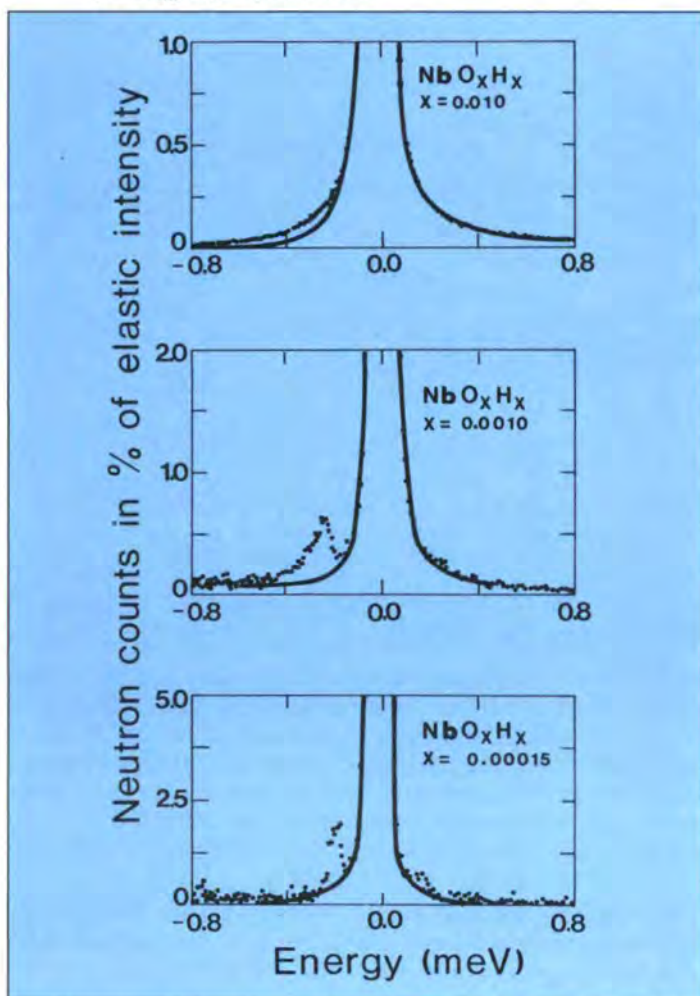


Figure 38: Inelastic scattering from the tunnel-split ground state for H in NbO_xH_x at various concentrations x . The measurements were performed at 1.3 K. The solid line gives the instrumental resolution.

tion of the hydrogen occurring between pairs of T sites separated by 1.3 Å and iii) a slower long range diffusion taking place via the O sites (Fig. 37). Furthermore it became clear that not all the protons are involved in the local jump, a given fraction being immobile on the timescale of the measurement. This suggests, that either these protons occupy alternative sites or are in some way trapped on a tetrahedral site. Measurements of the local mode frequencies (Exp. 6-14-63) surprisingly revealed two peaks; one at 136 meV which can be attributed to a hydrogen on a regular tetrahedral site together with a second peak at 102 meV. The relative intensities of these peaks do not depend on the amount of impurities such as oxygen, but are affected by the thermal history of the sample.

Quasi-elastic measurements of hydrogen diffusion in amorphous metals like $\text{Pd}_{0.80}\text{Si}_{0.20}$ or $\text{Ni}_{24}\text{Zr}_{76}$ (Exp. 6-14-17, 6-14-30) reveal spectra which cannot be described by a single Lorentzian line corresponding to a single diffusion process. It has been proposed that the hydrogen first occupies the deep potential wells where it is relatively immobile. With increasing hydrogen concentration less favourable and probably shallower sites are also occupied leading to a rapid hydrogen diffusion and a broad spectrum of dwell times at high concentrations.

Nb with a small amount of hydrogen bound at low temperatures by equal amounts of interstitial impurities such as oxygen is the only system known so far where the delocalisation of a hydrogen atom over two almost equivalent sites has been clearly observed. This year earlier data were greatly improved using the instrument IN6 (Exp. 6-14-61). Fig. 38 shows the influence of the defect concentration x in NbO_xH_x on the inelastic scattering. At low concentration $x = 0.00015$ a tunnel splitting of the ground state of 0.17 meV is measured with almost the instrumental resolution. With increasing concentration the interaction of the defects via their strain field becomes more and more important leading to locally varying asymmetric double well potentials. Asymmetric potentials have an increased ground state splitting which will, however, be measured with reduced intensities. The lineshape measured at $x = 0.0010$ directly evidences this mechanism. At even higher concentrations $x = 0.010$ the inelastic scattering is smeared out over a large energy range and can only be measured with low intensity.

Diffusion in Bulk Material

Progress has been made in the study of the diffusion of Co in β -Zr (Exp. 6-14-53). Because single crystals are difficult to grow due to the phase transition from α - to β -Zr earlier experiments were carried out on polycrystalline samples. This obstacle has now been overcome by alloying Nb to Co-Zr thereby stabilizing the β -phase at room temperature. First measurements on $\text{Zr}_{69}\text{Nb}_{30}\text{Co}_1$ showed an anomalous fast diffusion of Co.

The self-diffusion of polycrystalline Ti in its high temperature β -phase has also been measured at the backscattering spectrometer IN10 and the spin echo spectrometer IN11 (Exp. 6-14-51, 6-14-35). The quasi-elastic linewidth as a function of temperature is compared in Fig. 39 with results from tracer measurements. The width at 1160° C agrees with the tracer results. However, at higher temperatures there is a significant difference between the results from the two techniques. The quasi-elastic linewidth seems to follow a linear extrapolation of the low temperature tracer measurements.

In-Beam NMR Spectroscopy

The study of the layered compound LiC_6 by the observation of β -radiation detected nuclear magnetic resonance and polarisation transients of ^8Li has been completed. The temperature dependence of the ^8Li quadrupole coupling constant measured in the range from 10 to 500 K shows an anomaly near 230 K. This is also reflected by a discontinuity in the spin lattice relaxation rate T_1^{-1} , which was measured in the range from 70 to 700 K for various magnetic fields and for two crystal orientations. The T_1^{-1} data above room temperature indicate two low-dimensional Li-diffusion processes.

In the glass $\text{Li}_2\text{O} \cdot 3\text{B}_2\text{O}_3$ T_1^{-1} was measured for the two probe nuclei ^8Li and ^{12}B . For $T < 200$ K a weak magnetic field and temperature dependence was observed, similar to results from β -NMR on a silicate glass. This can be explained by quadrupolar coupling to thermally activated defects typical for glasses. From 300 to 500 K T_1^{-1} is dominated by the Li diffusion. The activation energy is only half the value obtained from conductivity measurements. This may be attributed to a partly localized diffusion.

Quantum Liquids

The scattering function of liquid and solid hydrogen has been measured over a wide Q -range from 1 to 7 \AA^{-1} (IN4). With increasing momentum transfer up to $\sim 4 \text{ \AA}^{-1}$ the rotational lines, the single phonon transitions and the elastic line diminish due to the Debye Waller factor. For $Q > 5 \text{ \AA}^{-1}$ the spectra show one broad recoil line centered at $\omega = \hbar^2 Q^2 / 2m$, where m is the effective mass of the recoiling system (Fig. 40). Theoretical arguments show that the impulse approximation holds in a Q -range for which the Debye-Waller factor is small. Thus the momentum distribution and the kinetic energy of condensed hydrogen can be derived from the shape and the width of the recoil line.

The experimental work on liquid He^4 has also been continued, examining the interactions between the elementary phonon-roton excitations with resolution in energy and wavevector hitherto unobtainable. The measurements of the

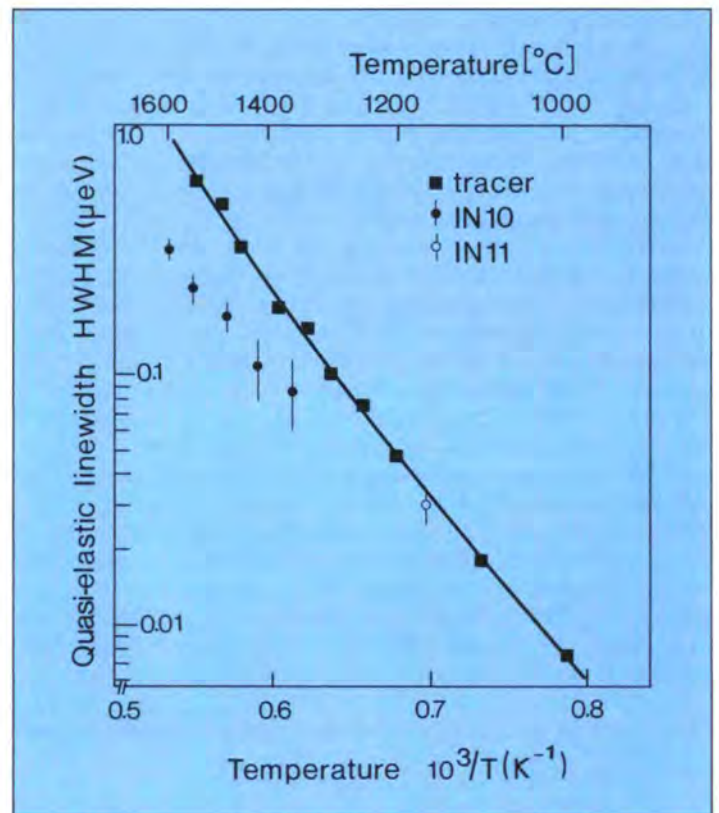


Figure 39: Temperature dependence of the quasi-elastic width from the self-diffusion of Ti compared with results from tracer measurements. Data are shown for $Q = 1 \text{ \AA}^{-1}$.

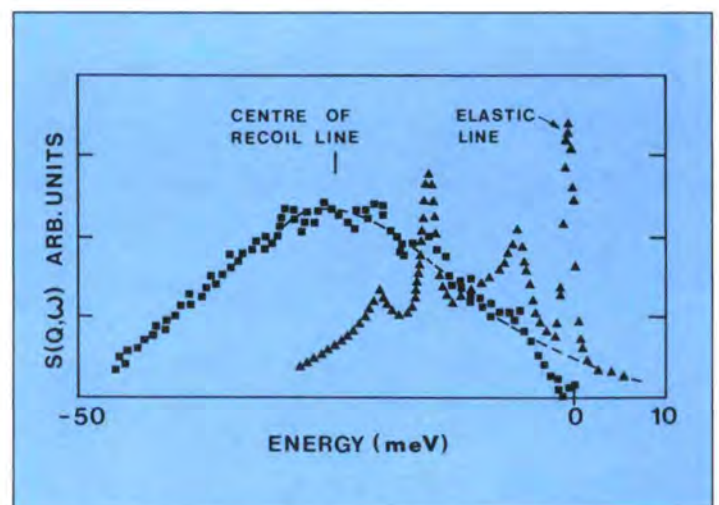


Figure 40: Scattering law $S(Q, \omega)$ of solid hydrogen at $Q = 3.9 \text{ \AA}^{-1}$ ($\Delta\Delta$) and at $Q = 5 \text{ \AA}^{-1}$ ($\square\square$). Data at high Q are fitted with a Gaussian function (—).

lifetimes of phonons in superfluid He^4 have been extended using the triple-axis spectrometer IN12 (resolution ~ 20 to $40 \mu\text{eV}$). Additional wavevectors were examined, including the "maxon" at $Q = 1.13 \text{ \AA}^{-1}$, and particular attention was devoted to temperatures higher than those reported earlier (Exp. 6-01-84). With these data fairly complete information on the phonon lifetimes is available, permitting a detailed comparison with theoretical predictions.

Another field of activity involving the interactions between excitations in liquid helium is the study of bound states of two rotons. Two-roton resonances or bound states are expected to make a significant contribution to the multiphonon continuum observed at higher energies than the phonon-roton excitations. A reexamination of the pressure-dependence of the inelastic scattering from liquid He^4 has recently been initiated on IN12. Although data analysis is as yet preliminary, it is clear that the multiphonon continuum displays more structure than previously believed. For example, at the "maxon" wavevector $= 1.13 \text{ \AA}^{-1}$, the continuum has a definite extra peak in the neighbourhood of twice the roton frequency. This peak tends to decrease in intensity with increasing pressure, as predicted by theory. By comparison with theoretical lineshapes, it is hoped to extract the effective roton-roton coupling parameters as a function of both pressure and wavevector.

Secretary: A. Magerl

Random (close) packing

From the viewpoint of the study of atomic-scale structure of the condensed phase, the crystal/glass difference is substantial. While for crystalline solids the crystallographic data yield detailed and quite complete information about the equilibrium positions of the atoms, providing an advanced initial outpost from which to progress further in our understanding of the material, for amorphous solids the nature of the atomic arrangement is itself a difficult and hard-to-win objective. The lack of long-range order and of its afferent selection rules makes it very tedious to extract structural information from the diffraction experiments. The picture of amorphous structure that has gradually emerged turns out to be concordant with homogeneous, continuous filling of space in which chemical-bonding considerations are challenging randomness.

Three notable types of continuous-random models have been proposed, namely:

- Continuous random network appropriate to the structure of covalent glasses.
- Random coil model, appropriate to the structure of polymeric organic glasses.
- Random close packing appropriate to the structure of some simple metallic glasses.

When a large number of hard spheres of uniform size are quickly poured and packed into a container having irregular surfaces, the disordered but stable configuration which results can be characterized, with varying degrees of completeness, by the same sort of numerical and functional measures as used for crystals but generally take on the form of statistical distribution.

However, some quantities are, empirically, remarkably well defined and reproducible. One good example is the filling factor (fraction of space contained within the spheres) found to be 0.637 in a variety of experiments of the type. The 0.637 filling factor for the random close packed (RCP) structure means that for balls of the same size, random close packing is about 86% as efficient a filling of space as is crystalline close packing (the filling factor is 0.7405 for the fcc and hcp lattices).

It is natural to wonder if there exists a purely mathematical derivation of the RCP structure in analogy to the inevitable occurrence of the fcc and hcp structures in the systematic study of symmetric lattices. An alternative description of space filling by atoms is the partitioning of space into cellular neighbourhoods. The corresponding atomic polyhedron or Wigner-Seitz cell (WS) surrounding a given atomic site is defined as the polyhedron whose interior contains all points which are closer to that site than to any other (Fig. 41). The WS cells generated by a random array fill space in such a way that every face is surrounded by two

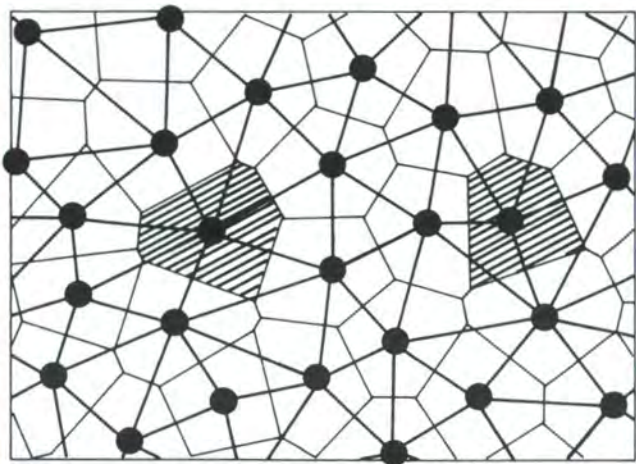


Figure 41: Polygonal divisions of a plane defined by an irregular array of sites. The heavy dots denote the atomic sites, the Wigner-Seitz atomic cells are shown by the light lines (two cells are shown shaded), and the heavy lines denote the bonds.

cells, every edge is surrounded by three cells and every vertex is surrounded by four cells. The first is obvious, the second and third follow because the locus of positions equidistant from three (four) unrelated points is a line (point). Now the question is whether or not there exists a regular division of space by identical polyhedra, each polyhedron bounded by identical regular polygons, with these topological specifications. For a three dimensional network of polyhedra there is an Euler-Poincaré relation:

$$V - E + F - N = 1$$

in which V is the number of vertices, E is the number of edges, F the number of faces and N is the number of cells. When applied to a single isolated polyhedron ($N = 1$), this relation gives for instance:

$V = 8$, $E = 12$ and $F = 6$ for a cube
 $V = 14$, $E = 24$ and $F = 12$ for a rhombic dodecahedron, etc.

The "averaged" cell of a RCP structure, as explained above, has three faces (and edges) meeting at each vertex, 2 faces meeting at each vertex and of course each polygonal face (p edges) is in contact with p edges (and vertices), so that:

$$3\bar{V} = 2\bar{E} = p\bar{F}$$

which substituted into the Euler-Poincaré relation gives

$$\bar{F} = \frac{12}{6 - \bar{p}}$$

or expressed in another way

$$\sum_{p=0}^{\infty} (6-p)F_p = 6N$$

where F_p is the number of faces with p sides.

It can be shown that for the distribution in p the most common occurrence is:

$p = 5$ (41% of the faces) followed by $p = 6$ (29%), $p = 4$ (19%), $p = 7$ (6%), $p = 3$ (4%) and $p = 8$ (1%).

The averaged value $\bar{p} = 5.12$ is also the "possible" number of regular tetrahedra that can share one edge. The corresponding $\bar{F} = 13.6$ is also the averaged coordination number.

In conclusion the RCP structure has empirical and mathematical existences indeed and is actually the amorphous modification of fcc and hcp crystals. Of course it means also that other symmetric lattices must have amorphous modifications: as crystalline metals have not only fcc or hcp structure, amorphous alloys have not only RCP structure neither.

Partial pair distribution functions in amorphous materials

Information on the environments of atoms in binary amorphous materials is contained in partial pair distribution functions

$$G_{\alpha\beta}(r) = \frac{4\pi r}{C_{\beta}} [\rho_{\alpha\beta}(r) - \rho_0]$$

derived from the partial structure factor $S_{\alpha\beta}(Q)$ where α and $\beta = 1, 2$ corresponds to the type of atoms, C_{α} or C_{β} are the concentrations, $\rho_{\alpha\beta}(r)$ is a local density describing the number of β -atoms in a unitary volume at a distance r from the α -type atom.

Partial structure factors $S_{\alpha\beta}(Q)$ are components of the total structure factor $S(Q)$ which in turn is derived from diffraction data. In neutron diffraction there are advantages in dissecting $S(Q)$ into "Bhatia-Thornton" partials so that:

$$S(Q) = \frac{1}{\langle b^2 \rangle} [\langle b \rangle^2 S_{NN} + 2\langle b \rangle \Delta b S_{NC} + (\Delta b)^2 S_{CC}]$$

with:

$$\begin{aligned} \langle b \rangle &= C_1 b_1 + C_2 b_2 \\ \langle b^2 \rangle &= C_1 b_1^2 + C_2 b_2^2 \\ \Delta b &= b_1 - b_2 \end{aligned}$$

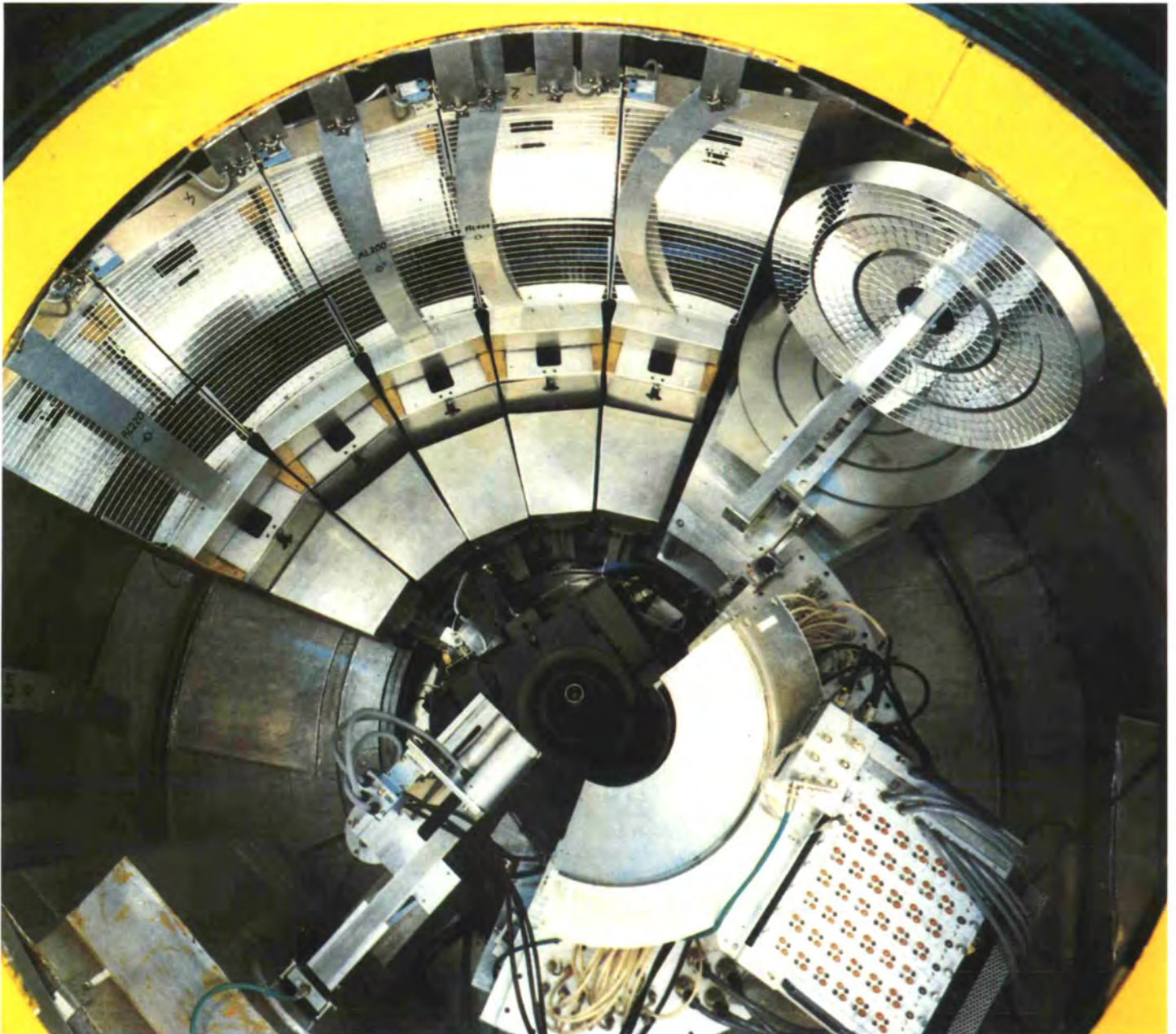
The S_{NN} function is related to the Fourier transform of the total atomic pair distribution and contains the same information as the interference function in the monoatomic case. It is the structure factor of the topological network of the atomic sites without any reference to chemical aspect. The S_{NN} function may be regarded as the amorphous modification of the Bragg peak set for a Bravais crystal lattice. S_{NN} is directly measured in neutron diffraction if an alloy with $b_1 = b_2$ can be prepared, using for instance isotopic or isomorphous substitution.

The S_{CC} gives directly the degree of chemical order and is particularly informative when Fourier transformed to give a "radial concentration correlation function". Formally S_{CC} is related to the averaged difference between the distribution of like and unlike bond pairs. S_{CC} in amorphous alloys is the equivalent of diffuse scattering as measured in crystalline alloys. Maximum values of S_{CC} occurs either between or at the S_{NN} "peaks" depending on chemical ordering or clustering tendency, respectively. The S_{CC} function is directly given by measuring neutron diffraction on a so-called "zero alloy" ($\langle b \rangle = 0$) using again isotopic or isomorphous substitution techniques.

1

The S_{NC} function describes cross-correlation effect and is related to the difference between pair distributions (like + unlike) around the two types of atoms. S_{NC} does not exist in a crystal since atoms occupy well defined lattice sites with

the same total number of neighbours in their coordination shells. S_{NN} , S_{NC} and S_{CC} as they are defined here oscillate around 1,0 and C_1C_2 respectively.



Top view of the backscattering spectrometer IN10.

COLLEGE 8 AND EMBL GRENOBLE: BIOCHEMISTRY

Members of the College

I. At ILL

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C. Devaux
A.J. Dianoux
K. Ibel
M.S. Lehmann
S. Mason
R. May
R. Oberthür
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F. Borrás-Cuesta
J. Chroboczek
S. Cusak
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A. Gabriel
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GENERAL SUMMARY

The experiments carried out within the aegis of the college cover a wide range of biological problems. Structure remains the dominant interest but studies on solvent-protein and membrane surface interactions and protein dynamics are also in progress. Structures in crystals, partly ordered systems and of particles in solution are being investigated. Small angle solution scattering has been principally used with complexes by exploiting the indigenous differences in scattering length density between different components (usually between protein and nucleic acid, lipid or polysaccharide). Specific deuteration is being used to manipulate relative scattering densities so as to focus on chosen components (e.g. ribosome, triptophan synthase).

These studies provide low resolution models of the solution structure of complexes which are usually large and difficult to crystallise and study in detail. Low resolution crystallography again with the benefit of contrast variation is providing more detailed structure information in some complexes. The models obtained are taken over to advance the X-ray diffrac-

tion analysis to higher resolution when good isomorphous derivatives are lacking. The dynamic behaviour of proteins is being explored in two very different ways. By using high resolution crystallography to monitor H/D exchange of individual sites and by making inelastic scattering measurements in solutions.

SCIENTIFIC TRENDS AND HIGHLIGHTS IN 1984

A meeting of the French Biochemical Society for young scientists, "Forum des Jeunes Chercheurs", was held in Grenoble. Six of the participants brought samples and on one day on D11 they were able to make radius of gyration and molecular weight determinations. In three cases the oligomeric state of the enzyme was different from that anticipated. Thus by direct experimentation the young scientists obtained insight into the use of neutron scattering. This innovation was considered to work well by all concerned.

Low Resolution Crystallography

Matrix porin is a major transmembranar protein isolated from the outer membrane of *E. Coli*. It can be readily crystallised from aqueous detergent solutions including octyl glucoside. In this system the protein is solubilized as a trimer ($3 \times 36,000$) and crystallises in space group $P4_2$ with $a=b=154 \text{ \AA}$, $c=172 \text{ \AA}$ with two trimers per asymmetric unit. Crystals contain 40% protein, 20% detergent and 40% water. X-ray diffraction extends to 2.8 \AA but attempts to produce isomorphous derivatives have met with a number of difficulties, delaying all attempts at structural analysis. Neutron diffraction studies have been carried out to 16 \AA resolution with the objective of localizing the protein and detergent (11% D_2O) using structural information obtained from electron microscopic reconstructions of 2-dimensional lipid membranes and modelling the shape of the trimer by an array of cylinders of constant density. Model parameters are refined by minimizing the R-factor. The trimer has been positioned in the unit cell with orientation angles found independently in rotation function analysis of X-ray data between 10 and 30 \AA . The model phases allow calculation of reasonable density maps at 30 \AA resolution. Refinement to 16 \AA will be attempted after localization of the detergent which is not in a bilayer arrangement (Basel, EMBL, ILL).

The complex of yeast aspartyl-tRNA synthetase (MW 125 000) with two molecules of its cognate tRNA (MW 24,160) crystallises in the cubic space group I432. The neutron diffraction

data collected previously at different contrasts on D17 have been analysed. Using the data to 40 Å resolution collected when the tNRA is contrast matched (i.e. 65% D₂O) the proteins have been located giving the first picture of the molecular packing in the crystal. The tRNA molecules have been then located at 25 Å resolution using neutron (H₂O buffer) and X-ray data. Finally the resulting model was refined against 15 Å resolution X-ray data. Electron micrographs from thin sections of the crystals confirm the molecular packing. This provides a second example, the first being the nucleosome core particle, of a low resolution structural determination with neutron diffraction providing a base for X-ray analysis to higher resolution (EMBL, ILL, Strasbourg).

Data collection from tomato bushy stunt virus crystals was extended to 16 Å resolution for three contrasts 0%, 70% and 100% D₂O. Data reduction is almost complete, the data sets appear to be of very high quality although there is a rapid decrease in intensity beyond 19 Å resolution such that the fraction of observed reflections in the 20-16 Å range is rather small (EMBL, ILL, Strasbourg).

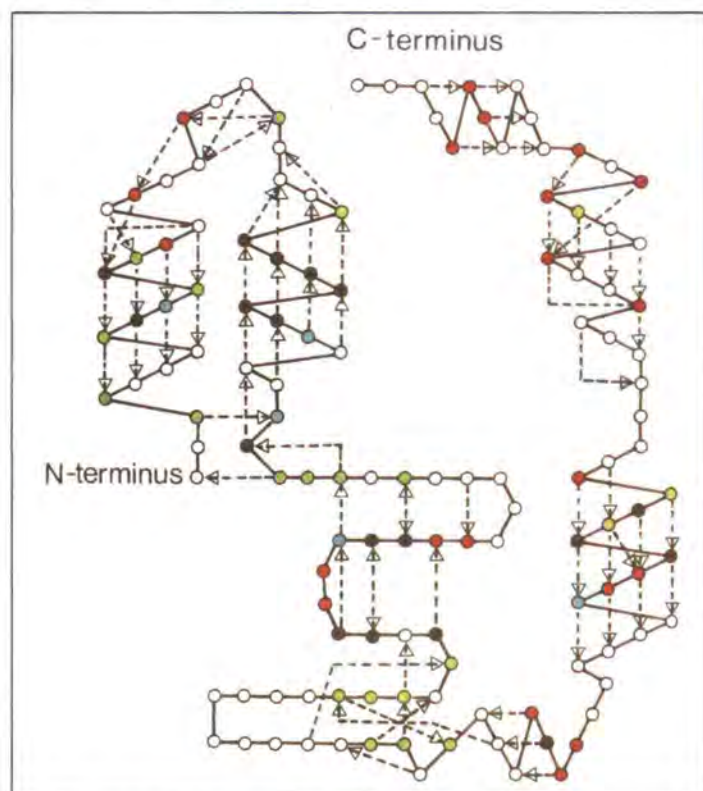


Figure 42: The H/D exchange pattern of the amide hydrogens of lysozyme as determined by four separate neutron diffraction measurements. The arrows indicate the direction from the donating (NH) to the accepting (CO) groups in the protein secondary structure. The relative ease of H/D exchange of the peptide amide groups increases in the order: black, blue, green, red and white.

High Resolution Protein Crystallography

The structure of a protein, as determined by X-ray crystallography, gives a time average model of the molecule with only a limited picture of its dynamic behaviour in the form of the derived thermal parameters. The process of H/D exchange between the protein and D₂O buffer, can be followed by neutron diffraction and it has been shown that significant fluctuations from this time averaged structure occur. In particular, careful control of exchange of the peptide amide hydrogens, which serve as common markers throughout the entire molecule, can be exploited to obtain dynamic behaviour that is not necessarily evident in the "static" model of the protein. Recent experiments on lysozyme using D8 and D19 have shown that this can be achieved through judicious choice of pH and temperature while soaking the crystal in its D₂O mother liquor. The preliminary results are illustrated in figure 42.

It is particularly noteworthy that the data collection times, as for the ethanol-soaked lysozyme reported in College 5, were equivalent to only 10 days on the four-circle diffractometer D8. The success of these experiments convincingly demonstrates that when the basic structure of a protein is known, neutron diffraction experiments need not be prohibitively long (ILL, EMBL).

E. Coli 50S Ribosomal Subunit

In the study of the spatial arrangement of proteins within the large subunit of *E. Coli* ribosomes, this year emphasis was given to measurements of protein distances. Three new protein shape parameters were determined (proteins L9, L17, L20), making a total of 15 proteins. Data for 22 new protein pairs nearly doubled the number of completed distance measurements, which now amounts to 43. Currently, efforts are being made to combine all data into a common file for simultaneous treatment. Groups of protein pairs have been chosen for the measurements. Thus, the number of proteins that can be included in an initial model of spatial arrangement is increased with respect to a random choice of protein pairs. On the assumption that the distance measurements are all correct, a basic structure consisting of seven proteins (L2, L3, L4, L13, L20, L22, L23) can be calculated without further information. The distances of five more proteins (L1, L9, L15, L21, L24) to any three of the proteins of the basic structure is known. In cases where additional information (e.g. immuno EM) is available or where volume exclusion can be assumed, the positions of some of those five proteins can also be fixed (MPI Berlin, ILL).

Virus in solution

Experiments were performed on the temperature sensitive mutant ts112 of adenovirus which lacks one of the major core

proteins, some other protein and is DNA depleted. Comparison with the native virus indicates that the mutant particle has a structure much more like a hollow shell from which some of the protein is missing (EMBL, ILL).

Bromegrass mosaic virus can be decapsidated with a pH jump and can be progressively reassembled by lowering the LiCl concentration. The kinetics of reassembly have been followed with small angle scattering at different contrasts in order to separate the behaviour of the protein and RNA components (EMBL, ILL). The bacteriophage T7 was studied on D17 during orientation in a shear gradient. No anisotropy in the scattering was observed although birefringence measurements indicate high orientation. A test experiment on D11 showed that the virus was amenable to a contrast variation study. These preliminary results indicate that there is much less protein in the core than has been proposed from X-ray studies (ILL, Moscow).

Membranes

Myelin membranes are insulative layers wrapped around the nerve axon. For the myelin sheath to maintain its structural and functional integrity, adhesion must occur at both the cytoplasmic (intracellular) and extracellular surfaces. As the temperature and pressure response of a system allows a characterization of the nature of the interactions in the system at equilibrium, these thermodynamic variables have been used together with neutron diffraction to study the mechanism of adhesion at each surface. The scattering density profiles in figure 43 show the bilayer membrane to thicken and the cytoplasmic space to increase with increasing hydrostatic pressure. The cytoplasmic effect appears to be due to ionic bonding between the negatively charged membrane surfaces and myelin basic protein. High pressure dissociates these ion-pairs and opposing membranes repel each other. A very similar result was obtained with the model system made of negatively charged multilamellar lipid vesicle dispersions containing myelin basic protein. The membrane thickening effect results from the highly anisotropic compressibility of the bilayer; the hydrocarbon chains pack closer together with a consequent elongation of the lipid molecules perpendicular to the membrane plane. This effect is also found with lipid bilayers. Decreasing the temperature at ambient pressure has a similar effect to increasing the pressure at a fixed temperature (figure 43).

Below 25° C the extracellular space increases abruptly from 53 to 80 Å on increasing the pressure. Lowering the temperature causes this to occur at a lower pressure indicating the interaction across the extracellular space to be between membrane associated hydrophobic groups.

Prothrombin (MW 72,000) is an extrinsic membrane protein which in the presence of calcium binds to the acidic phospholipids on the platelet membrane where it is converted to thrombin by the prothrombinase complex. Using solution scatter-

ing the binding curve of prothrombin to negatively charged single bilayered lipid vesicles has been obtained (figure 44). It was also found that this rather elongated protein bound with its long axis perpendicular to the membrane surface without penetrating the bilayer (ILL, CEN-Grenoble). Efforts are also being made to determine the molecular weight and radius of gyration of intrinsic membrane proteins reconstituted into lipid vesicles (EMBL, ILL).

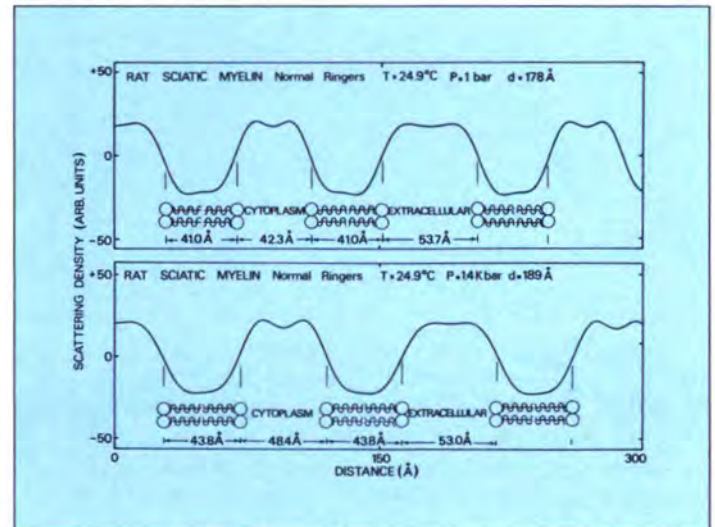


Figure 43: Scattering density profiles perpendicular to the membrane plane at ambient pressure and at 1.4 K bar, as shown, derived from seven Bragg order of diffraction.

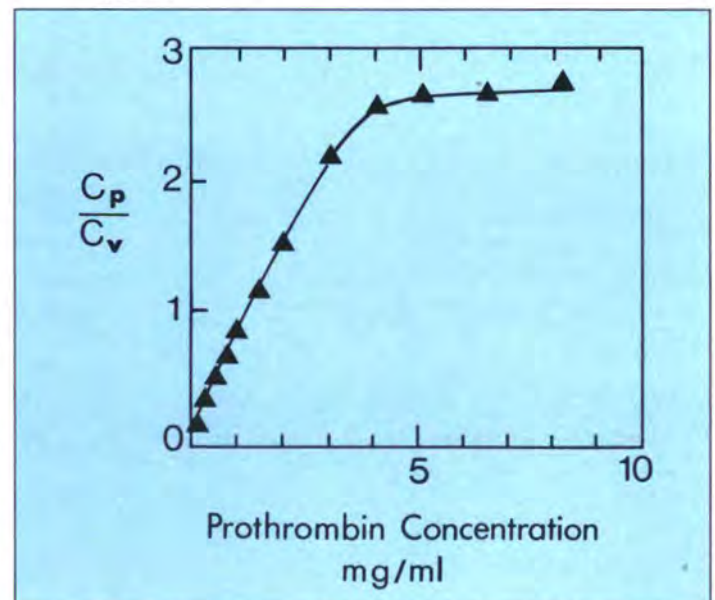


Figure 44: The binding of prothrombin to single shelled lipid vesicles. C_p = bound prothrombin concentration. C_v = lipid concentration.



Dismantling of D11 (status of October 1984) in preparation for the re-build.

Work on the purple membrane of halobacteria has continued with the position of the chromophore retinal reported last year being confirmed (Berlin). Characterisation of the structure and hydration at liquid nitrogen temperature with the optical cycle frozen in has also been done (ILL).

Diffraction studies were carried out on oriented layers of matrix porin reconstituted into planar lipid bilayer. Location of the channel is in progress, the results will complement the low resolution crystal work discussed above (Berlin).

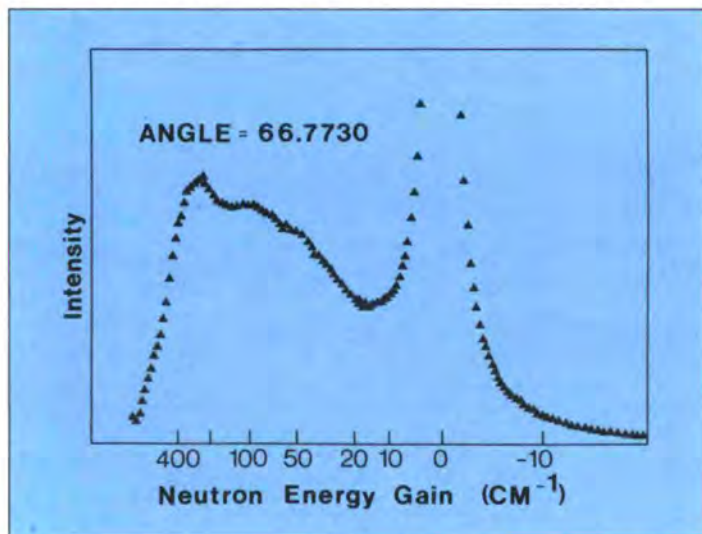


Figure 45: Inelastic scattering spectrum of bovine pancreatic trypsin inhibitor measured on IN6. (J. Smith, S. Cusack, J. Finney. May 1984). Current theoretical research is directed at explaining the form of this curve using models of protein dynamics (with M. Karplus).

Proteins in solution

Tryptophan synthase from *Escherichia coli* is a multi-enzyme complex (MW 143, 430) of two α subunits and two β subunits. Small-angle neutron scattering involving deuterium labelled isomers revealed the quaternary structure of the enzyme at the level of the β_2 subunit and the two structural domains P_1 and P_2 which constitute the α subunits. Within the $\alpha_2\beta_2$ complex, the two α subunits are completely separated. They are situated on opposite sides of the β_2 subunit. The most probable distance between the two α protomers has been measured to be 10.5 ± 1 nm; the nearest distance is 5.8 ± 0.5 nm, and the largest distance is 13.5 ± 0.5 nm. The two domains of the same α subunit are intimately juxtaposed. The distances between two like or unlike domains belonging to opposite α subunits are roughly equal. All domains exhibit about equal distances to the β_2 subunit which is situated in the centre of the complex. Thus the cleft between P_1 and P_2 , which probably contains the active site of the α subunit, makes intimate contact with the β_2 subunit. Neutron scattering allows a determination of the shape of the β_2 subunit within the complex. Comparison with data from the free dimer suggests a conformational change, upon assembly, from an elongated into a more compact form.

Halophilic enzymes function in conditions of extreme salinity and are inactivated in normal ionic environments. This behaviour in different conditions can therefore be used to investigate how proteins adapt to different solvent conditions. Using neutron and X-ray small angle scattering and analytical centrifugation it has been shown that halophilic malate dehydrogenase in 1 to 5 M NaCl behaves as a particle with invariant volume. The proportions of water and salt associated with the protein were determined, and considerable interpenetration of all three components was found to occur (ILL, Weizmann).

Inelastic neutron scattering

The application of inelastic neutron scattering to the study of internal protein dynamics has continued this year with theoretical and experimental advances in work on bovine pancreatic trypsin inhibitor (BPTI). Using the results of a normal mode analysis of BPTI it has been calculated that the incoherent scattering function has a simple dependence on energy transfer and that when resolution broadening and orientational averaging are taken into account this dependence is strongly influenced by the vibrational frequency distribution. Experimentally, data have been collected on BPTI in solution (figure 45) and powder form using IN5 and IN6. Methods of reducing the data and of comparison with the theoretical models are being investigated (ILL, EMBL, Harvard, London).

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

Low Resolution Structures of Biological Complexes studied by Neutron Scattering

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Neutron scattering has been an established technique in solid state physics for some 30 years and in the last ten years has had a significant impact in biological structure determination. This is especially true in the field of low to medium resolution structure, where complementary and competing techniques are electron microscopy, X-ray scattering and the more indirect biophysical techniques such as hydrodynamic measurements. Small angle neutron scattering from solutions of particles and diffraction from ordered or partially ordered arrays of particles has made it possible to examine *in-situ* the distribution of different components of a *biomolecular complex* by substituting D₂O for H₂O in the molecular environment and/or D for H in the complex. Such investigations cannot be performed with other techniques. Several comprehensive reviews on applications of neutron scattering have been published in the last few years^(1,2,3). We propose in this review, after outlining the basis of the method, to show through selected examples how neutron scattering has taken its place alongside X-ray scattering and electron microscopy as a complementary technique for the analysis of biological structures.

METHOD

Contrast

An object may only be visualized through a scattering experiment when its scattering density is different from that of its environment. This concept is in fact very familiar in both light microscopy and electron microscopy where *staining* of specimens is a standard technique. In scattering experiments, the particle may be either in solution (disordered)

or in a hydrated ordered system such as a crystal, membrane or fibre.

For the purposes of low resolution scattering we consider the solvent to be a homogeneous continuum of scattering density ρ_s in which is immersed a particle of scattering density ρ . If we define contrast as $\rho - \rho_s$ it is clear that it can be varied by changing either ρ or ρ_s - the equivalents of +ve and -ve staining respectively in electron microscopy. But how do we do this? The answer lies almost entirely with the difference in scattering power between natural hydrogen (predominantly ¹H) and its heavier isotope ²H (D, deuterium). Thus the scattering density of H₂O is $-0.00562 \times 10^{-12} \text{ cm}/\text{\AA}^3$ whilst that of D₂O is $0.064 \times 10^{-12} \text{ cm}/\text{\AA}^3$ and H₂O/D₂O mixtures are a linear combination of these values. Note that at 8% D₂O, $\rho_s = 0$; an experiment in these conditions will visualise the particle as if it were in a vacuum. As far as the scattering density of a biological macromolecule is concerned, this is also a linear function of the deuterium content of its aqueous environment due to the exchange of its labile hydrogen atoms with those of the solvent. The variation of mean values of ρ for biological molecules and ρ_s for H₂O/D₂O mixtures is plotted as a function of percentage of D₂O in the solvent in Figure 46. This also shows the scattering density of molecules

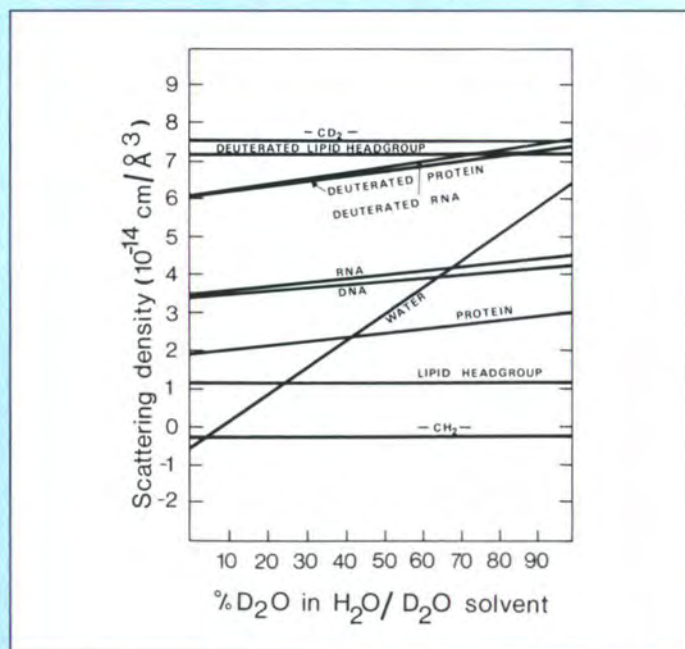


Figure 46: Scattering density of different chemical components of biological complexes as a function of the D₂O/H₂O mixture in which they are immersed. The scattering densities are calculated assuming that all labile hydrogens (i.e. those attached to O or N) do in fact exchange with the solvent except in proteins where a figure of 80% exchange is assumed. Horizontal lines (e.g. -CH₂-) are for compounds having no labile hydrogen.

where covalently bound protons have been exchanged for deuterium.

Changing of contrast by varying ρ_s is straightforward — it requires simply that a solution of particles be exhaustively dialysed against an appropriate D_2O/H_2O mixture. Contrast variation by changing ρ , the scattering density of the particle, can also be carried out by *in vivo* deuteration such that the non-labile hydrogen atoms of a molecule are replaced by deuterium through biosynthetic incorporation, and by chemical labelling.

Scattering and Contrast

As the scattering density of both particle and solvent must be linearly dependent on the deuterium content of the solvent we can write

$$\rho - \rho_s = (\rho - \rho_s)_{H_2O} + X(\rho - \rho_s)_{HD} \quad (i)$$

where the subscript H_2O refers to the structure in H_2O and HD to the scattering density increment in going from H_2O to D_2O . X is the mole fraction of D_2O in the D_2O/H_2O mixed solvent.

The wave scattered due to a molecule of scattering density $\rho(r)$ dissolved in solvent ρ_s is described by

$$F(q) = \sum_j [(\rho(r_j) - \rho_s)v_j \exp i q \cdot r_j] = F_{H_2O}(q) + X F_{HD}(q) \quad (ii)$$

where F is a vector quantity describing the amplitude and phase of the scattered wave (the structure factor) at point q in reciprocal space, from a particle of excess scattering density $\rho(r_j) - \rho_s$ at point r_j with associated volume v_j .

The observed intensity of this scattered wave depends on whether the particles are arranged in a crystal (or partly ordered system) or in solution. The difference between these cases is that in a crystal the scattered waves interact coherently and therefore their amplitudes add, whereas in solution the particles scatter independently and thus the intensities are added.

In the *crystal* case the scattered intensity is given by the square of the structure factor amplitude^(5,6).

$$I(q) = |F(q)|^2 \\ = |F_{H_2O}(q)|^2 + 2X |F_{H_2O}(q)| |F_{HD}(q)| \cos \Phi + X^2 |F_{HD}(q)|^2 \quad (iii)$$

As there is constructive interference, $I(q)$ is zero at all points except for $q =$ reciprocal lattice vector. Φ is the phase difference between F_{HD} and F_{H_2O} . In the case of a centrosymmetrical structure where $\Phi = 0$ or π then

$$I(q) = \left\{ |F_{H_2O}(q)| + X |F_{HD}(q)| \right\}^2 \quad (iv)$$

i.e. the square root of the intensity is linear with contrast.

Thus the amplitude $|F(q)|$ may be measured or calculated for any contrast and if the corresponding phase can be determined then the scattering length density at any point in the particle can be computed by the reverse of equation (ii).

In the *solution* case the measured intensity $I(q) = \langle |F(q)|^2 \rangle$ where $\langle \rangle$ denotes an average over all possible orientations of the particle. The scattering is therefore isotropic and q becomes a scalar quantity

$$I(q) = \langle |F_{H_2O}(q)|^2 + 2X \cos \Phi |F_{H_2O}(q)| |F_{HD}(q)| + X^2 |F_{HD}(q)|^2 \rangle \quad (v)$$

Thus again $I(q)$ is a quadratic function of X .

For a detailed discussion of this interpretation of contrast variation data the reader is referred to various reviews^(1,2,3).

The averaging in (v) means that $F(q)$ cannot be determined directly (except in the special case of a spherical particle). However, at resolutions corresponding to the particle size:

$$I(q) \approx I(0) \exp - q^2 R_g^2 / 3 \quad (vi)$$

$$\text{i.e. } \ln I(q) \approx \ln I(0) - \frac{q^2 R_g^2}{3} \quad (vii)$$

This is the Guinier approximation which is valid in the range $qR_g \leq 1$. Hence from a plot of $\ln I(q)$ v q^2 , $I(0)$ and R_g may be determined. These are two model independent parameters related to the contrast by:

$$I(0) \alpha [\Sigma(\rho(r_j) - \rho_s)v_j]^2 \quad (viii)$$

$$R_g^2 = \frac{\Sigma(\rho(r_j) - \rho_s)v_j r_j^2}{\Sigma(\rho(r_j) - \rho_s)v_j} \quad (ix)$$

(where r_j is the distance from the centre of mass of $\rho(r_j) - \rho_s$). $I(0)$, the intensity at zero angle, is related to the molecular weight and R_g , the radius of gyration, to the shape. The analytical behaviour of $I(0)$ and R_g as a function of contrast has been described in detail⁽⁴⁾.

APPLICATIONS

The utility of deuterium labelling and contrast variation derives from the different contrast behaviour of various components of a biological complex. It is, therefore, convenient to discuss applications of the technique in terms of the type of components forming the complex, e.g. proteins, nucleic acids, lipids... etc. In addition, the contrast may be manipulated in such a way as to highlight interactions between macromolecule and solvent.

Protein-nucleic acid complexes

Protein-nucleic acid interactions form the basis of many of the most important recognition and control systems of the cell. The electron densities of protein and nucleic acid are similar so that X-rays or electron microscopy cannot easily distinguish between the two chemical components. X-ray crystallography has been able to determine certain high resolution features of some complexes such as viruses ⁽⁷⁾ but in these cases inherent disorder has prevented even low resolution information from being obtained about a large part of the structure. Neutron scattering is particularly useful in this context due to the large difference in scattering length densities between the nucleic acid and protein and the technique has been applied successfully to a large number of protein-nucleic acid complexes in solution as well as to single crystals.

The Ribosome

Probably the most extensive neutron scattering studies carried out have been on the structure of the prokaryotic ribosome ⁽⁸⁻¹⁴⁾. The 70S ribosome of *E. Coli* is the site of protein synthesis. It can be simply dissociated into two subunits sedimenting at 30S and 50S. These particles contain respectively 21 and 32 different proteins, whilst the 30S contains one piece of RNA of MW $\sim 0.5 \times 10^6$ and the 50S subunit contains 2 pieces of RNA of $\sim 1.9 \times 10^6$ and 4×10^4 . The determination of the structure of these particles is clearly an enormous problem and one requiring the use of many techniques. In the early 1970's it was proposed that the distances between pairs of individual protein molecules in the ribosome could be measured by neutron scattering studies if pairs of specifically deuterated proteins could be incorporated into the ribosome ^(9,10). This was born the *label triangulation method*. The method has now been applied successfully to both the 30S and 50S subunits ^(11,12). Figure 47 shows a map of the protein positions in the 30S sub-unit. These positions on the whole agree with and complement the position found by immune electron microscopy. In this latter case the technique localises a specific antigenic determinant whereas the neutron measurement gives the position of the centre of mass of the protein.

An important adjunct to the measurement of interprotein distances within the ribosome has been the determination of the shapes of these proteins, especially in view of suggestions that ribosomal proteins are often unusually elongated compared to normal globular proteins. The first method used was to measure the scattering from single isolated proteins in solution ⁽¹³⁾. Contrast variation experiments on the complex between protein S4 (a constituent of the small sub-unit) and a 13S fragment of ribosomal RNA have also been carried out, allowing the radius of gyration of each constituent to be



Figure 47: Superposition of the neutron map on the electron microscopic image of the ribosomal 30S subunit. The contours represent the outline of the subunit as seen by negative staining in the electron microscope. Circled numbers are neutron-located proteins and uncircled numbers the positions of corresponding antigenic determinants as discovered by antibody staining. From ⁽¹¹⁾.

estimated at the match point of the other constituent ⁽¹⁴⁾, and showed the *in situ* radius of gyration of protein and RNA to be the same within error as that found for the free molecules.

Much recent work has been devoted to the measurement of *in situ* protein shapes in ribosomal sub-units by specific deuteration ⁽¹²⁾. In this method ribosomes are grown in various D_2O concentrations, dissociated and the components reassociated such that the average scattering length densities of the protein and RNA are the same whilst the one protein to be investigated is incorporated in its hydrogenated form. The radius of gyration is then measured where the contrast of the RNA/protein matrix is zero to yield direct information on the protein shape. This very elegant technique requires advanced biochemistry for dissociation and specific reconstitution. Most of the *in situ* radii of gyration measured tend to support the view that ribosomal proteins are compact.

Amino-acyl tRNA synthetase interactions with tRNA

Amino-acyl tRNA synthetases are specific enzymes which catalyze the formation of amino-acyl tRNA. This interaction is essential to the process of recognition in which the correct amino-acid is incorporated in the nascent polypeptide chain.

Solution scattering studies of the interactions have centred on the stoichiometry and structural change of the separate components by a monitoring of $I(0)$ and R_g as functions of contrast and tRNA-protein ratio. Such experiments involve a departure from the normal assumption of small angle scattering that we are considering a monodisperse solution of particles. Nevertheless, there are expressions for $I(0)$ and R_g for a mixture of different particles. The distribution of complexes can, therefore, be modelled by using association constants and the value of $I(0)$ and R_g . The analysis is simplified by contrast variation; the interactions being independent of contrast, the model for the particle distribution had to be compatible with contrasts where only protein contributed to $I(0)$ and R_g , and contrasts where tRNA also contributed. Thus protein-protein interactions were easily separated from tRNA-protein interactions. Results include a structural interpretation of anti-cooperativity in the methionyl-tRNA synthetase system of *E. Coli* (15), the measurement of the stoichiometry of tRNA binding in the aspartyl system from yeast (16) (a value which was controversial from biochemical techniques) and defining crystallisation conditions for that enzyme tRNA complex (17). Results clarified for the first time the importance of protein-protein interactions in these systems.

A contrast variation study was also carried out on aspartyl tRNA synthetase-tRNA Asp crystals and has allowed the localisation of the enzyme molecule within this complex in the unit cell (18).

Nucleosome

The nucleosome core particle is the fundamental repeating unit of the chromosome. It consists of two copies each of four basic proteins called histones, complexed with approximately 146 base pairs of linear double-stranded DNA. The protein and DNA each comprise about 50% of the particle weight thus making it an ideal subject for a contrast variation study.

Neutron studies from solutions of core particles were the first to demonstrate unambiguously that the DNA is situated on the outside of a protein core (19,20) and provided the overall dimensions of the particle. Experiments on nucleosomes and core particles at low ionic strength showed a structural transition related to unwinding of the ends of the DNA (21).

Nucleosome core particles were the first complexes to be studied successfully using contrast variation in single crystals (22,23,24). This study allowed the parameters of the DNA superhelix to be determined and the shape of the protein core to be seen. Crystalline aggregates of the histone core had also been studied by electron microscopy and image reconstruction. Figure 48 shows projections of the structure obtained by electron microscopy from the protein and by

neutrons from the nucleosome core particle in 65% D_2O where the DNA does not contribute to the scattering. The remarkable similarity between them shows how the shape of the histone core is unaltered by taking off the DNA.

Viruses

Viruses consist invariably of a protein coat enveloping a DNA or RNA genome which in simple viruses codes for the viral structural proteins and in more complex cases codes also for non-structural processing proteins. Some viruses contain also a lipid envelope which may or may not be derived from the host cell membrane.

Structural studies on viruses have been carried out particularly by electron microscopy. Some simple spherical plant viruses were amongst the first biological complexes crystallised over 50 years ago. X-ray crystallographic techniques however were not sufficiently sophisticated then and the atomic resolution structure of these viruses was not solved until the late 1970's. Now the structures of 3 spherical viruses, Tomato Bushy Stunt Virus (TBSV) (7), Southern Bean Mosaic Virus (SBMV) (25) and Satellite Tobacco Necrosis Virus (STNV) (26) are known but in each case the RNA and varying amounts of the protein are invisible in electron density maps. In the larger spherical viruses the distribution of the various components, protein, lipid and nucleic acid is practically impossible to determine except by the contrast variation technique. The first application of the technique to the

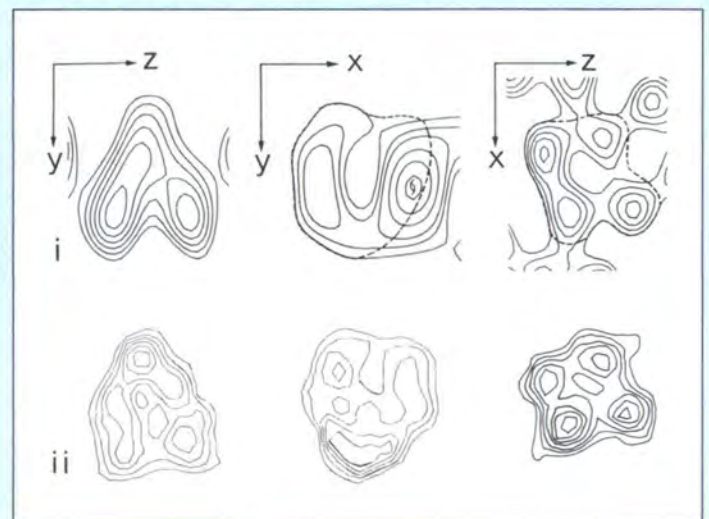


Figure 48: Comparisons of (1) projections of the nucleosome core particle in 65% D_2O buffer, where only the protein is visualised and (2) orthogonal projections of the three-dimensional reconstruction of the histone octamers from electron micrographs of tubular aggregates. The lack of similarity in the central example is due to partial overlap in the crystallographic projection. From (23).

small spherical plant viruses showed the RNA and protein not seen by crystallography (Fig. 49). In TBSV there is a bilobal distribution of protein ⁽²⁷⁾ and a more homogeneous distribution in SBMV ⁽²⁹⁾.

More recently the method has been applied to the much larger animal viruses such as adenovirus ⁽³⁰⁾ and influenza virus ^(31,32). In these cases the particles were originally less well characterised than the smaller plant viruses and such basic parameters as molecular weight were poorly known. Neutron scattering allowed the molecular weight of adenovirus to be determined and determined the radial distribution of DNA and protein in this virus (Fig. 49). In the case of influenza virus, a lipid-containing RNA virus, the molecular weight was redetermined and at the same time the chemical composition, in particular the protein/lipid ratio. The position of the lipid bilayer was also determined rather precisely. The model obtained is also shown in Fig. 49. In Kilham rat virus a bilobal distribution of protein similar to that found in TBSV has been found for empty capsids ⁽³³⁾.

Membranes and membrane components

Diffraction was first observed from biological membranes nearly 50 years ago. Schmitt, Bear and Clark correctly interpreted the diffraction pattern of myelin as being due to a "fluid crystal" of "lipids" ⁽³⁴⁾. Not until the 1960's, however, were membrane lipid structures characterised in detail and low resolution structures and phase diagrams were established for many systems ⁽³⁵⁾. Evidence accumulated for the lipid bilayer as a predominant component of natural membranes ⁽³⁶⁾.

Biological membranes are specialised structures with specific functional roles. They are made up of lipid and protein and other components such as cholesterol. Current thought regards the lipid as a support for the proteins, which are responsible for specific function. Lipid structure is nevertheless important in maintaining the permeability barrier and allowing optimum protein function. Membranes are amphiphilic with hydrophilic faces on either side and a hydrophobic interior. It is generally accepted, although by no means established in all cases, that the lipids are in a bilayer, a structure similar to that of lamellar phases observed in pure lipid-water preparations ^(33,34). In lipid characterization nomenclature, $L\alpha$ phases are liquid crystalline with fluid, disordered acyl chains giving broad diffraction at a spacing of 4.5 Å; the $L\beta$ phases are gel-like with ordered, close-packed acyl chains giving sharp 4.2 Å diffraction. Diffraction from myelin, for example, is similar to that of $L\alpha$ ⁽³⁴⁾. Lipid fluidity is important in membranes such as retinal rod outer segment discs, where function requires the protein to diffuse in the membrane plane ⁽³⁷⁾.

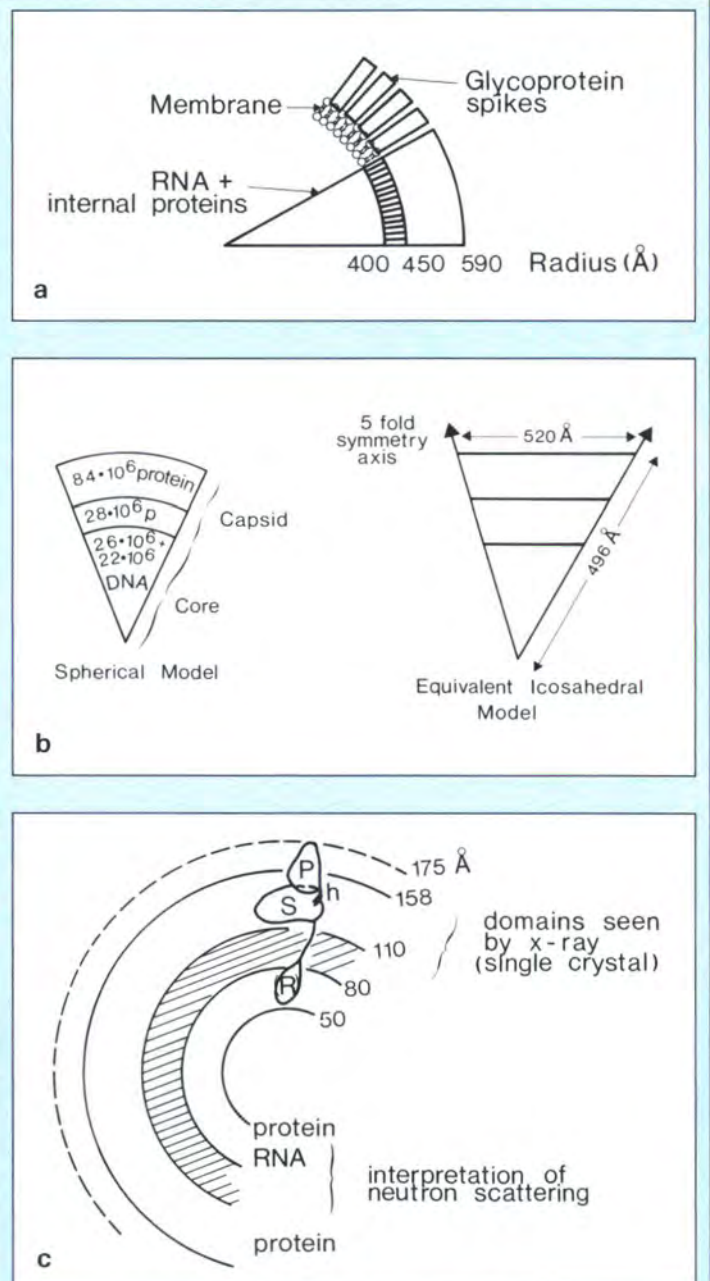


Figure 49: Information derived from small angle neutron scattering on spherical viruses.
 a) TBSV: this shows how the neutron scattering studies complement the high resolution X-ray crystallography in identifying the radial location of the RNA and disordered protein. Reproduced from (28).
 b) Adenovirus: dimensions of the nucleo-protein core and distribution of the protein in two shells of differing density. Reproduced from (30).
 c) Influenza virus: showing the radial location of the lipid bilayer and the absolute amount of protein constituting the spikes. Reproduced from (32).

Until very recently the molecular structure of membrane proteins remained elusive. Studies were limited by crystallographic difficulties (at best one-dimensional order was achieved from membrane stacks⁽³⁸⁾), and the complexity of membrane compositions. Extraction of membrane proteins to measure the most elementary structural information, such as sequence or molecular weight, for multi-subunit complexes, was very difficult because of the inadequacy of biochemical techniques to deal with their hydrophobic nature. Important break-throughs in membrane structure determination have taken place recently: the discovery of naturally crystalline membrane systems (purple membrane⁽³⁹⁾) and the development of detergents which allow extraction of active membrane proteins⁽⁴⁰⁾, and their crystallisation⁽⁴¹⁾.

Neutrons have provided a detailed description of the lipid bilayer, and recent work suggests they are going to be very useful in the study of solubilised membrane proteins and membrane protein crystals. In the case of whole natural membranes, retinal rod outer segment discs have been studied⁽³⁸⁾ and the complex structure of the myelin sheath is currently under study as a model for membrane adhesion (D.L. Worcester and L. Braganza, private communication). The purple membrane of *H. Halobium* might well be the first natural membrane to be described to atomic resolution and neutron diffraction studies have already contributed significantly to different aspects of its structure.

Lipid Bilayers⁽⁴²⁻⁴⁶⁾

The time-averaged structure of lipid molecules in bilayer profiles has been described in great detail by neutron diffraction. The bilayer profile of a specifically deuterated lipid is shown in Fig. 50. Hydration of the headgroups was measured by H₂O: D₂O exchange. The conformations of the two different acyl chains as well as of the headgroup were established by specific chemical deuterium labelling (CD₂ groups replacing CH₂). Experiments were performed in the L_α and L_β phases and for the two common headgroups of biological membranes: phosphatidyl choline and phosphatidyl ethanolamine. Specific labelling and contrast differences have also been used to describe the interaction of lipid water bilayers with cholesterol.

Purple membrane of *H. Halobium*

Purple membrane is naturally crystalline in two dimensions. The structure of bacteriorhodopsin, the only protein it contains, has been solved to 7 Å resolution by electron microscopy⁽³⁹⁾. Its function as a light-activated proton pump has been studied extensively and it was the first membrane protein to be sequenced; the chromophore is one

molecule of retinal bound to a lysine in the protein (reviewed in 47). Considerable complementary structural information on this membrane has been obtained from neutron diffraction (summarised in figure 51). H₂O: D₂O exchange has shown that hydration is predominantly around lipid

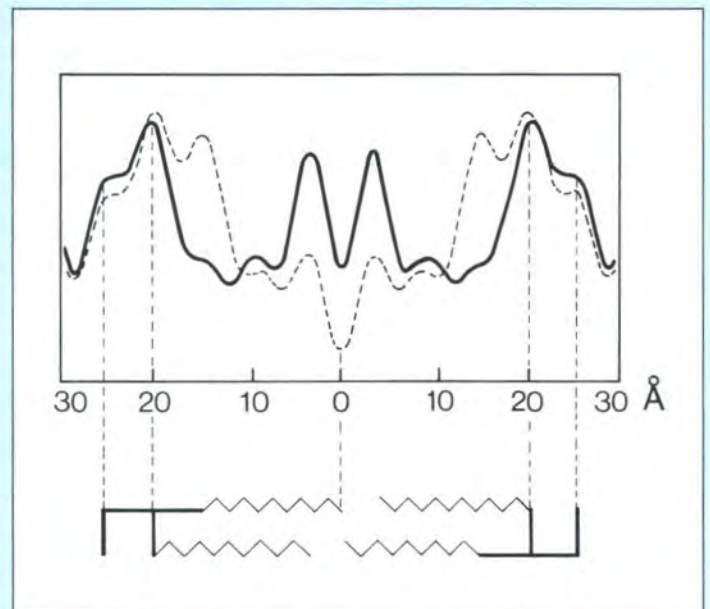


Figure 50: Scattering density profile of a dipalmitoyl phosphatidyl choline (DPPC) lipid bilayer at low water content in the gel phase. The full line is with the $-CH_2-$ at positions 15 in the alkyl chains replaced by $-CD_2-$ and the dotted profile for similar labels in the C.5 positions. Below, the molecule is shown schematically with structural features which have been shown to be common to the liquid crystalline and gel phases: headgroup parallel to the plane of the membrane and non-equivalent chains.

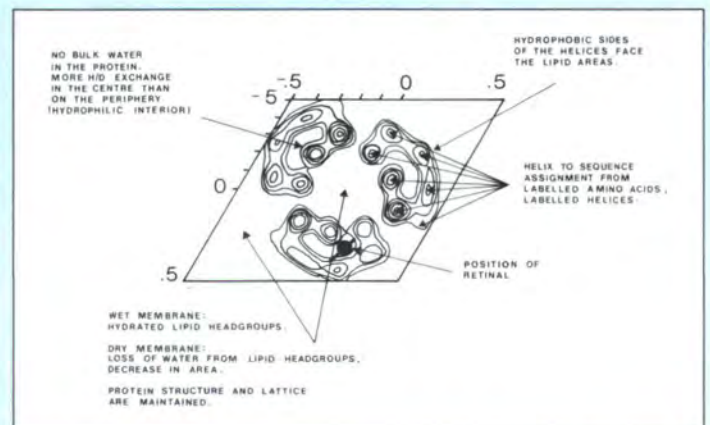


Figure 51: A unit cell of purple membrane showing the information derived from neutron diffraction experiments. The contoured area represents three symmetry-related molecules each comprising seven alpha helices and the intervening space is filled with lipids.

headgroups and that the protein does not have bulk water associated with it (48,49). This was an important result, excluding partial pores of bulk water in the proton pathway of the pump, or aqueous clefts either within a protein molecule or in between different protein molecules in the trimer.

In a neutron diffraction approach to a higher resolution structure, based on the low resolution structure and the sequence, specifically deuterated amino acids were incorporated in the structure by biosynthesis to act as labels (50). Diffraction experiments on these samples suggested that the protein α -helices are embedded in the bilayer with their hydrophobic faces towards the centre of the molecule away from the lipid. Sequence to helix assignments have also been suggested from these data (51). The position and orientation of the retinal in the projection has been determined by using a sample where deuterated retinal was incorporated biosynthetically into the membrane (52).

Solubilised proteins and membrane protein crystals

To successfully separate the radii of gyration of two components of a complex by contrast variation it is not sufficient that the mean scattering density of one of the components match the solvent, it should also be homogeneous to the resolution required. This is particularly problematic in the case of lipids or detergents where the scattering density of the headgroup and hydrocarbon chain may be very different and spatially separated. The difficulty may, however, be overcome by partial deuteration and was achieved in a very detailed study of rhodopsin micelle complexes in which the radius of gyration of rhodopsin was measured and the geometry of its interaction with the detergent was determined (53).

The *in-situ* molecular weight of membrane proteins is often a difficult parameter to determine, and the number of subunits in several membrane proteins remains controversial (54). Provided a pure system can be solubilised in detergent or lipid, a small angle neutron scattering experiment with contrast variation provides a straightforward molecular weight determination of the system in the given conditions. If the radius of gyration is not required with precision, the other component (detergent, lipid) need not be homogeneous in scattering density. The method was applied successfully to the ATP/ADP transport protein solubilised in excess detergent (55) and approaches using deuterated lipids are now under development.

Contrast variation is also applied in low resolution studies of membrane protein detergent crystalline complexes.

Preliminary neutron results are available from matrix porin crystals (M. Zulauf, P. A. Timmins, M. Garavito, private communication).

Solvent microenvironment of a macromolecule

The structure of a macromolecule in solution is determined in part by its interactions with solvent molecules, which in turn are perturbed by the macromolecule and may be structurally different from the bulk. A general model for a macromolecule in solution is a volume V_p containing the atoms of the macromolecule, a volume V' of perturbed solvent, and the whole surrounded by bulk solvent (Fig. 52). The dissolved *particle* measured in a solution scattering experiment is not the macromolecule alone in V_p , but the entire volume of composition different from bulk solvent, i.e. ($V_p + V'$). The microenvironment, V' , of a biological macromolecule could be very important in its functional interactions, yet there are very few experimental techniques available for its characterisation. Through the contrast variation approach, neutron scattering experiments from solution have been successful in separating the structure of a macromolecule from that of the perturbed solvent around it.

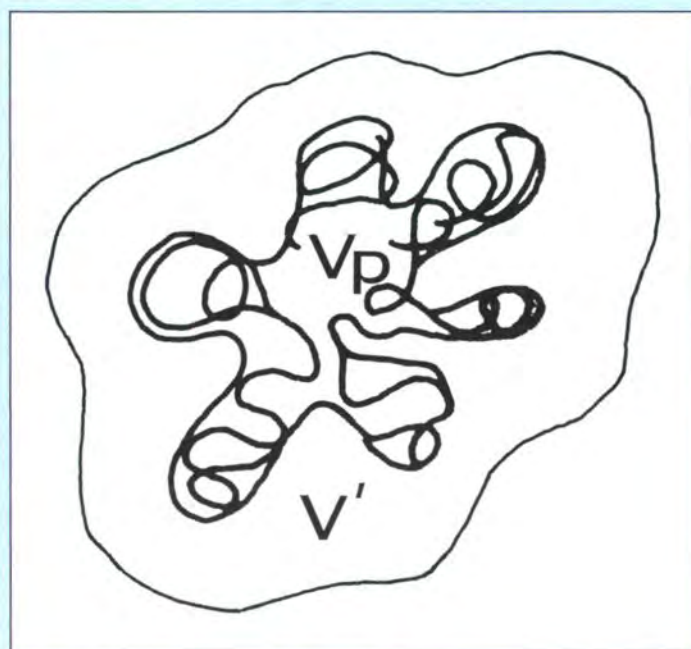


Figure 52: Schematic representation of the hydrated particle. V_p contains the atoms of the macromolecule, V' is a volume of perturbed solvent and outside this is the bulk solvent.

Transfer RNA, the case of polyelectrolytes

Charged macromolecules in solution have partial specific volumes which are functions of the salt composition of the solvent. This reflects volume differences in V' between the different conditions. Many cations, for example, have negative, partial specific volumes (electrostriction). It has been shown that, in an $H_2O:D_2O$ contrast variation experiment, a volume of dense solvent can be observed around the tRNA⁽⁵⁶⁾; and its composition and radius of gyration were measured for different conditions. This was interpreted in terms of the Donnan equilibrium in which salt is excluded from the immediate vicinity of the macromolecule with an accumulation of positive counter ions. Electrostriction due to these counter ions gives rise to the effective high solvent density observed. The method of neutron contrast variation between tRNA and its immediate environment should be generally applicable to charged macromolecules.

Hydration around proteins, a water volume excluding other solutes

A hydration shell around a macromolecule which excludes other small solutes can be measured directly by neutron small angle scattering if its contrast is different from that of the bulk solvent. In experiments on ribonuclease A, the hydration shell was investigated for glycerol and alcohol aqueous solvents⁽⁵⁷⁾. Experiments were done in D_2O and the contrast was changed by varying the concentration of deuterated glycerol $C_3H_5(OD)_3$ and ethanol $C_2H_5(OD)$. This approach has the great advantage that there is no H-D exchange of labile H during the series of experiments. A hydration shell corresponding to 0.2 g of water per g of protein was observed to exclude glycerol but no hydration shell was observed in the alcohol case, i.e. the protein surface is equally accessible to alcohol and water, but "repels" glycerol.

CONCLUSION

In this review we have attempted to point out some of the major contributions of neutron scattering to the field of molecular biology. We have been highly selective in our choice of examples and many important contributions have not been mentioned as our aim was to give an illustrative rather than an exhaustive review. Neutrons have been very useful, for example, for rapid measurements of molecular weight and radius of gyration of macromolecules in solution. These most elementary parameters are often not known and are difficult to measure by other techniques. Neutron scattering with a very small amount of sample (< 1 mg) in any buffer is a non-destructive technique which can provide a very

rapid characterisation. Moreover, the existence of "user" facilities can make such measurements rather efficient by enabling them to be carried out in a time-sharing context. We have considered only the *structural* aspects of molecular biology, although inelastic neutron scattering is now taking its first faltering steps into the investigation of the dynamics of biological macromolecules and their environment^(58,59). The next few years should clarify the usefulness of neutrons in this domain.

We have also omitted mention of high resolution neutron crystallography which has also provided many exciting results⁽⁶⁰⁾.

The growth of neutron small angle scattering can be traced to both a combination of biochemical advances and progress in neutron technology — particularly the development of high flux reactors, cold neutron beams and multi-detectors. Further progress will most probably depend more on advanced biochemistry. Specific deuteration has still not been fully exploited, partly due to the important investment in sample preparation. Advances in genetic engineering should allow pure molecules and complexes to be produced in the milligram quantities necessary for direct structural techniques rather than the micrograms or nanograms used for many functional characterisations.

Neutron scattering is, we should remember, a non-destructive technique and also one which is amenable to many different kinds of sample environment through the possibility of having strong, transparent sample containers. We can therefore look forwards to manipulations of thermo-dynamic parameters such as pressure or temperature. A few high pressure experiments have already been carried out (D.L. Worcester, L. Braganza, B. Schoot, G. Zaccai, private communication). With the use of low temperature techniques we can hope to map reaction intermediates and investigate (frozen-in) transitory conformations.

The future looks promising and although many experiments can and will be done with medium flux sources with appropriate instrumentation, a high flux of cold neutrons will always be necessary both for the more exciting and spectacular advances and for the more prosaic reason that large amounts of active biological material will probably remain very difficult to obtain.

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COLLEGE 9 CHEMISTRY

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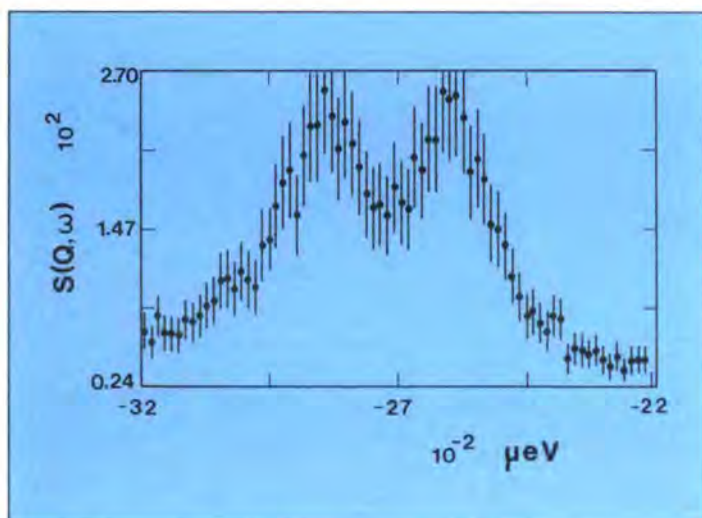


Figure 53: Tunnelling spectrum of toluene (4 K) showing the presence of two inequivalent methyl groups.

GENERAL SUMMARY

Individual experiments involving College 9 increasingly gather information from several instruments at the ILL, and often entail complementary evidence from non-neutron techniques. This tendency reflects the importance now placed on the characterisation of subsidiary spectral features, or subtle spectral changes, which frequently require supplementary studies before a meaningful interpretation can be attempted.

Instruments, sample environments and data treatment have, in general, been optimised to accommodate more elaborate experiments and more rigorous analyses. For example, it has recently been demonstrated where data are collected alternately in two external memories (e.g. IN4, IN5, IN6), a synchronisation of an external perturbation to the sample with memory-switching permits a rather precise comparison of spectra with and without the sample-perturbation. This technique promises to have some interesting applications.

SCIENTIFIC HIGHLIGHTS AND TRENDS IN 1984

Tunnelling and Librational Motions

The investigation of tunnelling transitions by neutron scattering has developed into a valuable spectroscopic technique and is increasingly used to probe the potential environment and interactions of molecular and ionic species. For example, the crystal-structure of toluene at 6 K is thought to involve two inequivalent methyl groups. These groups are comparatively free to rotate, and at low temperatures rotational tunnelling of the methyl groups is to be expected. A recent experiment (Bordeaux, ILL) using the energy offset facility of IN10, reveals two tunnelling features at 25.5 and 28.5 μeV (Fig. 53), demonstrating the motions of two inequivalent methyl groups.

A similar situation has also been encountered for ammonia-ligand tunnelling in $\text{Ni}(\text{NH}_3)_6\text{I}_2$ (ILL). Tunnelling of the NH_3 entities within the molecular octahedral hexamine species has been recorded using IN5 (Fig. 54) and is comprised of 3 peaks. This pattern of peaks suggests that the Ni atoms have molecular C_{3i} symmetry, invoking three inequivalent pairs of NH_3 ligands. The differing intensities of the tunnelling peaks may originate from coupling of the proximate NH_3 species. The analogous $\text{Ni}(\text{NH}_3)_6(\text{PF}_6)_2$ derivative shows a surprisingly large tunnel-splitting (Fig. 55), and both the intensities and the breadths of the tunnelling features may speculatively be attributed to coupling effects. In both of these hexamine derivatives, the tunnelling has been shown to persist, little

changed, as the temperature is increased to *ca.* 25 K, whereupon a structural phase transition leads to the spontaneous collapse of the tunnelling spectra into quasielastic components.

The tunnelling spectrum of the ammonium ion in NH_4PF_6 (ILL) was recorded using IN10 at high resolution, and represents the first example of tunnelling of a molecular tetrahedral species under C_2 rotational symmetry. This structural information was then included with other evidence and enabled the crystal structure of the low-temperature phase of NH_4PF_6 to be determined directly from powder neutron-diffraction data. It is interesting to note that whilst the observed splittings are in good agreement with the predicted energy-level scheme, the intensities are at variance with those predicted. Coupling effects can be excluded in this case as the ammonium ions are well separated, and at present the origin of the various tunnelling-peak intensities in NH_4PF_6 is unclear.

The torsional levels and ground-state tunnel-splitting of the methyl group in CH_3NO_2 (Bordeaux, NBS, ILL), as a function of pressure have been investigated using IN4 and IN10, respectively. Unexpectedly, this investigation found that the torsional levels decrease with increasing pressure whilst the tunnel-splitting increases, this being the reverse of all previously observed pressure dependencies. A potential which reproduces this effect has been found and is illustrated in Figure 56. The origin of the anomaly has been attributed to a repulsive component in the pair potential.

Vibrational Spectroscopy

The advent of the new IN1 BeF has greatly improved the potential of this instrument for the study of high-energy excitations in a wide variety of materials. The increased flux and absence

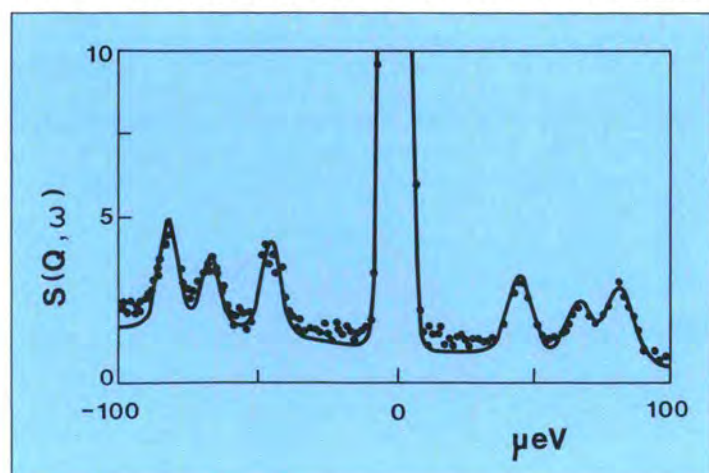


Figure 54: Tunnelling of inequivalent ammonia ligands in $\text{Ni}(\text{NH}_3)_6\text{I}_2$.

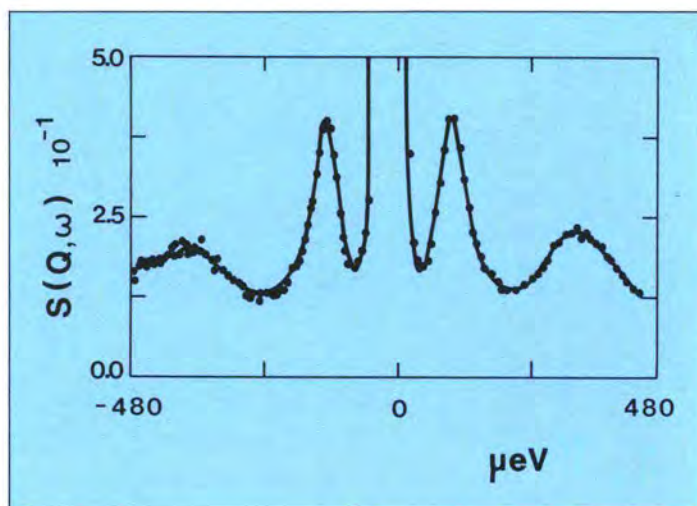


Figure 55: Unusually high tunnel-splitting in $\text{Ni}(\text{NH}_3)_6(\text{PF}_6)_2$ showing broad tunnelling features.

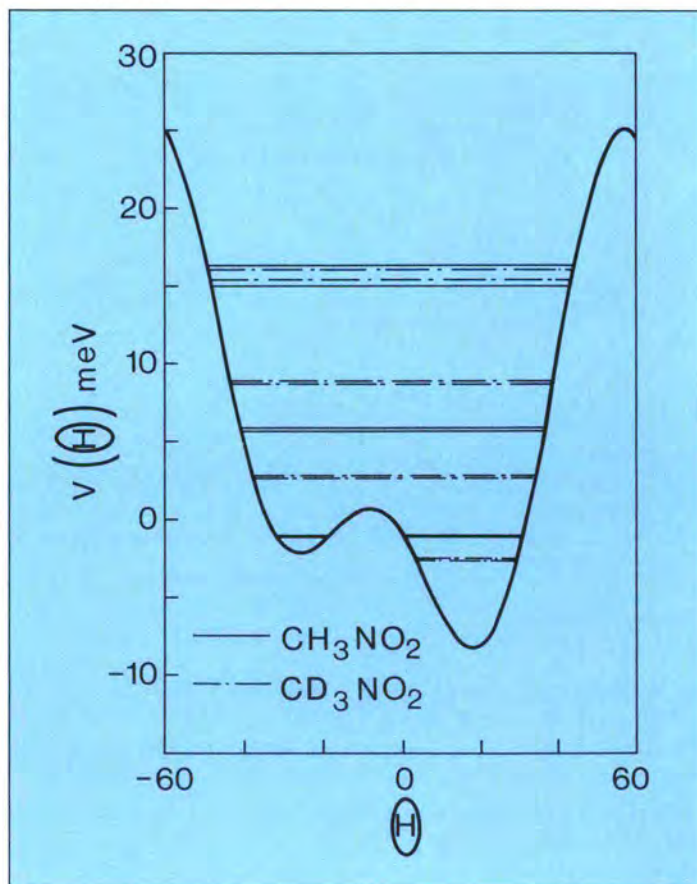


Figure 56: Illustration of the potential capable of reproducing the pressure dependence of torsional levels and ground-state tunnel-splitting in nitromethane.

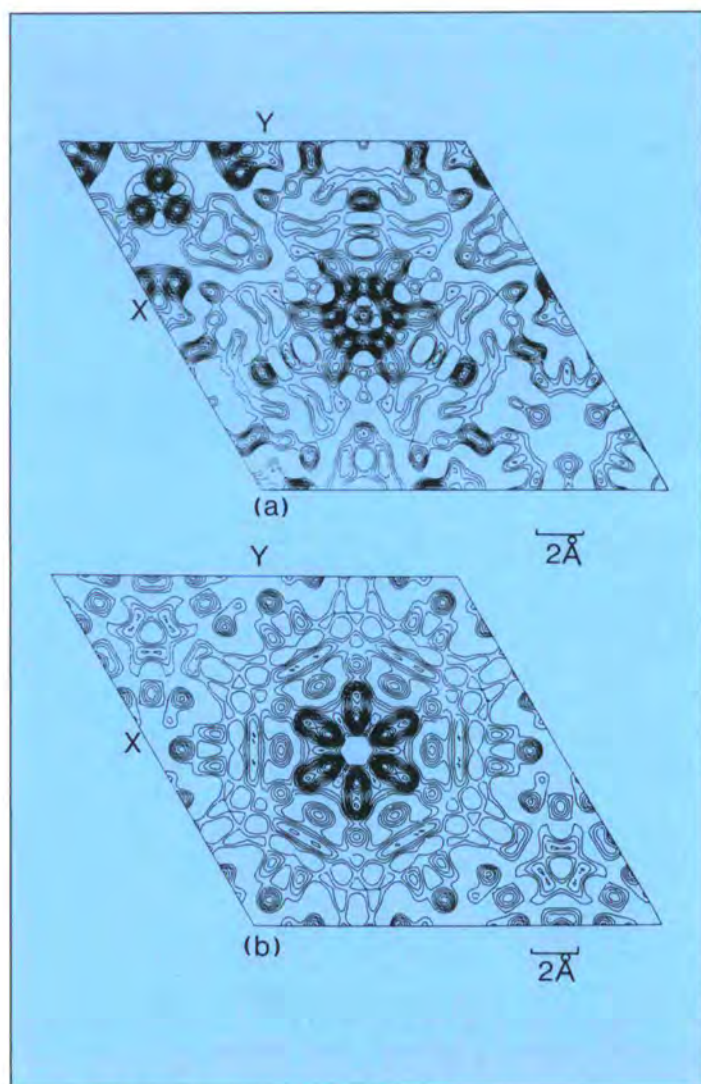


Figure 57: Fourier difference map showing the most readily occupied benzene-site in Y-zeolite (a).
Fourier difference map showing the less favoured "window-site" for benzene in Y-zeolite (b).

of background structure have enabled not only the study of smaller effective specimens, such as H_2 adsorbed in alkali-metal/graphite intercalates (ILL, Oxford), but also permitted the use of a high-resolution graphite filter as required.

The value of peak intensities, along with isotopic substitution and optical spectra, has proved useful in many experiments. In particular, the rather complex vibrational spectra of $UO_2HPO_4 \cdot 4H_2O$ (HUP) which contains a variety of aquo-species, has provided clear evidence of both H_3O^+ and

$H_5O_2^+$ ions (ILL), in agreement with the neutron diffraction data, and gave some insight into the form of the $H_5O_2^+$ ion vibrations.

A normal-coordinate treatment of the vibrational-frequency and structural data of the $H_5O_2^+$ ion in HUP shows there to be considerable mixing of the vibrations of terminal H_2O units when the formal $H_5O_2^+$ molecular mode contains a significant component parallel to the bridging structure. In contrast, other modes of this ion are well described as slight perturbations of internal and external modes of lattice water.

Replacement of the acidic cation in HUP by NH_4^+ ions leads to the formation of $UO_2NH_4PO_4 \cdot 3H_2O$ (AmHUP). The identity of the resulting "amine" species has been the subject of some discussion, diffraction studies seeming to imply the presence of discrete NH_3 molecules and H_3O^+ ions, rather than the expected NH_4^+ ion. A comparison of the IN1(BeF) spectra of HUP and AmHUP alongside a careful examination of the infrared spectrum enables positive identification of an ammonium ion, notwithstanding the presence of broad overlapping features in all spectra.

Zeolites

Powder neutron diffraction (PND) has been shown to be a successful technique for investigating both the framework structures and cation distributions found in zeolites. More recently, this technique has been shown to be applicable not only to the zeolite framework, but also to the localization of organic molecules adsorbed into the cavities of zeolites (Lyon, ILL). PND studies on a Y-zeolite, containing adsorbed benzene at two different concentrations, revealed the presence of two distinct benzene-sites in the cavities of the zeolite. At low coverage the benzene molecules are bound to the cations and located mainly in supercages, as illustrated by the Fourier map (Fig. 57 a). As the coverage is increased, van der Waals forces allow more of the benzene molecules to occupy less favourable "window-sites" formed between adjoining supercages (Fig. 57 b). The clustering of benzene molecules, observed by small-angle scattering, can be modelled on the basis of these two sites.

Physisorption

The behaviour of rare gases on *graphite* has been studied in the last year with different aims.

Deuterium has been adsorbed (Mainz, ILL) to study the peculiar transition between the commensurate ($\sqrt{3} \times \sqrt{3}$ -superstructure) and the incommensurate phase. There might be a

new phase between these phases, which melts around 7 K according to heat capacity measurements. This is now confirmed by neutron diffraction. In addition the melting of a second adsorbed layer on top of the solid first one has been observed. By melting the second layer the distortion of the first layer disappears, thus the crystallisation of the second layer influences the structure of the first one.

A solid-solid coexistence region in the monolayer of *Neon* on graphite has been shown by adsorption-isotherm work.

Unusual behaviour of the film could also be studied in the same region of the phase diagram using neutron diffraction (ILL, Mainz). However, a simple explanation of the phenomena has yet to be achieved. A wetting transition was observed with three adsorbed Ne-layers but it disappeared again after careful annealing.

The diffraction from *Argon* submonolayers (Kiel, Duisburg, ILL) to higher scattering angles and the first three 2-dimensional Bragg reflections have been studied as a function of temperature until the 2-dimensional liquid structure factor showed up. A slight distortion of the regular triangular lattice could be seen during the melting process, which might be connected to a small singularity in heat capacity measurements. This indicates a small first-order component of a higher-order transition.

The adsorption on *MgO*-(100) surfaces raises increasing interest. The study of CD_4 on *MgO* (Marseille) showed a commensurate $c(2 \times 2)$ superstructure for both the monolayer and the bilayer. However, the commensurate monolayer seems to melt with a first order transition for $T \geq 82$ K into a fluid phase.

Matrix Isolation Spectroscopy

Inelastic neutron scattering techniques have been applied to matrix isolated molecules only comparatively recently. To this end, a new technique has been developed in which it is possible to condense gas mixtures rapidly to form large solid samples in the interior of standard ILL cryostats. This approach has successfully permitted sufficient concentrations of impurity molecules to be trapped in the inert gas matrix; notwithstanding the insolubility of the impurity under equilibrium conditions.

Recent applications of this technique include the study of H_2 and H_2O rotations in argon (ILL), intermolecular vibrations and librations of CH_3CN in argon (Siegen, ILL) and intramolecular modes of hydrocarbons in argon (Durham, RAL, ILL).

Quasielastic scattering

Quasielastic scattering continues to play a major role in the investigation of the college. Extensive data-treatment and

analysis facilities have been developed to enable the separation of the more complex motions which are now being studied by this technique.

From quasielastic neutron scattering experiments performed in the rotator phase of n-alkanes (C_nH_{2n+2}), as a function of both n and temperature, two types of rotational diffusion have been detected (Orsay, ILL). The type B corresponds to a uniform rotational diffusion whereas the type A corresponds to a hindered rotation, probably limited to large amplitude oscillations. It is the first time that the type A rotational diffusion, given by the orthorhombic symmetry phase R1, has been observed. On increasing the temperature, this rapidly evolves towards the type B diffusion. Correlation times, which seem to be independent of the phase-type, are of the order of 5×10^{-12} s.

Quasielastic neutron scattering and heat capacity measurements, over a variety of temperatures, have been used to determine that the NH_3 groups in crystalline sulphamic acid undergo $2/3$ jumps (Paris, ILL). The values of the activation energy and residence time calculated from these data are in good agreement with those derived from NMR and Raman spectroscopies. The potential barriers from molecular interactions, estimated from atom-atom potentials, suggest that the dominant terms arise from hydrogen bonding.

IN13 has proved to be a useful asset in the study of short range motions, such as the proton dynamics in carboxylic acid dimers (Zürich, Würenlingen, ILL). NMR and infrared spectral interpretations of these dimers do not concur in explaining the disordered structure observed in such systems, the former technique suggesting a mechanism involving proton exchange between the acid groupings, whilst the latter favours a rotational mechanism. The jump distances involved in these two processes are quite different, 0.7 and 2.23 Å, respectively, and an examination of the quasi-elastic scattering from ring deuterated terephthalic acid was undertaken, using IN13, to elucidate which of the two mechanisms occurs. The observed and calculated quasielastic contributions have been compared, and it is clear that the rotational mechanism can be excluded.

An important experimental success has been achieved with the polarization analysis technique on the diffuse TOF scattering facility, D7, by separating coherent and incoherent scattering. It is only after this separation that reliable information on the elastic incoherent structure factor of C_2Cl_6 in its plastic phase (Tübingen, ILL) can be obtained.

Soap Films

For the first time and by use of a special beam arrangement, neutrons were scattered from a black soap film (Oxford). The film was drawn from a solution of normal (protonated) surfactant molecules and electrolyte in D_2O . Fig. 59 shows the change in neutron reflectivity as the film drains from a thickness of about 1000 \AA to about 50 \AA . The reflectivity profile at glancing angles, Fig. 60, is then related to the structure of the D_2O part of the film ("aqueous core"). The film obtained after about 40 min was found to contain a $16 \pm 4 \text{ \AA}$ thick D_2O layer. The overall film-thickness was $50\text{-}60 \text{ \AA}$ and the neutron result is therefore a direct confirmation of the sandwich structure of such films.

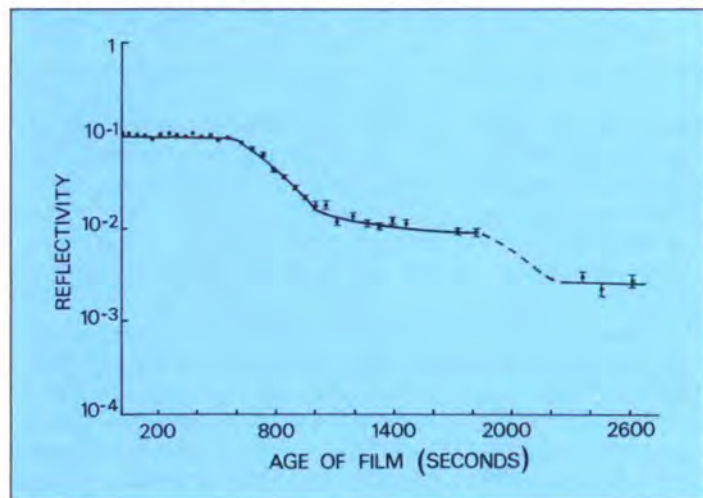


Figure 59: Reflectivity of thinning soap film at $2\theta = 0.044$ radians. (Oxford).

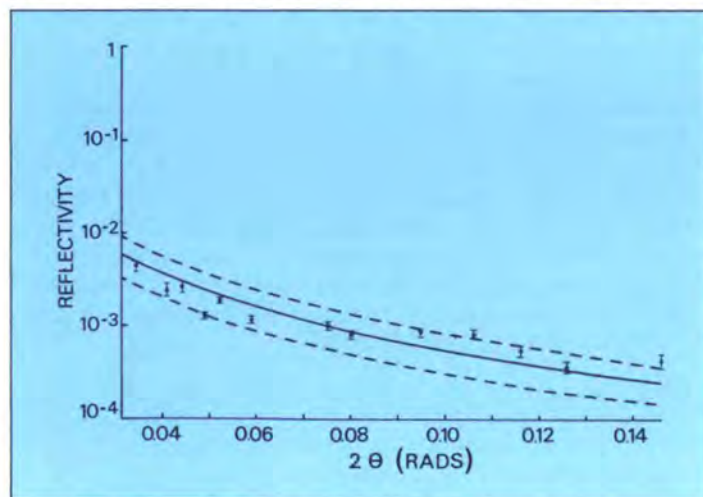


Figure 60: Measured reflectivity of a black soap film ($\lambda = 12 \text{ \AA}$) and calculations for slab profile of D_2O . Dashed lines are calculated for thicknesses of 12 and 20 \AA . (Oxford).

Microemulsions

Quasielastic studies have also been used to study the hydrodynamic motion of particles in dispersions of concentrated systems (Bristol). In microemulsion studies, a fast lateral motion of the surface active agent molecules around the surface has been observed. It has also been found that in "oil in water" microemulsions the diffusion coefficient of the oil molecules is comparable to that of the bulk liquid. In the case of "water in oil" microemulsions on the other hand, it was found that the diffusion coefficient of the water core was much smaller than in bulk water; this effect was attributed to the high concentration of counter-ions.

Colloids

An elegant small angle scattering experiment (Oklahoma, ILL) has been performed with polystyrene latex particles dissolved in D_2O (10 wt % sample). Different shear-rates were adjusted with a Couette flow shear-cell and lead to different amounts of order of the system. With zero shear a face-centred cubic structure of the colloids forms and a very small shear leads to an oriented arrangement (Fig. 61.a) without noticeable distortions. Relatively modest shear-rates ($s = 30 \text{ sec}^{-1}$) suffice for a marked slipping of (111) planes along the direction of velocity \vec{v} (Fig. 61.b). At a gradient of $s = 160 \text{ sec}^{-1}$ the long-range order is lost, but the same short-range order remains (Fig. 61.c). A further increase of the shear gradient to $s = 300 \text{ sec}^{-1}$, finally leads to a largely amorphous character of the structure.

Obviously, the application of external fields like shear-gradients greatly improves the sensitivity to detailed features of colloidal systems, e.g. like short-range order. In another case (cetylpyridiniumsalicylate) the alignment of anisotropic micelles in a magnetic field was observed as well as the re-establishment of disorder in a real-time experiment (Bayreuth). Several other interesting investigations comprise (1) a study of the internal structure of micelle (Paris, Strassburg) (SDS = sodium-dodecylsulfonate), (2) the micellation of copolymer molecules (Strassburg, ILL), particularly the disappearance of structure with increasing temperature, (3) indication of correlations of casein micelles from cow's milk (Reading).

Polymers

Innovative work in the general field of polymers continues. An example, in case is the material studies of the small-angle scattering from rubber under tension which have revealed the presence of quite long relaxation-times. The separation of coherent and spin-incoherent scattering by polarisation analysis on the diffuse time-of-flight spectrometer D7 has now also been applied to polymers. The samples studied comprise

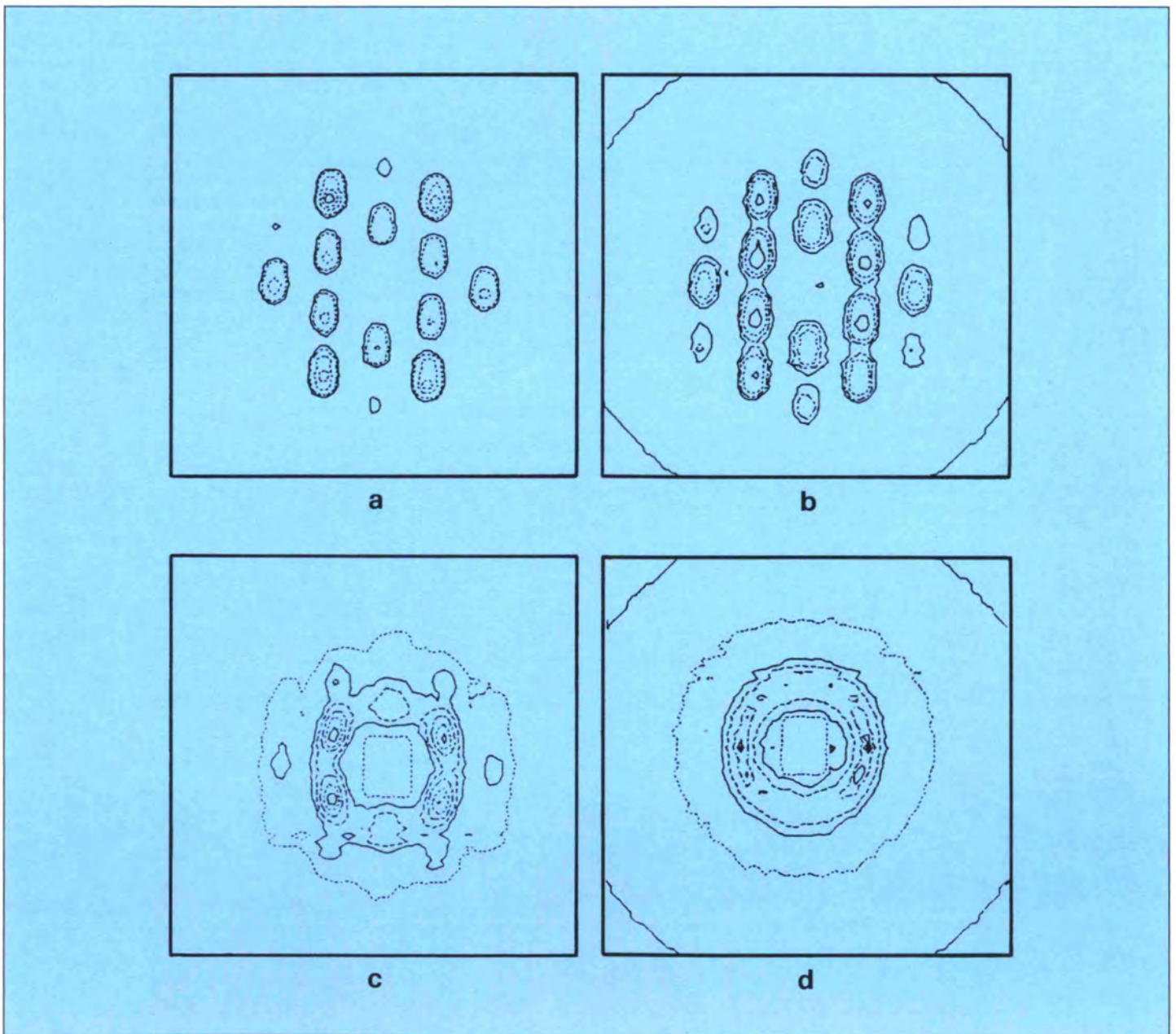


Figure 61: Small angle scattering of 0.105 μm diameter polystyrene latex particles in D_2O (highly deionized suspensions) at different shear rates; (a) $s=0$, (b) $s=30$, (c) $s=160$, (d) $s=400$ (all in sec^{-1}). (Oklahoma, ILL).

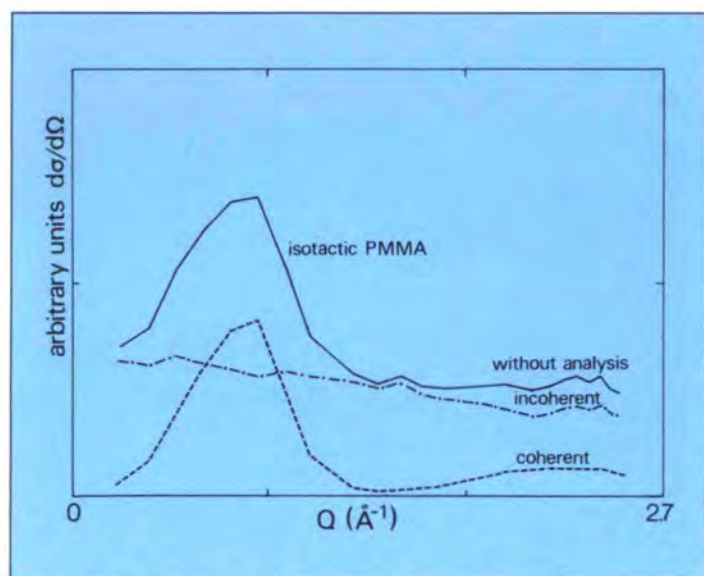


Figure 62: Fully deuterated isotactic PMMA measured without polarisation analysis (solid line) and the separated coherent (dashed line) and spin-incoherent (dot-dashed) contributions.

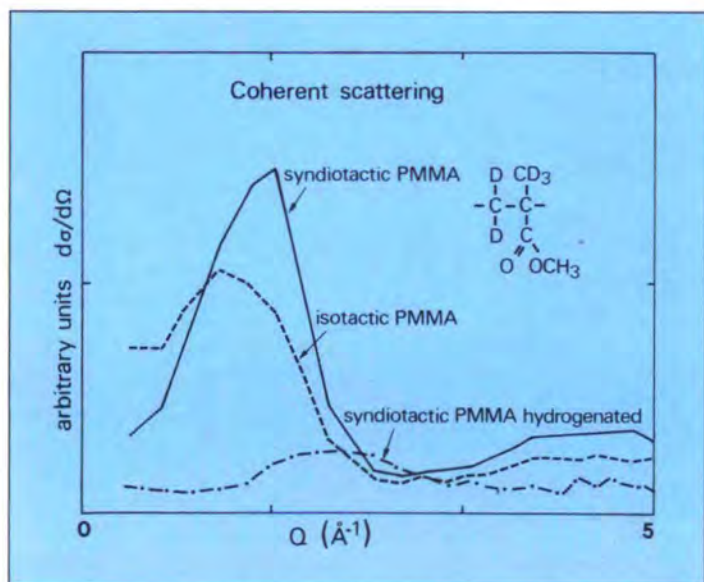


Figure 63: Coherent scattering from fully deuterated (i) syndiotactic PMMA (solid line) and (ii) isotactic PMMA (dashed line) as well as (iii) hydrogenated syndiotactic PMMA (dot-dashed line).

deuterated isotactic and syndiotactic polymethylmetacrylate (PMMA), polyvinylmethyl ether and polydimethyl siloxane (London, ILL) as well as isotactic polystyrene with various degrees of deuteration dissolved in CS_2 (ILL, Strassburg). Fig. 62 compares the spectrum of deuterated isotactic PMMA measured without polarisation analysis with the separated contributions. In particular, the coherent scattering shows a structure which would otherwise not have been visible. In Fig. 63, the coherent scattering of fully deuterated syndiotactic and isotactic PMMA has been isolated and is contrasted with that of fully-hydrogenated syndiotactic PMMA. In the latter case, the coherent contribution normally is neglected, when, for example, analysing the elastic incoherent structure factor. The separation and consequently rather detailed information is obtained when combining TOF and polarisation analysis.

Seminars

College seminars have again been organised on an approximately fortnightly basis and have covered a diverse range of topics. Invited speakers include: D. Schaefer (Albuquerque), J. Sauvajol (Lille), J. Besenhard (Munich), H. Jobic (Lyon), A. Vrij (Rijksuniversiteit Utrecht), Trommsdorf (Grenoble), S. Pawley (Edinburg), S. Trevino (NBS), G. Huggins (Stuttgart), J. Rundgren (Stockholm), R. Thomas (Oxford), K. Usha-Deniz (Bombay), A. Gukasov (Stalingrad), K. Hahn (BASF, Ludwigshafen), J.N. Israelachvili (Canberra, Australia), P. Lindner (ILL), L.J. Magid (University of Tennessee, USA), Micheron (Thomson-CSF, Orsay), A. Rennie (Universität Mainz), M. Stamm (KFK Jülich).

Edited by: G. Kearley/W. Press

Single particle rotations of molecules: Progress and complications

A large part of the College 9 activity is centred on incoherent neutron scattering and there, in particular, on the rotational motion of molecules in a great variety of solids. For several years already, the data are rather successfully analysed in terms of simple models based on single molecule rotations. "Single molecule", this means that rotational jumps or rotational diffusion as well as rotational tunneling and free rotation of a single particle are considered. In this context, the surrounding of the molecule is reflected as a static orientation dependent potential, to which a fluctuating contribution has to be added at high temperatures. The purely elastic scattering (EISF = elastic incoherent structure factor) yields information on the geometry of the motion, the quasielastic scattering (high temperatures) on the time scale on which the motion occurs and the inelastic scattering about librations in the static potential as well as about the overlap of wavefunctions in neighbouring potential wells (low temperatures).

Precise information depends on a careful data treatment and there, in particular, on corrections for multiple scattering and for the experimental resolution. While these corrections can be handled rather routinely, now — there is an additional question concerning the quality of the data, namely coherent contributions to the incoherent scattering. Progress is being achieved there as well: 2/3 of the incoherent scattering involve a spin-flip of the scattered neutrons. Polarised neutrons allow to measure the spin-flip scattering and the non-spin-flip scattering separately and thus allow the isolation of the incoherent part of the scattering. This is being done on the spectrometer D7 for about two years now and in certain cases (C_2Cl_6 , polymers) already has yielded more reliable information.

Complications mainly concerns the model employed. The jump motion of molecules between several equivalent orientations, for example, have been simulated on the computer (NH_4Cl). It turns out that the molecules indeed pass the low part of the potential barrier, but with the kinetic energy acquired, a second or third jump are likely to follow immediately. Now two 90° jumps of a tetrahedron at a site with cubic symmetry add up to a 120° jump, if two different rotational axes are involved and thus an analysis in terms of single jumps is bound to provide a distorted picture. Another complication — and models are only about to deal with this aspect — concerns the coupling of the rotational motion of a molecule with other degrees of freedom. Examples are the translational or vibrational motion of the molecule itself or the rotational motion of neighbouring molecules or molecular groups. The latter aspect is very clearly seen at low temperatures: Tunneling spectra of certain systems (Li-acetate,

Mn-acetate, CH_4) no longer can be understood strictly in terms of single particle motions. Instead a Hamiltonian involving the kinetic energy and the potential energy of (e.g.) two molecules *and* an interaction energy must be considered, giving rise to more complex energy level schemes. One might say — in a simplified view — that the rotational potential of a given molecule depends on the rotational states of one and more neighbours. Clearly the effect will be strong, if there are rather dramatic changes in the shape of the wave function involved.

While in the latter case the interpretation obviously fails with the neglect of an interaction term, the diffusive rotational motion still can be analysed in terms of the conventional models. Of course, there may be model parameters which in an obscure way absorb details of the more complex motion. But then, these complications only reflect the progress of the field.

2

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INSTRUMENT OPERATION DEPARTMENT



2

Introduction

The Instrument Operation Department has overall responsibility for the operation and improvement of all the scientific instruments for experiments around the reactor and in the neutron guide hall. This also involves all the technical assistance to guest scientists during their experiments. There is now general satisfaction with the results of the reorganisation implemented last year: in addition to the five instrument groups, there are the Central Group (providing a link for the physicists with the general services and the Reactor Department), the Sample Environment Group (standard cryogenics, vacuum, high temperatures, high pressures, magnetic fields) and the Special Cryogenics Group (superconducting magnets, dilution refrigerators).

Einleitung

Die Abteilung Instrumentenbetrieb ist verantwortlich für die allgemeine Verwaltung, den Betrieb und die Verbesserung aller wissenschaftlichen Instrumente, die für die Experimente in der Reaktor- und in der Neutronenleiterhalle eingesetzt sind. Der Aufgabenbereich umfasst ebenfalls die technische Unterstützung, die die Gastforscher während ihrer Messungen benötigen. Die im Laufe des vorigen Jahres eingeführte Struktur arbeitet jetzt zur allgemeinen Zufriedenheit, mit, neben den fünf Instrumentengruppen, der Zentralgruppe (Bindeglied zwischen den Physikern, den Allgemeinen Technischen Diensten und der Reaktorabteilung), der Gruppe "Probenumgebung" (Standard-Kryogenie, Vakuum, hohe Temperaturen, hohe Drucke, Magnetfelder), und der Gruppe "Spezielle Kryogenie" (supraleitende Magnete, Entmischungskryostate).

Introduction

Le Département Exploitation des Instruments assure la gestion globale, le fonctionnement et l'amélioration, de l'ensemble des instruments scientifiques permettant des expériences autour du réacteur et dans le hall des guides de neutrons. Cette gestion implique également toute assistance technique aux chercheurs invités pendant le déroulement de leurs mesures. Les structures mises en place au cours de l'année précédente opèrent maintenant à la satisfaction générale avec, autour des cinq groupes d'instruments, le Groupe Central (liaison entre les physiciens d'une part, les services généraux et le Département Réacteur d'autre part), le Groupe Environnement des Échantillons (cryogénie standard, vide, hautes températures, hautes pressions, champs magnétiques) et le Groupe Cryogénie Spéciale (aimants supraconducteurs, cryostats à dilution).

During 1984 the Building Services and Maintenance Group was transferred to the Instrument Operation Department, which increased the staff of the Department to approximately one hundred, and combined similar and/or complementary areas of activity in a single structure. This immediately resulted in greater flexibility in the use of the skills of the staff, particularly during the last three months of the year, when the Department was required to participate intensively in the dismantling work associated with the current reactor shut-down.

In addition to the operation of the ILL itself, the Department was also required to participate actively in the preparation of the various documents associated with the proposal to install the European Synchrotron Radiation Facility in the vicinity of the High Flux Reactor: studies of the possible location on the site, contacts with the public services concerned, preparation of drawings and plans, financial studies, etc.

Im Laufe des Jahres 1984 hat die Abteilung Instrumentenbetrieb die Gruppe "Einrichtung und Instandhaltung der Gebäude" übernommen, was seine Belegschaft auf ca. 100 Personen erhöht, und gleichwertige und/oder sich ergänzende Aufgabenstellungen in einer einzigen Struktur zusammenfasst. Daraus hat sich unmittelbar eine grössere Flexibilität im Einsatz des fachlich qualifizierten Personals ergeben, und dies insbesondere während der drei letzten Monate des Jahres, wo die Abteilung intensiv an den mit dem derzeitigen Reaktorstillstand verbundenen Demontearbeiten beteiligt war.

Ausserhalb des ILL-Betriebs selbst, hatte die Abteilung auch aktiv an der Ausarbeitung der verschiedenen Dokumente mitzuwirken, die mit dem Vorschlag, die Europäische Synchrotronstrahlungsquelle in nächster Nähe des Hochflussreaktors zu bauen, zusammenhängen: Untersuchung der Installationsmöglichkeiten auf dem Gelände, Kontakte mit den zuständigen Behörden, Vorbereitung der Pläne und Skizzen, Kostenstudien, usw.

Au cours de l'année 1984, le Département Exploitation des Instruments s'est vu confier le Service Aménagement et Entretien des Bâtiments, ce qui a porté ses effectifs à environ une centaine de personnes et a permis de rassembler, dans une même structure, des secteurs d'activité similaires et/ou complémentaires. Il en est immédiatement résulté une plus grande flexibilité dans l'utilisation des compétences de personnel, notamment pendant les trois derniers mois de l'année où le Département a eu à intervenir de façon intense dans les travaux de démontage liés à l'arrêt en cours du réacteur.

En marge du fonctionnement propre de l'ILL, le Département a dû également fournir une participation active dans l'élaboration des différents documents liés à la proposition d'installer la Source Européenne de Rayonnement Synchrotron près du Réacteur à Haut Flux : études des possibilités d'implantation sur le site, démarches auprès des services publics compétents, établissement des plans et tracés, études financières, etc.

CENTRAL GROUP

The role of the Group is to aid the smooth operation of the experimental programme and with this aim the Group is now installed in offices in the new experimental hall ILL 22.

During the first 9 months of the year the normal rhythm of reactor operation and experiments required the maintenance of the general services, assistance to ILL staff and visitors in the movement and installation of delicate scientific equipment, modification and improvement of experimental installations and provision of cryogenic fluids. The workload was substantially affected by the very large number of low temperature experiments and by the increasing number of short term special experiments requiring specific safety installations.

During the latter part of the year, the whole effort of the Group has been directed to the reactor shutdown.

The major part of our work is carried out with the assistance of and in direct collaboration with the other ILL Departments. The general routine operation has involved participation and supervision of:

The experimental zones from the point of view of safe operation.

15 experiments involving dangerous materials, the analysis of the risks involved, the preparation of special equipment, alarms, and operating instructions (e.g. PuSb on IN8, Tritium on S18 and Plutonium on S51).

The regular testing of the instrument safety interlocks and direct responsibility for all transport and handling within the experimental halls.

More specific attention has been paid to:

The quality of the guaranteed electrical supply (ARC) for the instrument computers, the consumption, quality, and extension of the network.

The situation is now critical and a second source is urgently required — until such time as it is installed no further instrument computers can be connected to a clean supply.

The modernisation of the general 220 V supplies in the experiment hall.

The improvement of the instrument cooling systems, with interlocks and monitored alarms.

The improvement of the reliability of the computer air-conditioning systems.

The development of the SADI alarm system which allows the surveillance of instrument and sample environment parameters in the Reactor Control Room.

The development of improved shielding materials, and the measurement of low level radiation backgrounds and fluxes.

In connection with the long reactor shutdown detailed schedules were made to:

a) ensure the effective use of all the Department's technical staff not directly concerned with instrument modifications by either transfer between Groups, temporary transfer to other Departments, or by attachment to other outside laboratories,

b) ensure the complete dismantling of 12 major instruments, their shielding and ancillary services to allow the beam line changes and technical improvements.

It will be impossible to start the reinstallation and recommissioning of these instruments until late in the shutdown, and the extremely heavy workload during a limited period may then lead to some delays in bringing all instruments into full operation.



Dilution refrigerator (CRTBT-ILL).

2

SAMPLE ENVIRONMENT GROUP

A - STANDARD CRYOGENICS

During all the changes in the Department, the Vacuum and Standard Cryogenics Groups were able to deal with requirements which became more demanding as the approach of the reactor shutdown was felt.

1. Cryogenic Fluids

Helium : price per litre of liquid supplied by CENG: 45 F excl. taxes
price per m³ gas: 35.5 F excl. taxes
consumption from 1.12.83 to 15.11.84: 71 800 litres
gas returned to CENG: 24 800 m³ (50%)
gas used at ILL by experiments: 10 620 m³ (21%)
losses on recovering: 14 800 m³ (29%)
consumption of gas: 48 m³/day of reactor operation.

Nitrogen: price per litre of liquid: 0.53 F excl. taxes
price per m³ gas: 0.82 F excl. taxes
monthly consumption: 40 000 litres in normal operation
monthly consumption: 60 000 litres for exceptional operation.

Analysis of consumption:

a) For helium: the distribution and measurement of helium are carried out with a very high degree of reliability (one error for 7000 operations). Two explanations may be given for the high consumption figure of over 7200 litres per month for the operation period:

- a very high utilisation of orange cryostats,
- the use of large high consumption cryogenic machines such as PERKEO, and CENG, and OXFORD INSTRUMENTS superconducting magnets.

A very large quantity of He gas was also used for the continuous flushing of flight paths.

b) For nitrogen: a close collaboration between Cryogenics, Central Group and the Reactor Department made it possible to resolve the problems of the reactor resulting in an increase in consumption of 50% during a 3-month period.

c) For helium recovery: the recovery loss rate is very high. A considerable modification is required to the existing installation, also a study of the consumption of helium gas on the instruments, and particular attention must be paid to the risks of leaks.

2. Cryogenics

Apart from the everyday service on the instruments we have succeeded in guiding visitors, resolving their problems and in any case giving them practical advice on working at ILL, with apparent firmness, but still heeding their wishes.

While providing maintenance of the cryostats, and despite reduced staff, we have been able to carry out design and development work, for example on stainless steel-aluminium joints.

Construction of an "orange cryofurnace" for 1.5° K-500° K.

Commissioning of a new orange cryostat.

Design and testing of thermostat equipment for DB21.
Design, testing and construction of a cold thermodilation valve.

The quality and simplicity of the results obtained for this last item are encouraging for the complete automation of the orange cryostat in the very near future.

3. Vacuum

In addition to the regular routine maintenance such as servicing of pumps, repairs to contaminated pumps, detection of leaks in the laboratory and on the experiments, not forgetting the tests on reactor beam tube liners carried out on the manufacturer's premises, we also undertook the necessary reconstruction of the mobile helium pumping sets, now equipped with Roots pumps, and of a new "high pressure" model pump with a very little amount of oil in the exhaust. In addition to the commissioning of several turbomolecular pumps, the design and construction of new pumps for the future D11 have been undertaken.

B - HIGH TEMPERATURES

The demand for furnaces for experimental programmes continued to be high in 1984 as was the demand for new or non-standard installations. Independent development and service sections have been created to cope with the work-load. The newly designed "3-Axis furnace" was put into service with satisfactory results. This furnace will form the basis for a new generation of general purpose furnaces. Three experiments at temperatures above 2000 ° C were successfully run during the year, and the 2500° C furnace achieved its design temperature. Automatic optical pyrometry is now available with this furnace.

Development

1) The precision mechanical support system for a small angle scattering furnace has been delivered; the hot components are being developed.

2) The design project for a non-magnetic furnace for IN11 has begun. The furnace will use a triple re-entrant element with 1 mm wall separation at the sample zone.

3) Off-beam tests of computer controlled temperature management have started using a CERBERE control unit. Preliminary results are very satisfactory.

The High-Temperature/High-Pressure Group is now installed in a new workshop ILL 22, next to the new guide-hall, which offers improved working space.

SPECIAL CRYOGENICS

ELECTRONICS

In addition to the general maintenance of the electronics associated with the sample environment, we tested completely under real experimental conditions the preliminary series of 6 temperature controllers of the model developed during the previous years. The feed-back which we have received from the users has significantly helped us and enabled us to up-date both the electronics and software, in order to deal as well as possible with the needs expressed. Apart from the usual cryogenic sensors (metal resistors and semi-conductors), this equipment can now operate with all types of thermocouples, which also makes it possible to control the temperature of the furnaces.

This equipment is completely automatic, connected to the instrument computer, and makes it possible to control the temperature as simply as the position in space.

We are on the point of placing an order for 20 additional controllers. If they are delivered on schedule, these controllers will go into operation when the reactor starts up.

SUPERCONDUCTING MAGNETS

7.4 Tesla Cryomagnet (THOR)

Because of transversal movements due to the presence of ferromagnetic parts on the instruments, it was necessary to rebuild completely the cold centring system, which can now withstand a force of 300 DaN, without any notable increase in the consumption of liquid helium.

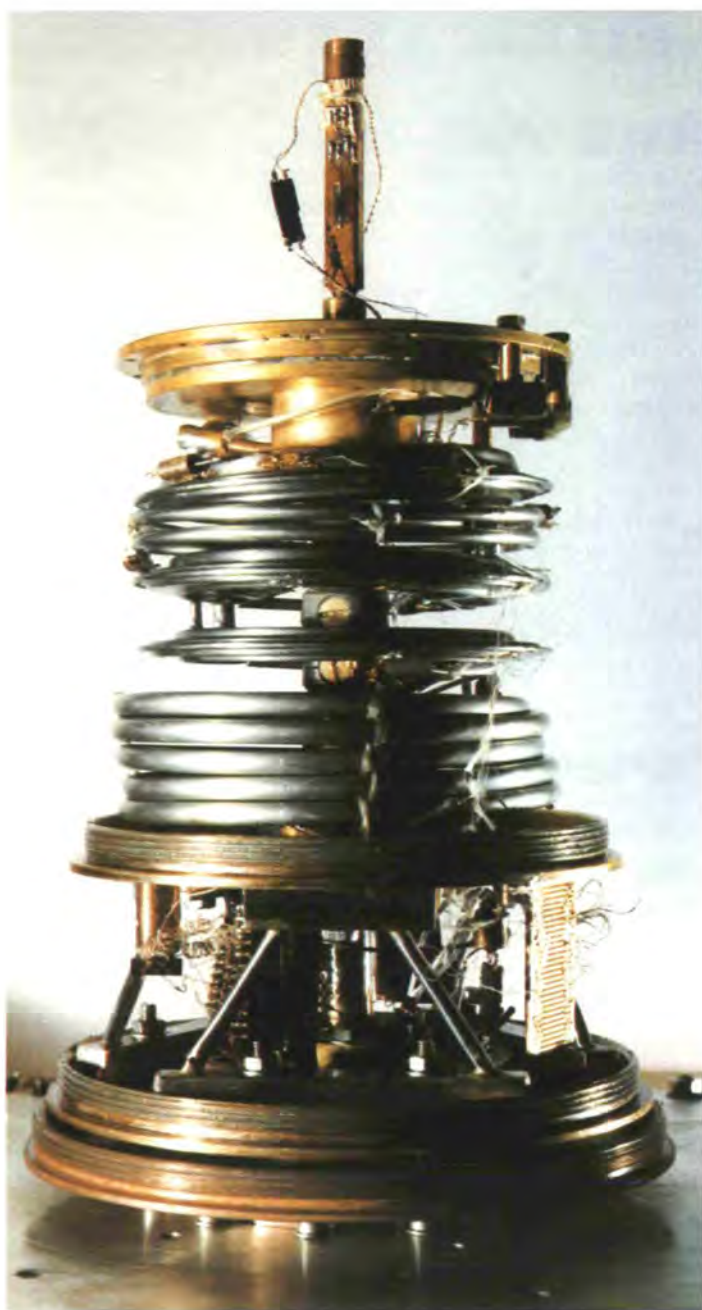
This cryomagnet, which is intended for general use, has been used on IN3, IN5, IN11, IN12. The total period of operation on these instruments has been 122 days. It has been used for temperatures from 1.8 K to ambient temperature, and magnetic fields from 1 Tesla to 7 Tesla.

It was found possible to operate regularly at temperatures below 4.2 K, without encountering the problems of impedance blockage found on the cryomagnet on D3.

This equipment can be considered as ready for the general use for which it was intended.

6 T Cryomagnet (OXFORD INSTRUMENTS) for 3-axis spectrometers

The main technical difficulties encountered by the supplier appear to have been resolved. Delivery of this equipment is expected at beginning of 1985 (i.e. 30 months late).



Double still dilution unit (CRTBT-ILL).

VERY LOW TEMPERATURES

The use of the OXFORD INSTRUMENTS dilution refrigerator is diminishing. It has been used for 3 experiments, one on IN12 and two on IN6. A 0.7 Tesla superconducting coil was mounted for the experiments with superconducting samples. Two "Neumaier" type dilution inserts are in use, for the 2 standard diameters of ILL cryostats (49 and 70 mm diameter), with respective basic temperatures of 25 mK and 20 mK. The time for changing a sample and return to 25 mK is 4 to 5 hours for an experienced user. They have been used on IN2, IN12, IN5, IN6 and IN10, with a total operating period on the instruments of 40 days.

Two of the new systems of dilution refrigeration developed in collaboration with the CRTBT (Benoit, Flouquet) have been built. This system, with direct access to the dilution stage while keeping the rest of the cryostat cold, permits a rapid change of sample, with a large amount of space available. It also has advanced automation, which simplifies its use considerably. The first such dilution refrigerator, with a simple tubular exchanger and a basic temperature of 50 mK, and a cooling time of 2.5 hours, has been used intensively at ILL on D10, D5, D7, D15, D13, at CENG at the Siloé and Mélusine reactors, and at the CRTBT, for a total of 197 days. The construction and testing of the second one, with 3 separate exchangers (sintered Ag), has been completed (13 mK, 5 hours). More detailed testing is necessary to achieve the desired performances (10 mK, 4 hours); this will be finished at the end of 1984. A He^3 cryostat and its pump have been built and tested (500 mK in continuous operation, 300 mK in 1 short operation).

SPECIAL EXPERIMENTS

The group was involved in the preparation and implementation of a number of experiments requiring special skills, for example:

Measurements on He^4 under pressure (IN11, IN12).
Construction, development and utilisation of an insert for measuring critical fluctuations of He^4 under pressure at point λ . (Stability and homogeneity of temperature within 1 micro Kelvin), in collaboration with B. MOSER of NBS.

INSTRUMENT GROUP FUNDAMENTAL AND NUCLEAR PHYSICS

- PN1: Fission product separator (LOHENGRIN) on beam tube H8 (H.R. Faust, R. Brissot, J.P. Bocquet, I. Gartshore, M. Taylor).
- PN2: Beta spectrometer (BILL) on the vertical beam tube V3 (K. Schreckenbach, G. Colvin, G. Blanc).
- PN3: Three curved crystal spectrometers (GAMS 1, 2, 3) one flat crystal spectrometer (GAMS 4) on the throughgoing beam tube H6/H7 (H. Börner, F. Hoyler, P. Geltenbort, G. Greene, M. Taylor).
- PN4: Ge(Li) pair spectrometer on the through-going beam tube H7 (F. Hoyler).
- SN5: Ultra-cold neutron (UCN) source on the inclined beam tube IH3 (P. Ageron, W. Mampe, A. Beynet, T. Manning).
- PN6: On-line mass separator for thermally ionized fission products (OSTIS) on neutron guide H23L (B. Pfeiffer, U. Stöhlker).
- SN7: Cold polarized neutron beam on guide H142 (W. Mampe).
- PN8: Fission product coincidence spectrometer (COSI FAN TUTTE) (P. Geltenbort, F. Gönnerwein, T. Manning).
- H17: Cold neutron guide: liquid helium UCN source (Ch. Jewel and RAL, ILL collaboration).
- H18: Cold neutron guide (W. Mampe).
- H22: Thermal neutron guide: neutron induced particle emission (H22D), R. Brissot), neutron induced fission (H22E, R. Brissot) γ - γ angular correlations (H22F, F. Hoyler, B. More).

INTRODUCTION

In 1984 the personnel in nuclear physics has experienced several important changes. R. Brissot (PN1), S.A. Kerr (PN3), B. Pfeiffer (PN6) and M. Taylor (PN1, PN3) have left the ILL. J.P. Bocquet has joined LOHENGRIN as Second Responsible and P. Geltenbort is now first responsible on PN8. In connection with the many new instruments which have been — or are to be — installed in the reactor hall it has become apparent that still more effort has to go into a better radiation shielding against background, stemming from both, neutrons and γ -rays.

Test measurements carried out on the H11 site have shown that the background level created on the GAMS 1 instrument has to be strongly decreased.

On the other hand studies have been undertaken in order to further reduce the background created by PN8, especially at the locations of IN20 and IN4.

In order to prepare the exchange of the remaining "first generation" beam tubes, foreseen in the long reactor shutdown, several nuclear physics instruments had to be dismantled in autumn 1984:

SPECTROSCOPY: GAMS 1, GAMS 4 (PN3); and pair spectrometer (PN4)

FISSION: COSI FAN TUTTE (PN8)

FUNDAMENTAL PHYSICS: UCN on the inclined beam tube IH3 (SN5) and liquid helium UCN source at H17.

All these instruments will be reinstalled during 1985 at their respective sites. In spite of this disruption, improvements and modifications have been continued on various instruments.

INSTRUMENT IMPROVEMENTS AND MODIFICATIONS

Fission : During 1984 the new ionization chamber installed at LOHENGRIN was used to measure rare events in the fission process, such as cold fragmentation in ^{239}Pu and isotopic identification in cold fragmentation of ^{233}U . It was shown that this chamber which now covers 45 cm of the focal plane, improves the detection efficiency of LOHENGRIN by a factor of 40 with respect to the former detectors. ($\Delta E \approx 600$ keV, spatial resolution in energy-direction ≤ 5 mm, spatial resolution in mass-direction ≤ 10 mm). This high efficiency permitted the investigation of mass and isotopic yields of fission in ^{238}Np which was bred by "double neutron capture" in a ^{237}Np target. Experiments are now possible on nuclei such as ^{229}Th which have cross-sections of the order of 30 barns or in other targets which necessitate multiple neutron capture.

In order to treat the information gathered by the ionization chamber the hardware installation needed for the 4-parameter measurements was completed and a corresponding software package is now available. This allows for the on-line treatment of the particle intensity image on the focal plane and the on-line identification of the mass and energy of fission products. After completion of final tests concerning resolving power and stability, the fission fragment coincidence spectrometer COSI

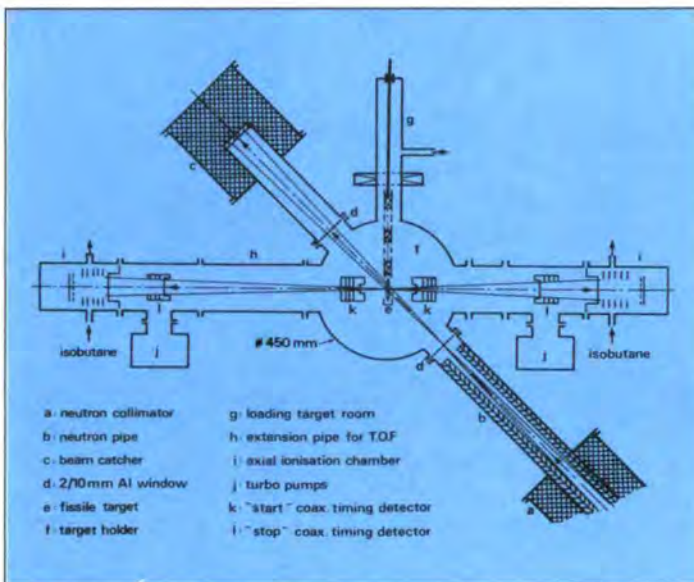


Figure 64: Schematic view of the energy-TOF spectrometer COSI FAN TUTTE.

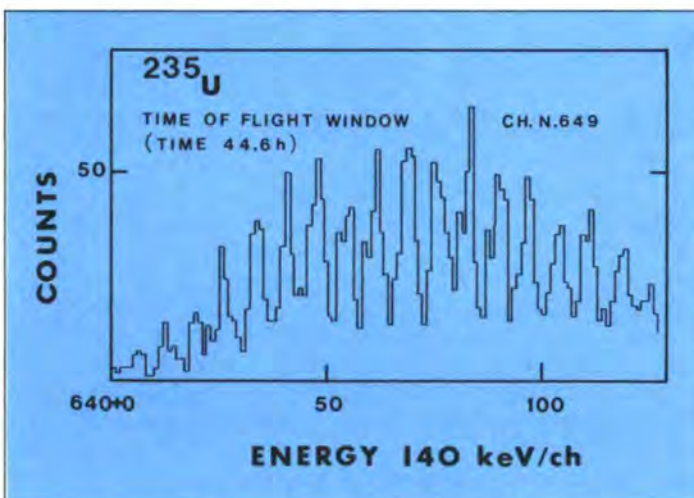


Figure 65: Energy spectrum of fission fragments from $^{235}\text{U}(n,f)$ for thermal neutrons with a time-window of 53ps set on the TOF. The peaks in the spectrum correspond to individual masses in the light mass wing of fragments.

FAN TUTTE was put into scheduled operation and first proposed experiments were carried out on thermal neutron induced fission (Fig. 64).

For a complete start-stop setup with 5 mm \varnothing devices in both the start and the stop detectors, a time resolution below 100 ps (FWHM) is standard. The energy resolution of the axial ionization chambers (counting gas: isobutane) is ~ 400 keV for typical light fission fragments (mass ~ 100 amu, energy ~ 100 MeV). Correspondingly a mass resolution of

$\Delta m/m = 0.5\%$ can be achieved for light fragments by measuring velocities and kinetic energies simultaneously and as can be seen from Fig. 65, all masses are resolved individually in this case.

During the reactor shutdown period this instrument will be used to study spontaneous fission in radioactive samples of ^{252}Cf .

Last year much experience was gained with high temperature ion sources at the On-Line-Mass-Separator OSTIS. These sources have currently become standard, replacing the thermal surface ionization sources. They allow work on a considerably extended range of elements: Ga, Rb, Sr, In, (Sn), Cs, Ba, long lived rare earth elements and their β -decay daughters.

Spectroscopy: The new 32-wire position sensitive proportional counter installed on the Beta spectrometer BILL is now used routinely and yields ~ 5 times higher intensity compared to previous counters.

The two axis flat crystal spectrometer GAMS 4 (NBS, ILL collaborations) installed at the end of last year became operational. It has been used to accurately measure γ -ray energies up to 3 MeV from the reaction $^{35}\text{Cl}(n,\gamma)$. The crystals and spectrometer have performed in a manner which clearly demonstrates that sub p.p.m. measurements of intense sources are possible in the 2 to 4 MeV region. Also a very successful precision measurement of the 2.2 MeV γ -ray from the reaction $\text{H}(n,\gamma)^2\text{H}$ was carried out.

Currently, studies are being made to improve even further both the precision and sensitivity of the instrument.

Considerable effort has been made to install a low background arrangement at H22F (in collaboration with the Institut Dolomien, Grenoble) used for γ -ray measurements in addition to the standard beam tube available for γ - γ angular correlations. This arrangement consists of 10 cm \varnothing perspex tubes with thin mylar windows and can be evacuated. Special care was taken to reduce background stemming from n-capture in target- and detector surrounding. This device is mainly used for PGAA (prompt γ -ray activation analysis) experiments on geological samples but is also available for nuclear spectroscopy.

Fundamental Physics: The inpile guide of IH3 has been lined with 0.2 mm Ni-tubes. These liners (developed at the TU-München) are produced by copying the outer surface of the glass tubes. The neutron reflectivity of the liners is as good as the one of glass with the advantage of a high Ni cut-off angle and the previous value for the UCN flux was again obtained. This means a gain factor of ~ 5 with respect to the value measured prior to this modification. The reasons for the time dependent guide degradation are understood.

Reflectivity measurements of various surface preparation procedures and materials (^{58}Ni included) have been carried out

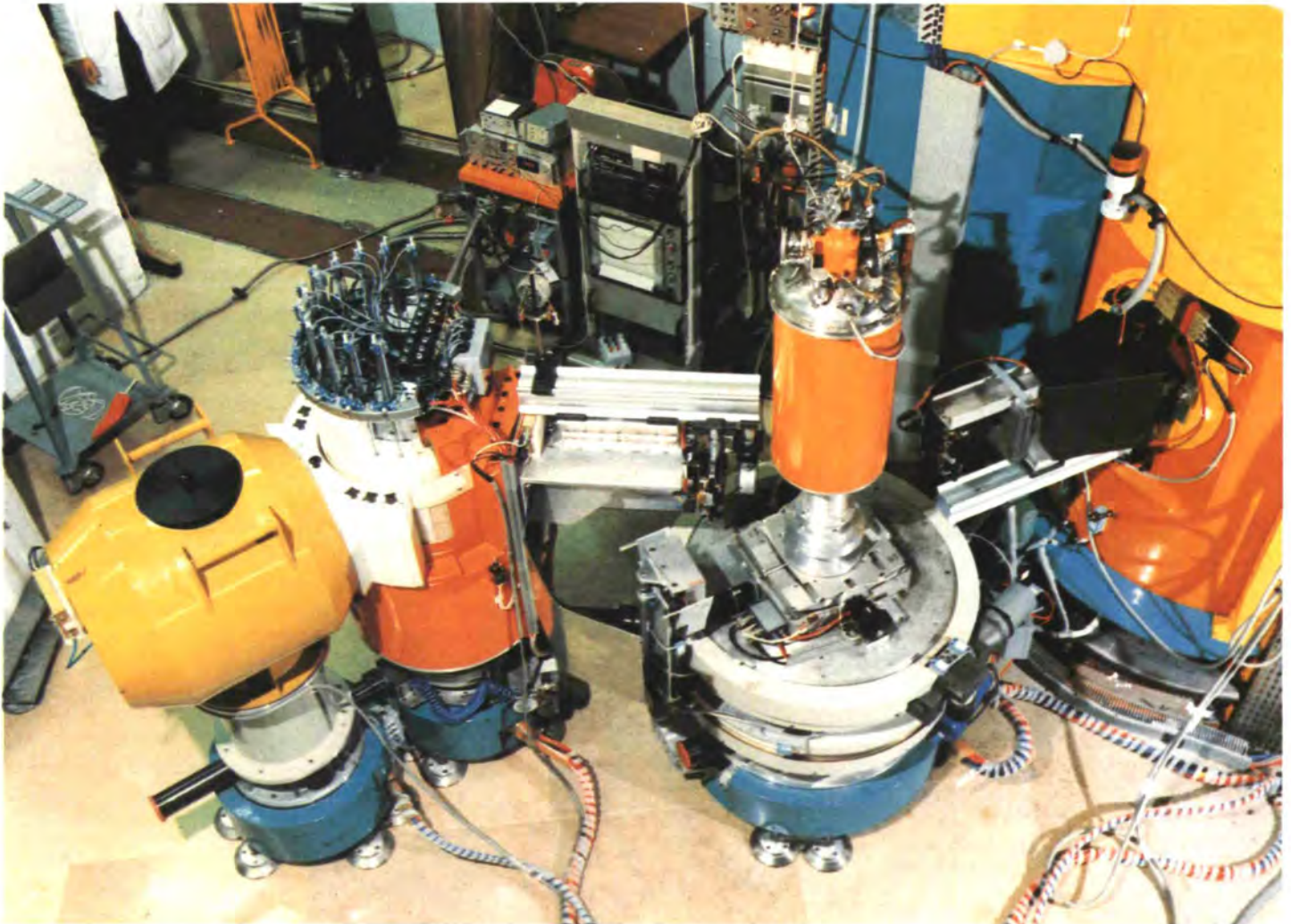
with very cold neutrons (VCN). These results will help in the construction of the inpile guide system of the vertical UCN source and the guide system of the new horizontal cold source. The 3 m long storage tube of the source installed at H17 has been coated with Beryllium by a specially developed sputtering procedure. A cold low loss UCN extraction system has been designed and manufactured in the U.K. It will be cryogenically tested during the reactor shutdown.

In order to prepare the neutron life time measurement on S52 the ^4He drift chamber for measuring the electrons following the β -decay of neutrons was tested in the monochromatic neutron beam at T16 ($\Phi_n = 6 \times 10^6$ n/s at 45 MW). These tests

were seriously disturbed by the high background level of γ -rays (~ 1 mrem) from the surrounding experiments.

The measurements for the study of β -decay of polarized neutrons were continued with the superconducting spectrometer PERKEO (Heidelberg, Argonne, ILL-collaboration). Sources of systematic errors, arising from electron-backscattering and effective source volume and detector solid angle were studied extensively and are largely eliminated. The energy dependence of the β -decay asymmetry has been measured for the first time and a new value was obtained for the ratio of weak coupling constants g_A/g_V .

Co-ordinator: Hans G. Börner



The most recent view (October 1984) of the IN8 spectrometer.

INSTRUMENT GROUP THREE-AXIS SPECTROMETERS

- IN1 : 3-axis and beryllium-filter spectrometer on the hot beam-tube H8 (U. Steigenberger, B. Dorner, H.J. Lauter, P. Cross).
- IN2 : 3-axis spectrometer with a double monochromator on the thermal beam-tube H13.
- IN3 : 3-axis spectrometer on the thermal guide-tube H24 (D. Paul, H.J. Lauter, R. Arthaud).
- IN8 : 3-spectrometer on the thermal beam-tube H10 (R. Currat, P. Frings, M. Hagen, A. Brochier).
- IN12: 3-axis spectrometer on the cold guide-tube H142 (W.G. Stirling, K.A. McEwen, D. Puschner).
- IN14: 3-axis spectrometer on a cold guide-tube on the second cold source (W.G. Stirling, W. Kaiser).
- IN20: 3-axis spectrometer with polarised neutron option on the thermal beam-tube H13 (R. Pynn, T. Bland, W. Kaiser, P. Flores).

MAJOR INSTRUMENT MODIFICATIONS AND IMPROVEMENTS

During the last year, the hot-source triple-axis spectrometer IN1 became completely operational, working with increasing reliability for scheduled experiments. A full set of variable-curvature analysers, P.G. (002), Cu (002) and Cu (220) is now available for use with the three copper monochromators. Further tests of resonance filters are required before general use of these may be made. During the 1984-85 shut-down the monochromator support is to be replaced and an additional CAMAC scaler unit will be installed.

The Be-filter spectrometer was able to handle all scheduled experiments since the rebuild of the IN1 monochromator. Improvements will be made for the 2 θ -arm of the monochromator which is not fully adapted to the high rate of usage of the instrument in the Be-filter mode.

A test experiment with a Be-graphite combination filter (both on loan from A.E.R.E. Harwell) showed an unexpected, high resolution of 0.34 THz and 0.6 THz at 11 THz and 28 THz energy transfer ($\Delta E/E_0$ is $\sim 2\%$ up to $E_0 = 45$ THz). Thus a new design for this version will become necessary as the test

unit allows only for the detection of neutrons from the sample in a small solid angle.

After twelve years of good and faithful service, IN2 was taken out of service in February: an informal "pot" celebrated this moving occasion. The mechanical installation of the new, thermal (polarised-beam) instrument IN20 was completed during the summer, at a temporary position outside the IN2 casemate. Preliminary tests with neutrons were made of the fully-functioning instrument and its control system. The Heusler alloy (111) monochromator was found to have a high polarizing efficiency, with an intensity enhancement of about six due to the vertical curvature; the curvature of the P.G. (002) monochromator increases the incident intensity by up to a factor of four. These tests indicate that the IN20 flux will be considerably greater than that of the (double-monochromator) instrument IN2, particularly when the monochromator drum is installed in its final position nearer the reactor.

Despite a variety of problems arising from the poor condition of the "tanzboden", the control electronics and the newly installed SOLAR computer, IN3 was used to carry out experiments for nearly all of the available beam-time in 1984. The single detector (5 cm diameter) was used most frequently, but the multidetector has always been available. The horizontally focussing analyser, too, was in frequent demand. During the long shut-down 1984-1985 the installation of a new monochromator system is planned. This system is a bifaced set-up with P.G. (002) and Cu (200) monochromators, both with variable vertical curvature.

A significant improvement in the instrument reliability of IN8 was achieved with the implementation of new PROM's in the existing motor-control units (Télématique CMP425 units: first generation). The new programs are adapted from those implemented in the second generation modules, as available on IN3 and IN20.

Following a recent policy decision within the group to introduce CAMAC scalers, a CAMAC crate was connected to the instrument's SOLAR and successfully tested, shortly after the reactor shut-down. The use of the CAMAC interface to operate a closed-loop motor-control unit is also envisaged, as a possible way to reduce positioning deadtimes on the casemate drum (A2 angle).

The main project to be implemented during the shut-down is the increase of the monochromator height from, currently, 70 mm to 140 mm. The aim of the project is to increase the vertical divergence, and hence the flux, available at the sample position. The modifications required are:

- i) The redefinition of the rotor apertures in the primary-beam shutter.
- ii) The installation of a new variable-curvature device and goniometer at the monochromator position.
- iii) Minor modifications to the casemate protection along the primary- and monochromatic beam paths.

Shortly before the reactor shut-down preliminary background measurements were performed in collaboration with the responsible for the H11 projects. These tests revealed a prohibitive increase in the epithermal-to-fast neutron background measured on IN8, due to the opening of the H11 primary beam. Additional shielding around the H11 beam-tube will be required in order to maintain acceptable working conditions on IN8. Simultaneously an effort will be made to improve the IN8-counter protection against epithermal and fast neutrons. Further tests will be needed at the reactor start-up. IN12 ran well during 1984 with few major modifications. Decreasing incident flux continued to be a worry on IN12, but this was eventually traced to problems with the H142 guide-

tube (possibly an oily deposit on the inner walls) which will be rectified during the shut-down. The computer-controlled ILL temperature controller continued to be a highly efficient and useful supplement to the instrument's capabilities. During the 1984-85 shut-down the new large-angular-range automatic analyser-detector system will be installed on IN12. Studies for the proposed IN14 instrument continued, with most effort going towards the design of the monochromator shielding. A "carousselle" system, in which concrete blocks rotate and then are lifted over the incoming/outgoing guide tubes, seems the most promising solution to the problems of instrumental and biological shielding, and beam definition.

Co-ordinator: W.G. Stirling



A view of the first Neutron Guide Hall (Vercors side).

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

- IN4 : Time-of-flight spectrometer on thermal tube H12 (A. Murani, W. Langel, A. Key).
 IN5 : Multi-chopper spectrometer on cold guide H16 (F. Douchin, G. Kearley, H. Blank, S. Jenkins).
 IN6 : Focusing TOF spectrometer on cold guide H15 (A.J. Dianoux, M. Bée, Y. Blanc).
 IN10: Backscattering spectrometer on cold guide H15 (C. Poinsignon, A. Magerl, P. Joubert).
 IN11: Spin-echo spectrometer on cold guide H141 (B. Farago, B. Sarkissian, J.P. Varini).
 IN13: Backscattering spectrometer for short wavelengths on thermal guide H24 (W. Petry, A. Heidemann, I. Anderson, J.F. Barthelemy).
 D7 : Diffuse scattering spectrometer on cold guide H15 (O. Schärpf, W. Just, R. Rebesco).
 D11 : Small angle and diffuse scattering spectrometer on cold guide H15 (P. Timmins, A. Wright, R. May, R. Baker).
 D17 : Low Q, High Resolution spectrometer (R. May, J. Torbet, P. Timmins, M. Cruz).

INTRODUCTION

Improvements to the performance of all instruments in this group are described. For D7, the improvements are the subject of a special chapter at the end of this report.

INSTRUMENT RESOLUTION AND FLUX IMPROVEMENTS

By increasing the number of analyser plates covered by polished Si(111) crystals, diffusion processes studied on IN10 can now be followed over a high Q-range with increased resolution. This possibility will be very useful with the flux increase achieved by the new cold source. Furthermore, circular analysers can now be translated in order to compensate for

the path differences between analysers and detectors, with respect to the ideal backscattering configuration imposed by the sample environment. In addition the accuracy of diffusion coefficient measurements at low Q (e.g. ionic solutions) has been improved significantly.

Considerable work has been carried out for the IN10B project in particular, the development of a prototype for a new drive system. This has a faster speed (3.5 m/s), with a transparent monochromator of $30 \times 80 \text{ mm}^2$, and has been tested both optically, and for a short time, in-beam.

Efforts to increase the effective flux on IN13 have resulted in two major improvements. Firstly extensive tests have shown that thicker monochromator crystals can increase the flux by a factor of approximately 2 without significant loss of resolution. Thus for most experiments at present, 1 cm thick monochromator crystals are used instead of the currently used 3 mm thick crystals. Some thicker analyser crystals have also been ordered to study the possible flux increase at the secondary spectrometer.

On the other hand one can increase the flux at the sample at the expense of the energy resolution by applying a temperature gradient across the monochromator crystals parallel to the beam direction. Such a monochromator gradient furnace has been constructed and used successfully during tests and for one experiment.

Another project aims at lowering the low-temperature limit of the monochromator furnace down to 77 K. In order to calibrate the energy scale of the instrument at these low monochromator temperatures, the lattice expansion of CaF_2 between 77 K and RT has been measured. This opens an energy-transfer range from $\sim 200 \mu\text{eV}$ to $350 \mu\text{eV}$ with an energy resolution of $7 \mu\text{eV}$ now available on IN13. A corresponding monochromator cryo-furnace is under development.

For IN5 it has been reliably established that the neutron-rate can be increased substantially for experiments using sample temperatures around 10 K. For tunnelling and magnetic experiments this has made the use of long wavelengths (up to 15 \AA) a practical proposition, with resolutions of $6.0 \mu\text{eV}$ having been realised. More recently, dephasing techniques have shown that there is considerable scope for modifying the instrumental resolution at a given incident wavelength and with the advent of magnetic bearings, both chopper speeds and phasings can be employed to supplement the independence of the Q and $h\omega$ ranges of the instrument.

Considerable effort has been made to reduce the "background" scattering of instruments, i.e. to discriminate the scattering from the sample environment such as furnace or cryostat walls. On IN6, the use of an oscillating collimator enabled this parasitic scattering to be reduced to less than 1 count per hour and per detector. A similar system will be installed on IN5 over the range 5° - 135° . Furthermore, with the help of a Monte-

Carlo simulation of the IN13 backscattering spectrometer it was demonstrated that placing a collimator between sample and analyser could give excellent results on this instrument. A number of small improvements to D11 were made in the first part of 1984 but the major effort was devoted to plans for the rebuilding of the instrument during the long shutdown of 1984/85.

The 40 m detector flight tube will be replaced by a wider one in which the detector will travel on a trolley. Thus the sample to detector distance will be continuously variable between 1 and 38 m. Construction of the mechanical parts was started in April 1984 and the new set-up of D11 was installed in February 1985. The detector position will be automatically controlled by computer as will the positioning of the beam-stop. The time for changing detector position will be reduced to a maximum of about 10 min.



Modification of the monochromator shielding of D7.

ELECTRONICS AND DETECTORS

A particular effort has been made to improve the reliability of the IN5 detector system, including the test and the repair of defective elements at the beginning of each experiment. This has been made easier by the provision of facilities for the setting of detector power supplies outside the instrument. Moreover tests with wider detectors (of the IN6 or IN4 type) permit future consideration of a totally fixed detector system. On IN11, the following improvements are planned: a complete check and replacement of some electronics parts, replacement of certain current power supplies, in particular the high current supplies.

ANCILLARY EQUIPMENT FOR SAMPLE ENVIRONMENTS

New ILL temperature controllers are now available and linked to the instrument computers (IN6, IN13). The main advantages are (1) Automatic scans of the sample temperature (elastic-window measurements on backscattering spectrometers, successive runs during the night...). (2) An easy and secure handling by the users. (3) The possibility to interrupt the data acquisition in the case of an accidental deviation of the sample temperature. (4) A standardisation of the temperature controller system for all the instruments (the intrinsic constants of the cryostat are introduced into interchangeable ROM).

This system permits a temperature control in both the low and high temperature range (1 K-500 K). A cryofurnace, built from a standard "orange" cryostat is now available on IN10. The cooling and heating loop of IN6, working with nitrogen gas and allowing very rapid changes of the sample temperature, will be adapted to this controller.

Finally, the standard IN5 cryostat is under modifications and will be completed by a second cryostat (common with IN6) adapted to very low temperatures and also to cryofurnaces working over a wide temperature range.

Associated with the modifications to the flight tube of D11 are improvements to the sample position including better accessibility from ground level and an improved definition of the beam and sample axes. The possibility of working in air will be much improved.

MAGNETIC BEARINGS

During the last cycle (August-September 1984), a new Fermi chopper working on magnetic bearings was installed on IN4. The maximum speed of the chopper is 30.000 rpm, which gives

a neutron pulse of 7 μ s width. Tests with graphite C(002) and C(004) and Cu(220) monochromators have been carried out with positive results. Modifications to IN4 to install the Fermi chopper on a permanent basis in the single monochromator configuration with a reduced flight path of 2 m, have now to be decided.

The prototype of the IN5 chopper working on active magnetic bearings using a maximum of permanent magnets, developed at IGV-KFA in Jülich by the group of M. Fremerey was delivered at ILL and tested in April-May. The results obtained after an improvement of the electronic and minor modification of the mechanical assembly were excellent. (Phase stability of 0.01° for all rotation speeds up to 20000 rpm). The IN5 choppers were removed in October from the instrument and will be modified in the same way.

SOFTWARE AND INSTRUMENT CONTROL IMPROVEMENTS

A new instrument control program has been introduced on IN6, including the remote control of the sample temperature and the possibility of interrupting the data acquisition in the case of temperature variation outside a given range. On IN10, a new disk unit, with three disks allows the storage and the access of data collected over a whole reactor cycle. A complete set of data correction and analysis programs is now available for IN13. In particular, the correction program SQW, dealing with data from IN10 and IN13 to produce corrected scattering law data in a standardized format compatible with the time-of-flight machines, is operating very successfully.

The 10 years old PDP 11/40 of D11 is being replaced by a Vax 11/730 which has already been delivered and is currently being tested. This improvement should greatly augment the D11 computing facilities particularly concerning on-line data treatment. The replacement of RK05 disks by RL02 disks on D11 as well as on D17 earlier in the year has already allowed 1000 spectra to be stored on a single disk rather than the 220 possible on an RK05. Advantage of all the mechanical modifications on D11 is also being taken to rebuild and slightly displace the cabin and so to improve the maintenance of computer and electronics by having them in an air conditioned part of the cabin separated from the normal working area.

First steps were taken to prepare computer control of the detector rotation of D17 about the sample axis and of the wavelength setting. Five identical closed-loop microprocessor modules are to serve these functions as well as the sample changer and Eulerian cradle motions. All settings will be verified by absolute encoders.

Standardisation of the instrument control software of D17 in parallel with that of D11 has been continued. We plan to fur-

ther match essential control commands as far as low-Q scattering is concerned.

Low-resolution crystallography will be supported on D17 until DB21 is commissioned.

MAJOR MODIFICATIONS ON D7

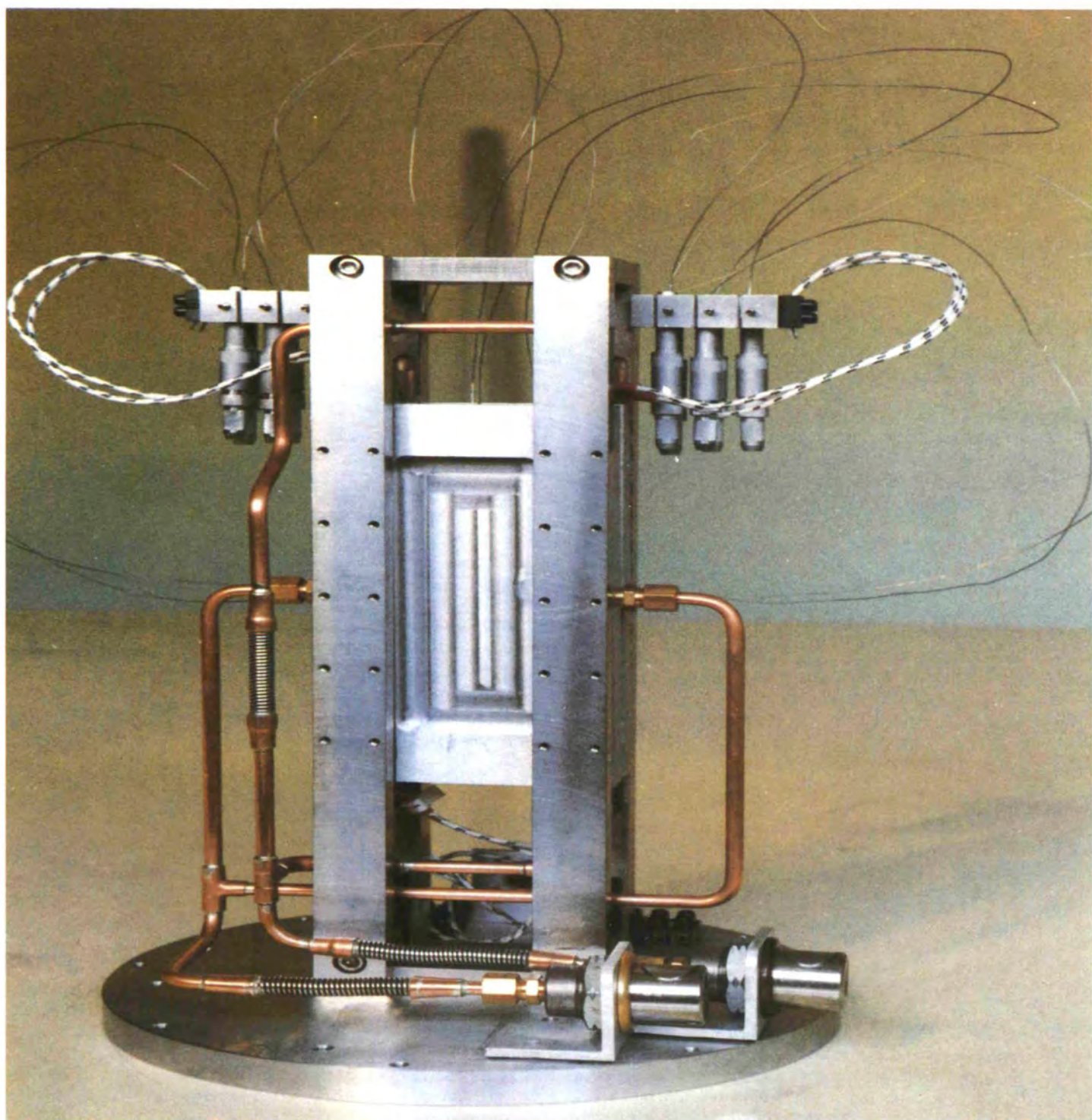
The monochromator shielding was modified to avoid all interferences of D7 with adjacent instruments. The three beam-holes are now equipped with lead-windows which are operated pneumatically. The instrument and its shielding are movable on air-cushions and can be positioned by a single person. To improve the Q and TOF resolution a detector box of 16 detectors (12 mm wide, 3 mm thick each) has been installed at the ends of each horizontal bank.

A fourth horizontal detector bank has been equipped for polarization analysis (PA). Experiments requiring PA were run by using 24 analysers initially and 28 subsequently. Analysers conceived for a range $\lambda > 4 \text{ \AA}$ were successfully used even at $\lambda = 3.1 \text{ \AA}$ (on liquid Na) despite the bad transmission. A promising project is the use of at least one bank having a cut-off at $\lambda = 23 \text{ \AA}$ by setting aside the 4th bank until further mirrors are available. Altogether 3200 mirrors (1600 are already available) will be required to equip the whole bank with these analysers. Thus a fairly rapid investigation of higher energy transfers will become possible.

Data from all experiments are stored on a new Winchester disk, thus avoiding frequent changes during data analysis.

Tests with various TOF methods revealed the following. Using the normal *mechanical chopper*, fairly good TOF spectra were recorded in 30 min, whereas with a *Fourier chopper* 4-8 h were required for yielding an equivalent result (a better resolution is only obtained for high intensity peaks). The tests with the *pseudostatistical spin-flip chopper* revealed inherent problems due to background subtraction. The only sensible application of the latter method is for inelastic scattering experiments with ferromagnetic materials, where the difference between spin-up and spin-down measurements can be obtained immediately. D7 programs and electronics were used for a 14 day experiment on D17 measuring the critical scattering from an Fe⁵⁷ crystal by using a pseudostatistically chopped Drabkin-monochromator. A resolution of 25 μ eV was achieved and TOF spectra with high Q and ω resolution near the critical point were recorded.

Co-ordinators: R. May/M. Bée



Monochromator furnace of IN13.

INSTRUMENT GROUP DIFFRACTION INSTRUMENTS

- D1A : High resolution powder diffractometer on thermal guide H22 (A. Hewat).
- D1B : Two-axis diffractometer with multidetector on thermal guide H22 (Ph. Mangin, A. Fitch, K. Ben Saidane, P. Agnes).
- D2B : Very high resolution powder diffractometer (in preparation) (A. Hewat, J. Kirby).
- D3 : Two-axis polarized neutron diffractometer with lifting counter on thermal beam H5 (F. Tasset, M. Bonnet, A. Dorn).
- D4B : Liquids diffractometer sharing the hot beam H8 with IN1B (P. Chieux, R. Meyer, A. Hawes).
- D5 : Three-axis polarization analysis spectrometer on hot beam H4 (K. Ziebeck, J. Schweizer, P. Agnes).
- D9 : Four-circle diffractometer on hot beam H3 (W. Kuhs, M. Lehmann, J. Archer).
- D10 : Four-circle triple-axis spectrometer on thermal guide H24 (neutron spin echo option) (C. Zeyen, G. McIntyre, R. Chagnon).
- T12 : Neutron camera on thermal guide H23 (A. Wright).
- D15 : Four-circle MK6 diffractometer on the inclined thermal beam IH4 (J. Brown, S. Wilson, J.M. Reynal).
- D19A: 2D multidetector for tests on thermal guide H24 (R. Stansfield, M. Thomas, M. Berneron).
- D20 : High flux multidetector (in preparation) (J.J. Panetier, P. Convert, J. Torregrossa).
- DB21: Four-circle diffractometer with PSD for biological macromolecules (M. Roth, A. Bentley, G. Bentley, M. Thomas).
- S18 : Neutron interferometer on thermal neutron guide H25 (T. Wroblewski, A. Rumpf, G. Schmid).
- S21 : Double crystal diffractometer (C. Zeyen, R. Chagnon).

INTRODUCTION

Considerable effort has been expended in 1984 for the building of new instruments and the renewing of existing facilities. As a result the group is involved in the installation of D2B at the H11 beam-port and the commissioning of an interim version of D20 which will replace D2. Another major modification will be D9B, the renewed version of D9.

Aside from these major projects an important concern of the group is the modernisation and standardisation of the motor control and shaft positioning electronics. It is now generally accepted within the group that the ILL designed "Munnier" microprocessor based closed loop control modules, provide a satisfactory standard. Consequently a large slice of the investment budget of the group for 1984 and 1985 has been committed to the replacement of the old Carine electronics on D1A, D10 and D9. This replacement should be completed by the end of the shut-down in the summer of 1985, by which time the only instrument in the group still using Carine electronics will be D5. A further significant fraction of the group budget is committed to equipping more of the instruments with computer directed high precision temperature controllers.

The other changes and improvements planned are those which are either made necessary by the work being carried out on the reactor, or exploit the long shut-down to carry out work which would otherwise take the instruments concerned out of normal operation for one or more reactor cycles. The more important projects are listed separately below.

— Interchange of the monochromator positions of D1A and D1B.

— Modification of the D5 monochromator and shielding.
— Advantage will be taken of the shut-down to extend the marble floor of D4/IN1 into the D4 preparation area. This will allow delicate equipment to be set up on D4 whilst IN1 is operating and subsequently transferred smoothly into the operating area.

In addition to the more important projects outlined here, most of the instruments plan other minor improvements either in their operating characteristics or in their software support.

MAJOR INSTRUMENT MODIFICATIONS

D1A and D2B

The instrument (see picture) has been completed and set up for testing behind D1A/D1B. The 160° detector shielding, weighing over 1 ton, gives excellent results. The mechanisms, belt driven, with direct encoding, are capable of positioning the detector to the required precision of $\pm 0.005^\circ$ (individual microprocessor positioning electronics, driven by a PDP11/24 computer and linked directly to the PDP10). The focussing monochromator (300 mm high) has not yet been completed, but test data were obtained using an old flat Ge crystal. D2B is now being moved to the H11 beam inside the reactor hall, and should start its operation there soon after the reactor start-up. Fig. 66 shows the calculated performance which will be unequalled for the solution and profile refinement of moderately complex crystal structures.

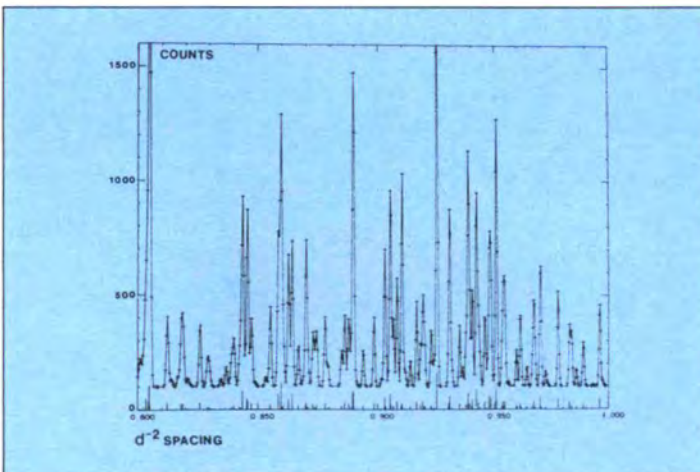
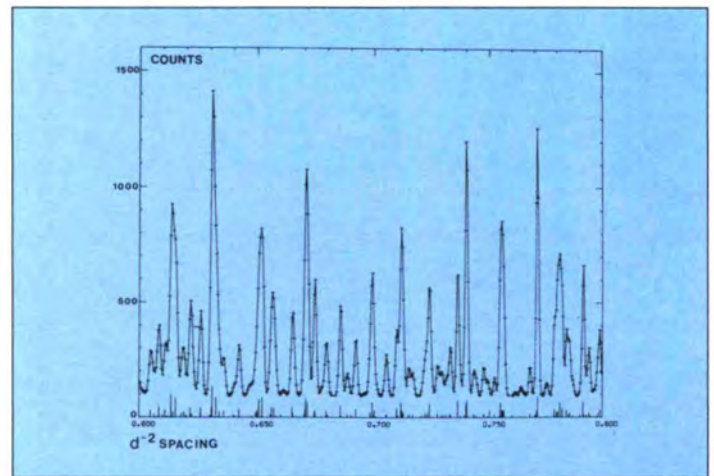
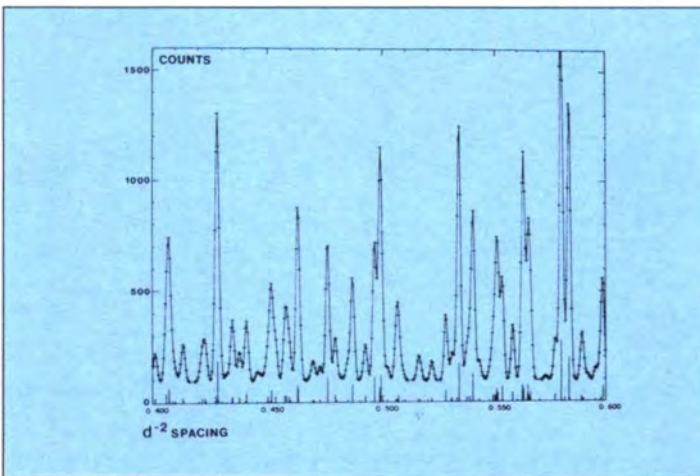
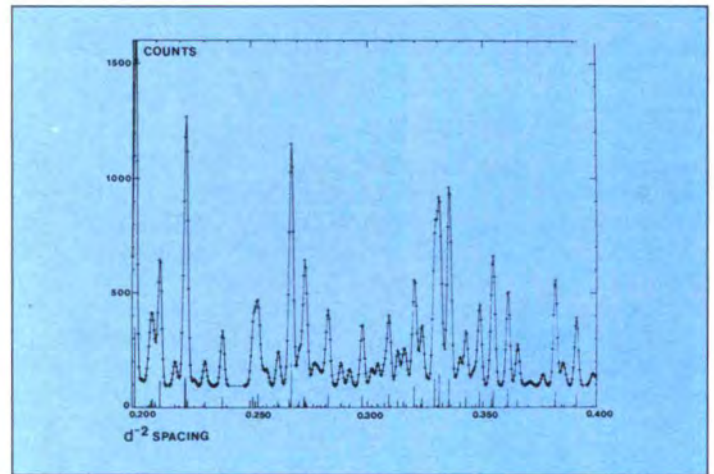
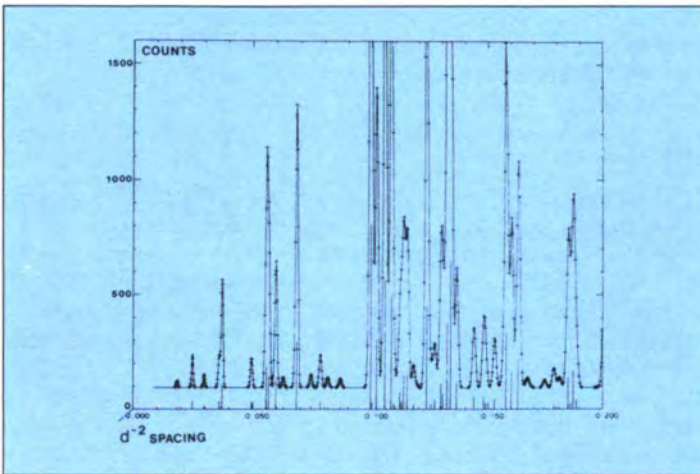


Figure 66: D2B calculated diffraction pattern for Tutton's salt, a monoclinic 750 Å³ cell (B.J. Hathaway and A.W. Hewat (1984) *J Solid State Chem* 51, 364-375).

D1A is being refurbished (electronics and computer identical to D2B) and will serve as a special diffractometer for experiments requiring longer periods than the normal 2-3 days for D2B.

D1B

Several improvements are under way:

- The instrument will be shifted up-stream to the first position of the H22 guide which should yield a better stability of the incident flux. This is of great importance for spin glass and physisorption experiments.
- A focussing graphite monochromator will be installed (flux increase by ~ factor 3 at $\lambda = 2.52 \text{ \AA}$).
- A new ILL precision temperature controller (ILL-PTC) will be installed and interfaced with the data acquisition system so that automatic T scans in both the cryostat and furnace will become possible.

2

— The use of polarized neutrons will be facilitated. D2 has been taken out of commission in February 1984.

D3

In conjunction with the replacement of the H5 beam-tube substantial work was invested in renewing motor control electronics and some ageing mechanical parts. Although the instrument showed a reliable performance throughout the year, the scientific programme was restricted to measurements above 4.2 K due to instabilities in the 4.6 Tesla cryomagnet sample chamber. An automatic liquid He valve has been developed for solving this problem [1] and the long reactor shut-down will be used to incorporate this device in the D3 cryostat. Progress was made with the reliability of the liquid nitrogen refilling system: an optoelectrical sensor (based on optical fibre techniques) is used which detects the sudden changes of the refraction index at the liquid-gas interface.

[1] Brevet français No. 84 10673 by F. Tasset, S. Pujol, P. Morin (ILL) (5.07.1984) Vanne droite à commande électrique proportionnelle.

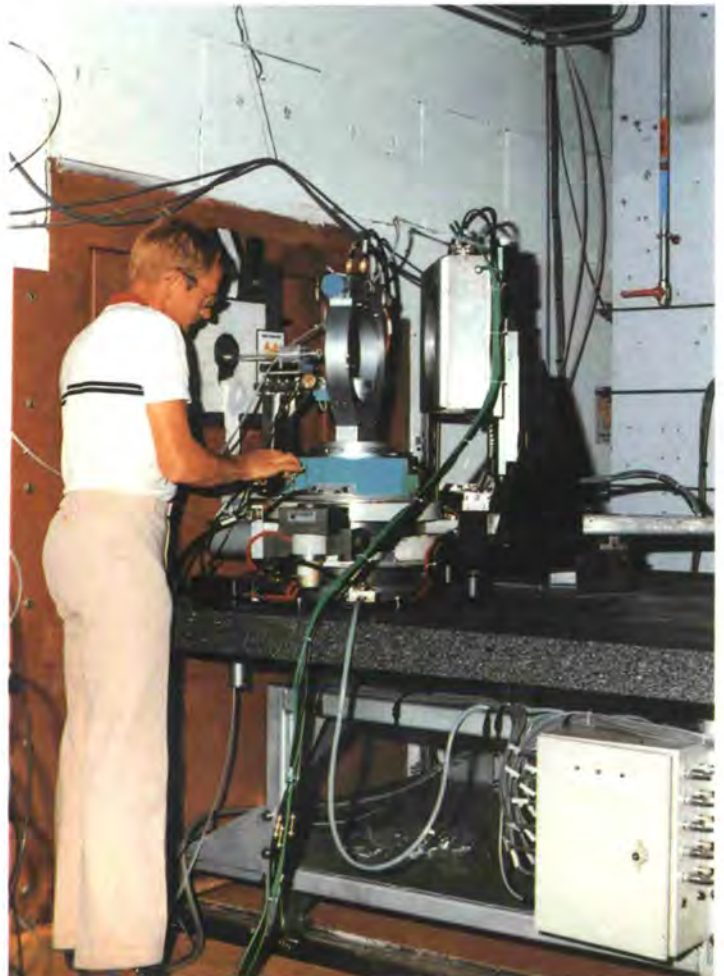
D4B

The pressure for beam-time during this first year of operation of the new D4B was rather high due to the time sharing system (with IN1B) and the long waiting list of users. Practically all the different groups had access to the machine and most sample configurations were tested (isotopic substitution technique; low and high temperature; pressure vessel tests). The average duration of an experiment was less than 4 days. This short time, in addition to the increased instrument complexity and accuracy, requires more skill from the experimentalist. Various new experimental requirements (2 multidetectors at various distances from the sample, new background problems related to new geometries; the handling of the multidetectors at very high accuracy etc.) had to be developed at the expense of the ongoing experimental programme, as there was no test time available. Immediate data evaluation has become possible due to fully corrected and regrouped "intensity versus angle" plots. The gain of the data collection rate, compared with the previous D4 equipped with a 20 cell detector, is about a factor 100. Roughly one order of magnitude is gained by the monochromator and by the improved geometry. The small angle background has been significantly improved, the loss in resolution being $\sim 10\%$. Calibration of the new 64 cell ^3He detectors can now be achieved within an accuracy of 10^{-3} in a few hours. During most experiments a statistical accuracy of $3 \cdot 10^{-3}$ was achieved and in some cases 10^{-3} . The impact of the new D4B on the scientific programme cannot be fully assessed, but it certainly simplifies considerably partial structure factor determinations using the isotopic substitution

technique. The one year experience also showed that sample quality and/or sample environment stability (high temperatures!) require the utmost care.

D5

The instrument was equipped with new collimators which can be evacuated, and with solid Boron carbide slits, both additions reducing the background substantially, particularly at small angles. The temperature range, by using the ILL/TBT dilution refrigerator, was extended to the mK region. An extensive range of temperatures, field and pressure configurations now exist. The dismantling of D5 due to the H4 beam-tube exchange will enable a complete overhaul of its mechanical parts. D5, improved by a new monochromator, will be reinstalled during the summer of 1985.



M. Thomas adjusting the test set-up for DB21 at the H14 guide.

D9

D9 will be almost completely renewed and is expected to be completed as D9B by mid 1985. The old D9 finished its service in 1984. Part of the activity in 1984 was dedicated to the definition of new control electronics. Likewise, the new Eulerian cradle was tested, and the first construction of a new cryostat holder for a two-stage displax cryorefrigerator was completed.

An essential part of D9B will be the new monochromator shielding to be placed ~ 3 m closer to the core (compared with the former set-up). The protection is presently being fabricated and new monochromator holders are being designed. This design is aiming at the use of a horizontally focussing monochromator compensating for the high vertical anisotropy of the hot source beams, and at the same time, shifting the focusing to slightly higher scattering angles. An area detector (gas type) with 32×32 elements and 2 mm interspacing is presently under construction.

D15

D15 was reinstalled in November 1983 after the beam tube exchange and restarted scheduled experiments in December. Since then a full schedule of experiments has been carried out over a wide range of temperature, pressure and applied field. The new X, Y, Z table allows more rapid and precise centering of samples held in cryostats and furnaces. After temporarily using a painters scaffold a narrow high level platform has been installed to allow access to the sample with the 4.6 T superconducting magnet in place. Modifications which make the control of sample position within the magnet compatible between D3 and D15 have been made. A successful experiment on EuAs_3 using the superconducting magnet allowed the identification of three different magnetic structures, two incommensurate and one commensurate, induced by applied field.

D16

Use of the machine has been considerably eased for some small angle scattering users by the introduction of an automatic sample changer, with up to 16 sample positions.

During the shutdown, new machine control software will be introduced. This will be similar to that of other multidetector machines in the group and will facilitate the use of D16 in the single crystal mode. At the same time, better software for the sample changer will be included. More comprehensive data treatment programs are being written for the DEC10, to be used from the Tektronix in the cabin.

The possibility of separating the machine from the Be filter support is being studied, so that for some experiments it will

be possible to put the specimen about 70 cm nearer to the monochromator, so increasing the maximum possible flux on the specimen by a factor of about two.

There is also a longer term study which has the aim of putting the filter and first slits inside the monochromator housing. For many experiments this would improve the resolution by a factor of about two for the same intensity, and also cut down the general background level.

D19A/H24

Since November 1983 the instrument has been exploited for experimental data collection while at the same time developing the associated software. A massive effort has been expended over the last ten months in improving programs for the acquisition and analysis of data. The D19 VAX 11/750 is used to perform a sophisticated, *on-line* reduction of the three-dimensional data array to Bragg intensities.

The first protein sample investigated was a crystal of triclinic lysozyme. Approximately 7000 reflections were collected in 30 d. At the end of this experiment, the instrument was working on-line reliably. Four outside user experiments were performed.

The "banana" position sensitive detector, built by the ILL detector group appears to be very reliable now, with stability and homogeneity of $\sim 1\%$.

D20

This instrument will be installed at the H11 beam port during 1985. As a large "banana" PSD will not be available before 2-3 years from now, D20 will be temporarily equipped with a 128 cell PSD. This latter, built by Jacobé, Feltin et al has been tested before the reactor shut-down in September 1984, and revealed a good stability and low background; however, the cell efficiencies are still too different and have to be better matched. The new data acquisition system developed by Epaud and Klesse allows for stroboscopic measurements which enable the detection of periodic phenomena, such as the microscopic response of a sample under cyclic perturbations (mechanical stress, electric and magnetic fields etc.). A striking illustration of this technique was the recording of the two-dimensional (ω , 2θ) reflectivity profile from a rotating crystal of grafoil with 30° mosaicity. The rotational speed was 3000 rpm. The period of the recorded phenomena being 20 ms had to be resolved into 80 equal slices, i.e. 64 different counts from different 2θ PSD cells had to be stored every 250 μs . A counting time of 80 s yielded a total counting time of 1 s per ω position, each position being set 4000 times during this period of

time. Fig. 67 shows two peaks of equal intensity, indeed a breaking of the "Friedel"-symmetry rule would require higher rotational speeds!

DB21

This joint ILL/EMBL project is a four-circle diffractometer equipped with a two-dimensional PSD, for low resolution crystallography of biological macromolecules. The instrument was tested at the H142 guide for about 4 weeks in 1984. It was designed for the use of a two-dimensional PSD with a spatial resolution of <2 mm. The detector initially available was of the "multistrip avalanche chamber" type operating with a Gd-foil as neutron-electron converter. The present state of the art, however, showed that this type of detector is not suited for DB21, due to its intrinsic high γ -ray sensitivity and low neutron efficiency. For that reason two other types of PSD are being prepared and are expected to be available by mid 1985: 1) a multiwire ^3He multidetector and 2) a scintillation detector of the Anger Camera type. During the first half of 1985, DB21 will be transferred to its definitive position at H15 and is expected to be operational by the end of that year.

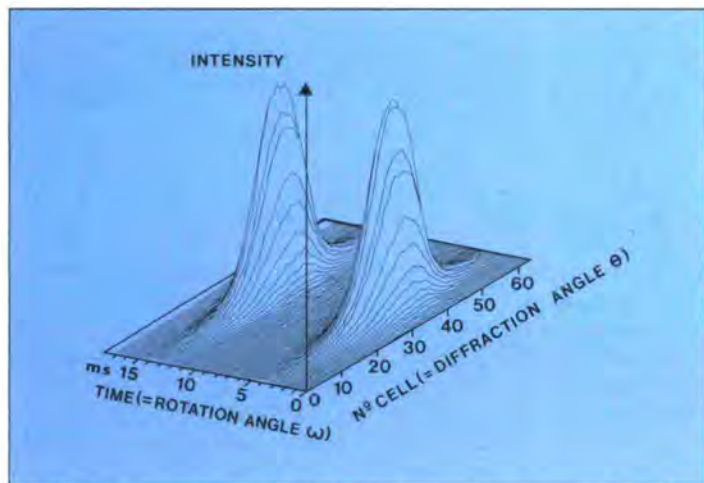


Figure 67: Stroboscopic recording of the reflectivity profile from rotating grafoil, on D20.

S18

Two new interferometer crystals providing space for larger samples have been manufactured and tested successfully. They were used for experiments requiring more space, such as the measurement of the coherent scattering length of tritium (with a pressure cell) and of the Fizeau effect for neutrons (with a rotating sample). A third interferometer (two separate crystals will provide even more space and is presently being developed. During the long reactor shut-down the instrument electronics will be modernized.

S21

After a long measurement of vacancy concentration in gold the instrument was used for a variety of experiments starting on April 24th 1984. Macroscopic concentration modes in the Nb-D_x system were extensively studied via the lattice parameter distribution in samples loaded in situ. The measurements were completed by radiographic studies of the samples. The instrument was used as a high resolution triple axis (PG, Si, Si) spectrometer to resolve the Zeeman splitting of neutrons in a magnetic field (1.2 Tesla, splitting observed ~ 0.14 μeV).

This experiment was preliminary to a forthcoming study of neutron - optical effects in acentric crystals. A Ir¹⁹² (50 Ci) γ -source was tentatively installed so that on-line γ -diffraction can be performed to yield simultaneous and very accurate (10^{-6}) information on both lattice parameter variations and tilting of lattice planes. These might both be due to domains or simply parasitic sample rotations of the sample holder. The importance of this has been demonstrated for the case of lattice deformation under electric field of KDP close to its ferroelectric phase transformation. Previous results obtained by X-ray diffraction were corrected using the new technique. In this particular example spontaneous shear effects introduced errors of the order of 30% of the measured quantity. During 1985 S21 will be shifted to the H25 thermal guide and will benefit from much better neutron flux conditions.

Information received from F. Tasset
Report edited by B. Maier

Special Studies of experimental and instrumental techniques

by P. Ageron

To solve problems raised by users or due to reactor modifications, various methods have been developed including:

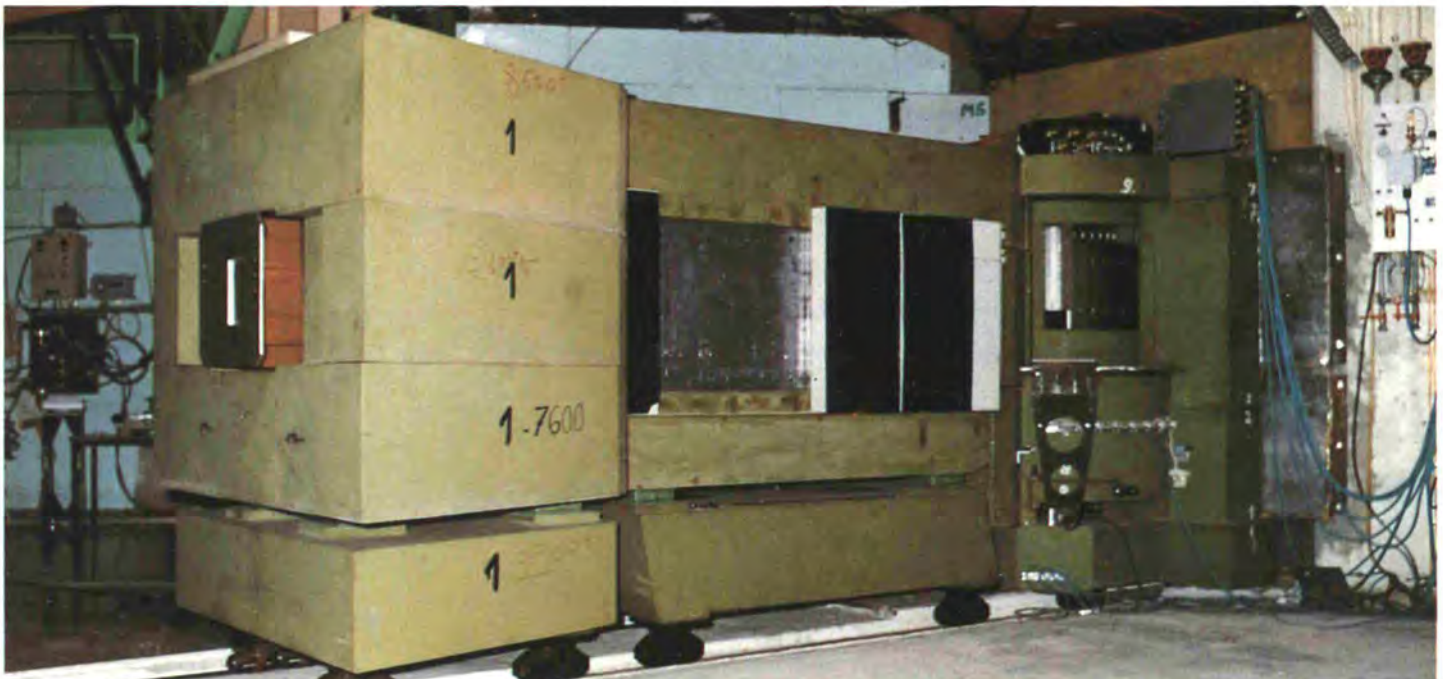
- 1) Means of calculation, i.e. adaptation of existing or creation of new programs by A. Robert:
 - a program for calculating energy transfer cross sections in hydrogen and deuterium
 - the DOT program (two dimensions, multi-energy groups of neutrons) for thermalisation and void perturbation studies
 - different programs such as ANISN (one dimension, multi-energy groups of neutrons slowing down) or MERCURE for shielding, nuclear heating, activation studies in unusual conditions
 - a Monte Carlo program for calculations of the transmission of neutrons in guides of any geometry or in systems including crystals or focalising devices

— a program for wave propagation in any combination of parallel layers, for studies of multi-layers of interfaces.

- 2) Experimental devices developed by W. Mampe and A. Beynet presently installed on PN5, and using:
 - very cold neutrons (50-100 Å) for transmission measurements using multiple reflexions in real or scaled down guides, reflexion curve measurement for interface studies and development of multi-layer monochromators
 - ultra cold neutrons for studies of neutron life times in bottles and of UCN transmissions by membranes.

Among the different problems treated or being studied are:

- the improvement of the vertical cold source with a cavity and a vertical guide
- the optimisation of the second (horizontal) cold source
- the perturbation caused by the enlargement of a beam-tube (e.g. H11)
- nuclear engineering problems associated with the cold sources (in cooperation with the Reactor Team and the Health Physics Group)
- the qualification of metallic neutron guides (in cooperation with Garching, FRG)
- the improvement of the superfluid helium UCN source, membranes, neutron life time (in cooperation with Rutherford Appleton Laboratory, UK)
- the optimisation of neutron guide systems (for the second ILL cold source and for Jülich, FRG)
- the improvement of UCN life-times in bottles.



3

EXPERIMENTAL ACTIVITIES IN 1984

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WORKSHOPS AND CONFERENCES

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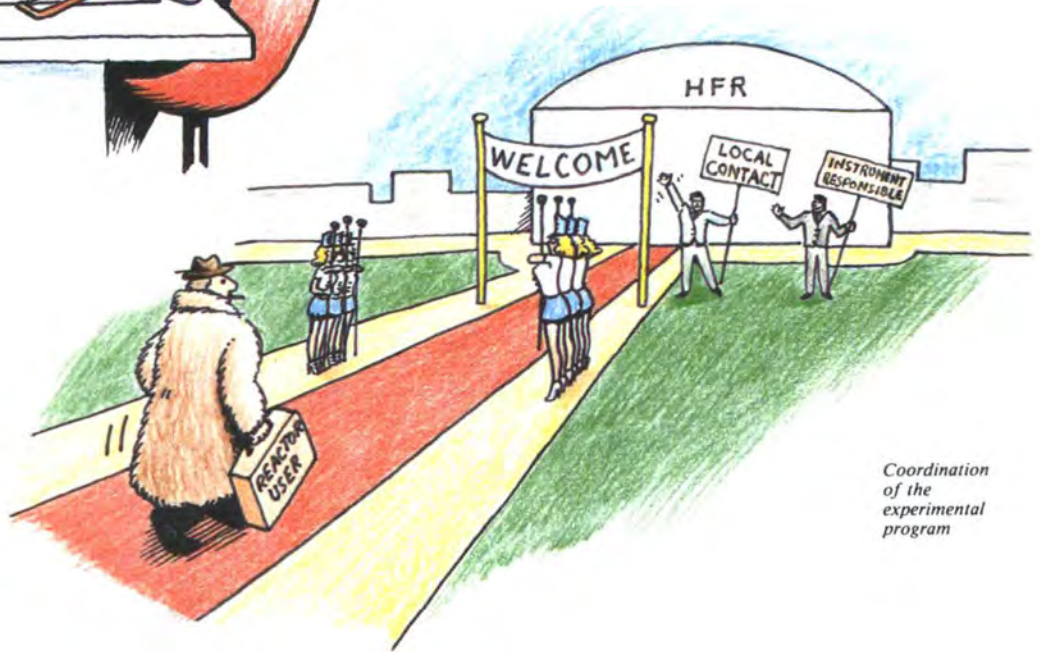
PUBLIC RELATIONS

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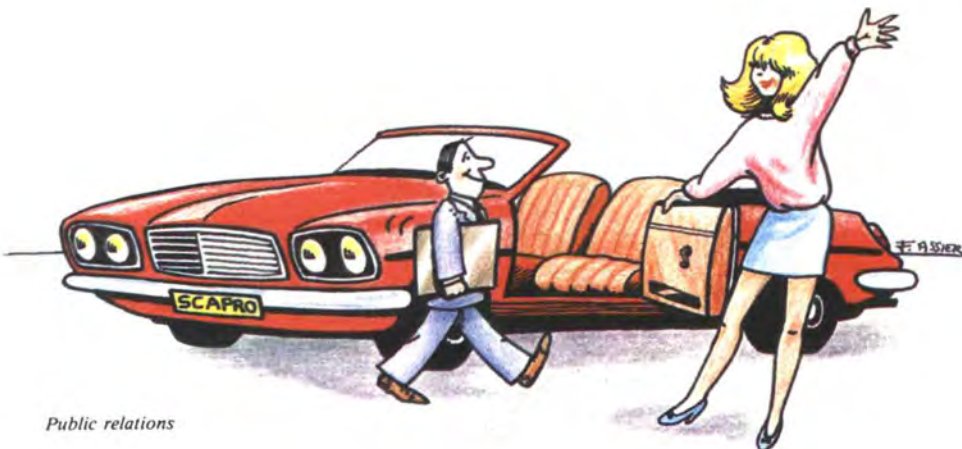
SCIENTIFIC COORDINATION AND PUBLIC RELATIONS OFFICE



Workshops



Coordination
of the
experimental
program



Public relations

3

EXPERIMENTAL ACTIVITIES IN 1984

The announcement that the reactor would be shut down for approximately 10 months from the end of September 1984 marked the beginning of an intense period of scientific activity. Beam-time applications from groups wishing to complete on-going scientific programmes before the shut-down, showed a considerable increase and the specially arranged meetings of the sub-committees in February 1984 was the last opportunity for some 18 months to apply for, and carry out, experiments at the ILL. In addition, delays in the programme during 1983 caused by reactor problems, had resulted in a large back-log of approved experiments which, together with the newly approved proposals in February, presented the office with the formidable task of co-ordinating 707 urgent experiments to be compressed into the remaining 5 reactor cycles. That the last of these 707 experiments was concluded in an emergency prolongation of the 5th reactor cycle, makes it worth-while recording here, our thanks to all those who contributed to the success of the operation:

- the ILL scientists, instrument responsables and technical staff who had themselves a considerable in-house programme of neutron test experiments directly concerned with commissioning requirements of new instruments
- external scientists who showed considerable patience with repeated re-arrangements of the programme during its course, designed to ensure that neutron beams were intensely used
- the reactor staff who provided the basic means (neutrons) of completing the programme and often under very difficult conditions towards the end of the 5th cycle.

The absence of an active external scientific programme during the last few months of 1984 was not allowed to detract from the vigorous scientific atmosphere usually associated with the Institut. An enhanced programme of scientific seminars and workshops began and will continue for the duration of the reactor shut-down and of course the forum for discussions, of which the Institut is justifiably renowned, will be scrupulously maintained by a programme ranging from invitations for long term visitors to the welcome given to transitory scientists wishing to call in for a few hours for talks with in-house colleagues.

The instrument availability and usage from January to September 1984 is given in table 1.

TABLE 1

Beam-time Allocation and Instrument Statistics

The reactor operated for 5 cycles between 3rd January and 4th October 1984. Three cycles were interrupted by short shut-downs, the lost time being recuperated by a prolongation of the operating period. The 5th cycle ended with 11 days at 70% of full power during which time the scientific programme was able to continue with some experiments being given compensatory increased beam-time allocations. The following figures are based on an equivalent full power operating period of 217 days.

TABLE 2

Special Beam Experiments (under preparation, in progress or carried out in 1984)

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)	47		47					18	Time-sharing BeF + D4 Time-sharing 3-axis + D4 Removed for installation of IN20 Installation of a dedicated computer
IN1 (BeF)	28				10		18	16	
IN2	48		23		25			0	
IN3	115		93				22	102	
IN4	150		64		33			67	
IN5	177		45		21	16	95	40	
IN6	165		50		24	26	65	52	
IN8	151		141		10			66	
IN10	166			2	50	4	110	51	
IN11	158		87	4	21	5	41	59	
IN12	159		115		44			58	
IN13	164				63	11	90	53	
IN20								30	Pre-commissioning tests
D1A	163			157	6			54	
D1B	162			101	10	6	45	55	Instrument removed (March 1984) for H11 installation
D2	70			37	33			18	
D3	182			182				35	Time-sharing 3-axis + BeF and final commission
D4	80				73	7		28	
D5	174		55	119				43	Instrument removed (March 1984) for H11 installation
D7	159		30	87	22		20	58	
D8	69			40		29		19	
D9	163			161	2			54	
D10	100		7	64	25		4	117	Tests include Spin-Echo feasibility programme
D11	172			22	20	57	73	45	
D15	174			174				43	
D16	164			20		77	67	53	
D17	203		13	12	26	55	97	14	
PN1	182	182							
PN2	167	167							
PN3/4	190	190							
PN6	202	202							
PN8	220	220							

Beam Position	Proposed by	Title	Time Allocated
H142	University of Heidelberg	β -decay of polarized and unpolarized neutrons	3 cycles
H16	Berlin and Munich Universities	Determination of range profiles and lattice positions	long-term
H17	R.A.L. ILL	Upgrading of superthermal UCN source	2 cycles
H17	Sussex Univ., Harvard Univ., R.A.L.	Search for the neutron EDM	Long term
H18	Rouen Univ., Uppsala Univ., CENG	Boron-labelled probes in physiology and oncology	42 days
H21	P.T.B., Braunschweig	Experimental determination of h/m (initial stage)	Long-term
H22D	Gent University	Study of n-alpha and n-fission reactions	4 cycles
H22E	Darmstadt and Bordeaux Univ.	Multiparameter measurements of light particle-associated fission of ^{241}Pu	4 cycles
H22F	Munster, Bochum Univ. and ILL	Stellar reaction rate of Al^{26} (N.P.) Mg^{26}	14 days
H22F	Manchester University and ILL	Gamma-Gamma correlation studies	21 days
H22F	Sussex University and ILL	Level structure determination, directional correlation measurements and low spin state studies	1 cycle
H22F	Surrey University	Fundamental aspects of neutron tomography	14 days
H22F	Sussex University	Neutron capture by Krypton	21 days
H24	Stuttgart University	Macroscopic and microscopic thermal expansion studies	2 cycles
H24	Ispra and ILL	Dual polarized beams	30 days
H25	Munich University	Concentration profiles by (n, γ) and (n, p) reactions	Long-term
H25	Marburg University	In-beam NMR studies	5 cycles
H25	Dortmund Univ. Vienna, Dubna	Neutron interferometry studies	Long-term
IH3	Sussex Univ., Harvard Univ., RAL	Search for EDM of the neutron	Long-term
IH3	T.U. Munich	Neutron microscope studies	3 cycles

3



IN2 the first operational instrument at the High Flux Reactor (1972), was dismantled in Spring 1984 prior to being replaced by IN20. On the occasion of its removal from the ILL a celebration was organised around the "old IN2". The pictures from left to right: a) B. Dorner delivers the "funeral speech". b) P. Flores presents the "last sample" on the IN2 sample table, a Bavarian "Leberkäs".

c) U. Steigenberger demonstrates how a neutron detector can convert neutrons into a delicious Beaujolais. d) The ILL Jazz Band provided the instrumental accompaniment (from left to right: Y. Lefebvre, R. Klesse, W. Stirling and S. Heathman).

WORKSHOPS AND CONFERENCES

The office has organised four workshops in 1984:

- 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. Zaccai, CNRS-Grenoble).
- 4) "Powder Diffraction", 2-3 August 1984 (Responsible: A. Hewat).

Except for the 4th workshop all the proceedings are available (Published in *Journal de Physique*).

The workshops/conferences to be organised in 1985 are:

- 1) "Diffusive Molecular Motion", 4-15 March 1985 (Responsibles: J.P. Beaufils, M. Bee).
- 2) "Interpretation and Uses of Electronic Distributions", 26-29 March 1985 (Responsibles: P.J. Becker, P.J. Brown, F.L. Hirshfeld).
- 3) "3rd International Conference on the Structure of Non-Crystalline Materials", 8-12 July 1985 (Responsibles: C. Janot, A. Wright).
- 4) "Investigations of Higher Order Correlation Functions", 15-16 July 1985, (Responsible: J.B. Suck).
- 5) "Evaluation of Data from PSD's", 4-8 November 1985 (Responsible: M. Roth).

The following workshop will be organised jointly by the ILL and IFF/Jülich.

"Atomic Transport and Defects in Metals by Neutron Scattering", (Responsibles: C. Janot, W. Petry (ILL), D. Richter, T. Springer (IFF)).

PUBLIC RELATIONS

In addition to the brochure "ILL Neutron Beam Facilities Available for Users" (edition January 1984), the Office has produced an ILL guide which is mainly a description of the ILL infrastructure ("Guide-lines and Regulations for Reactor Users, Long-Term Visitors and New Scientific Staff", edition March 1984).

In addition to the usual "ILL Newsletters for Reactor Users" SCAPRO has edited two "Special Editions" of the Newsletter (N° 8 and N° 10) on the occasion of the ILL's case for

consideration as a site for the ESRF (European Synchrotron Radiation Facility). Both publications are available on request from this office.

A short general leaflet about the ILL has been edited in September 1984 (French and German versions are available, an English version is being prepared).

The ILL "Open Day" on September 22, 1984 organised by this office in collaboration with P. Blum (Department Instruments and Methods) was a considerable success (about 800 people from the Grenoble area visited the Institut).



In the picture B. Maier, head of SCAPRO, is showing Professor Haensel (Universität Kiel) the series of publications edited by his office during 1984.

4

MECHANICAL CONSTRUCTION

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ELECTRONICS

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MULTI-DETECTORS

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MULTI-LAYER LABORATORY

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SPECIAL INSTRUMENTS

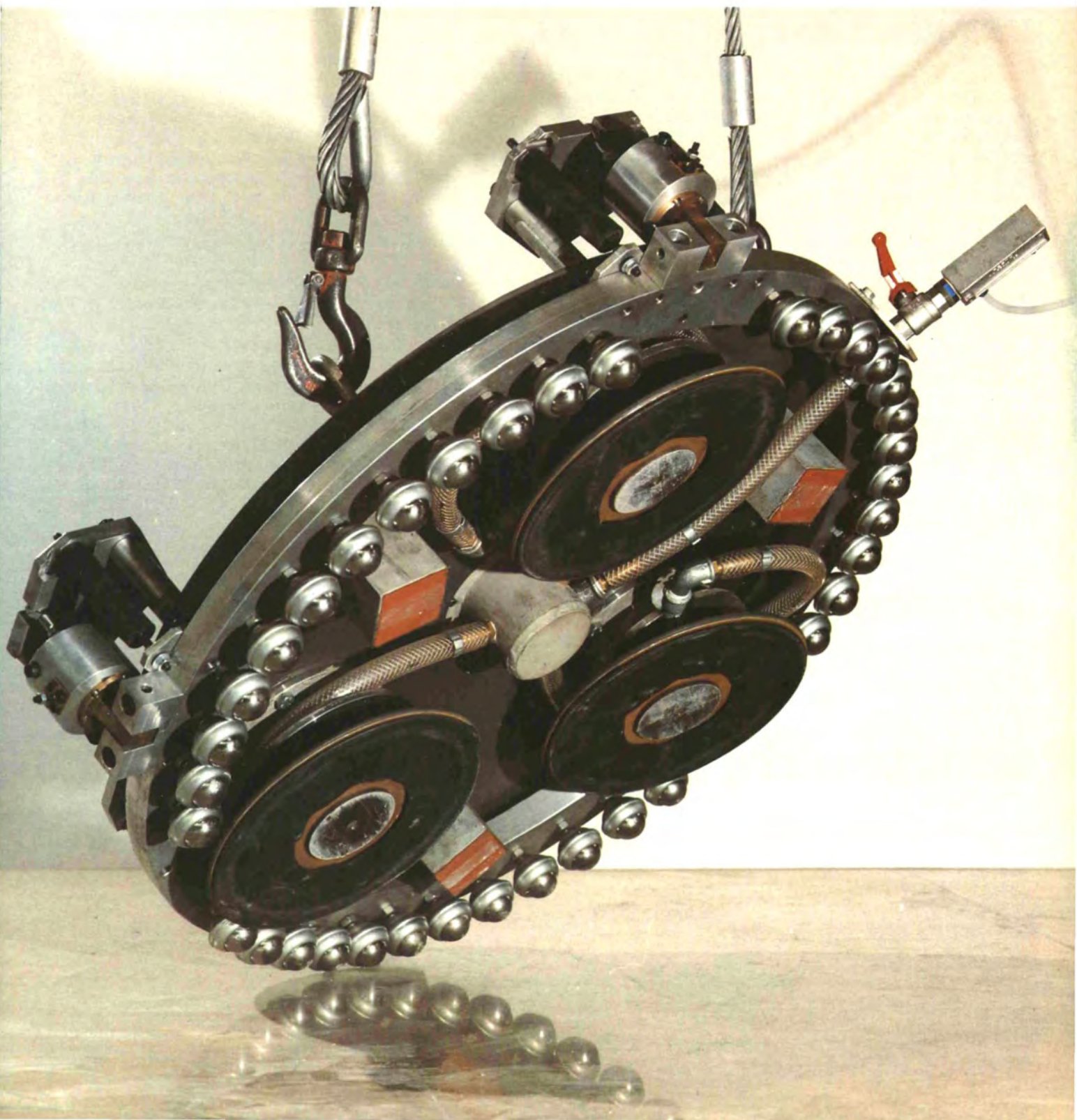
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MONOCHROMATORS

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Standard module of an instrument support (version with 3 cushions) for heavy loads equipped with a ball bearing ring. ►

DEPARTMENT INSTRUMENTS AND METHODS



4

Introduction

The functions of the Instruments and Methods Department cover both the construction, modification and maintenance of the instruments available to visitors and also the maintenance at the best possible level and the development of neutron measurement methods.

The major events include the shut-down of IN2 and the installation of IN20 in its place; the first neutron tests took place in July. Similarly D2 and D8 have been definitively shut down,

giving way to the new instruments D2B, D19 and D20, which should start operation in 1985.

In the field of development of methods a contract with the Max Planck Institut should permit the production of beryllium monochromators, while at the ILL the furnace for growing copper crystals started operation. The multidetector production group has been provided with a dust-free workshop. Finally the evaporator installed in 1983 became operational, permitting the production of polarisation analysers for D7B and of various supermirror assemblies for external laboratories.

Einleitung

Die Aufgaben der Abteilung für Instrumente und Messmethoden umfassen den Bau, die Umrüstung und die Instandhaltung der den Reaktorbenutzern zur Verfügung gestellten Instrumente. Ausserdem obliegt ihm die Aufgabe, Messmethoden für Neutronen auf dem neuesten Stand zu halten und weiterzuentwickeln.

Unter die wichtigsten Ereignisse im vergangenen Jahr war die Stilllegung von IN2 und die damit verbundene Installation von IN20 zu zählen. Erste Neutronentests fanden im Juli statt.

Ebenso wurden D2 und D8 abgeschaltet, um Platz für D2B, D19 und D20 zu schaffen, die ihren Betrieb gegen Ende 1985 aufnehmen werden.

Im Bereich der Methodenentwicklung sollte der Vertrag mit dem Max-Planck Institut Stuttgart zur Entwicklung von Beryllium-Monochromatoren, sowie die Inbetriebnahme eines Ofens zur Züchtung von Kupferkristallen erwähnt werden. Die Multidetektorgruppe erhielt eine staubfreie Werkstatt. Schliesslich sei auf die Inbetriebnahme der im Jahre 1983 installierten Aufdampfanlage verwiesen, die die Verwirklichung der D7B Polarisationsanalysatoren und die Herstellung verschiedener Serien von Superspiegeln für auswärtige Labors ermöglichte.

Introduction

Le Département Instruments et Méthodes a pour mission, d'une part la construction, les modifications, la maintenance des instruments mis à la disposition des visiteurs, et d'autre part, le maintien au meilleur niveau et le développement des méthodes de mesure avec neutrons.

Parmi les faits marquants on peut noter l'arrêt de IN2 et l'installation sur le site de IN20, dont les premiers tests en neutrons ont eu lieu en juillet. De même D2 et D8 ont été

définitivement arrêtés au profit des nouveaux instruments D2B, D19 et D20 qui devraient démarrer en 1985.

Dans le domaine du développement des méthodes un contrat avec le Max Planck Institut permet d'espérer la réalisation de monochromateurs en Beryllium, tandis qu'à l'ILL le four de tirage des cristaux de cuivre devenait opérationnel. Le groupe de réalisation des multidétecteurs s'est vu doté d'un atelier hors poussière. Enfin, l'évaporateur, installé en 1983 devenait opérationnel et permettait la réalisation des analyseurs de polarisation de D7B et de divers ensembles supermiroirs pour des laboratoires extérieurs.

1. MECHANICAL CONSTRUCTION

The Mechanical Construction Group includes four sectors: mechanical design, production workshop, industrial relations and sub-contracting, assembly and testing.

In 1984 there was a considerable increase in priority work requested by the Reactor Department in connection with the long shut-down, while in parallel with this there was construction of experimental equipment with a particular effort on mechanical devices for focusing neutron beams. As regards construction work, it was found that of 5500 hours, 30% were devoted to the reactor and 70% to the instruments. The sub-contracted work diminished by 30%.

The work of the group was essentially in its traditional fields: new construction, maintenance and modification of equipment in operation, inspections and tests, technological developments.

NEW INSTRUMENTS

In 1984 there was full utilisation of the test position in the test hall. This permitted mechanical, electrical and electronic testing of complete assemblies or sub-assemblies for IN20, DB21, D2B and D20 before their installation on the beam port. D4B which consists of a modified version of the old D4, adapted for direct encoding, started operation in summer. Simultaneously the first neutron tests were carried out on IN20 together with the evaluation of the D19B shielding. The construction of the mechanical parts of D11C made good progress and installation in the neutron guide hall was started in December 1984. S2M, the first rotor on magnetic bearings with Soller collimator, which will be used on IN4, has operated at 30000 rpm. The first mechanical tests on the test position of the IN5 chopper on magnetic bearings from Jülich took place shortly afterwards. An ILL-type air bearing chopper adapted to D7 is under test.

MAINTENANCE

Maintenance covered the mechanical structures in operation, velocity selectors, choppers, etc., and also involved participation in the reactor maintenance work, particularly on the main neutron guides (H1-H2).

INSPECTION AND TESTING

This work takes place on request or in the form of support for maintenance. The acquisition of a digital reading T 2000 theodolite and the maintenance at the best possible level of the metrology equipment (vibrations, displacements, dimensions, etc.) make it possible to provide efficient assistance to all the other Departments.

TECHNOLOGICAL DEVELOPMENTS

Components: Circular orientation units (rotating disks with vertical axis), with integrated direct encoding have been developed. One model has been tested with ball bearings, and another on an air film, the results of industrial cooperation between ILL, SEIV, SLAM, PRECILEC and THOMSON.

Table spectrometer: Construction of an X-ray and Gamma spectrometer on air cushions with modular FRANKE-HEYDRICH or SLAM components with integrated encoding.

Displacements on air cushions: general introduction of combined air cushions incorporating pressure skirts and ILL air pads which equip the IN11B spin analysis lines. In parallel with these systems designed for marble floors, combined air cushions with shock absorbers have been developed for marble or resin floors: air cushions with a single central skirt or with several skirts.

As regards the technology for the floors which is associated with these air cushions, tests have shown how to handle a resin, which has been adapted to the aerostatic conditions, but is not resistant to thermal shocks (such as liquid nitrogen falling on it), against which only marble is resistant. In these uses of resins, for which some tests remain to be done, structures must be designed with protective features to avoid cold liquids falling on them. This solution of resin with a layer of special concrete costs only half as much as the present marble floor.

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2. ELECTRONICS

The Electronics Group itself, is responsible for the construction and maintenance of instrument control systems. If no account is taken of the collaboration with industry which has been more or less important at different periods, with on the one hand the neutron detection team and on the other the computing staff responsible for the data processing and the general design of instrument automation, one can say that the Electronics Group has changed relatively little since the first years of the ILL.

Despite an almost unchanged staff complement, this group has successfully dealt with the construction and development of a large number of instruments (more than 30) and a fundamental change in the technologies used. During this period of some 10 years, electronics has moved from the transistorized circuit to the integrated circuit, and the microprocessor appeared, developed and finally became predominant. Microprogramming has very quickly become one of the major tools of the electronics specialist.

Within the group this trend was accompanied by a certain number of divergent developments on generally connected problems. This variety again results in problems of maintenance which are the more serious because the technologies used become obsolescent more rapidly.

In 1984 the Electronics Group of the Instruments and Methods Department developed on several planes: the structure of the group, the laboratory equipment, the standardisation of the basic electronic modules and the extension of the rooms.

STRUCTURE OF THE GROUP

Since the beginning of 1984 the majority of the design, construction and maintenance work for the instrument control systems has been carried out by two groups instead of three. All the 3-axis spectrometers and all the standard diffractometers have been entrusted to one group, while the second group is responsible for instruments with special operating conditions: high data acquisition rate requiring memories and fast display of spectra, time-of-flight analysis with specialised electronics and phasing of fast velocity selectors.

Two persons outside this group deal with maintenance and control of general equipment, stores, documentation and work on material using analogue electronics.

LABORATORY EQUIPMENT

To deal with the increasing requirements for development of microprocessor systems while limiting the number of different

types of these components, the laboratory has been provided with a centralised development system. By means of a system of interconnection and a multi-user operation system, the electronics technicians of the entire ILL have available a PDP 11/24 computer equipped with a large capacity memory, printers and a universal programmer. Among other features the software includes cross assemblers permitting the use of the main microprocessors used at the ILL, in particular the new 16 bit micros.

STANDARDISATION

A support for future developments has been introduced in the form of the "VME standard" which will conveniently complement the NIM and CAMAC standards every time problems require it. This new standard has the advantage of having a single bus permitting dialogue between electronic modules each built around a 68000 microprocessor. This standard has been adopted following CERN and a large number of European laboratories.

Among the immediate applications may be mentioned the development of TOF electronics with programmable parameters, the development of a rapid display system for spectra during acquisition, and the remodelled IN10 data acquisition system.

The gradual introduction since 1981 on new or renovated instruments of a closed loop motor control module using CAMAC continued in 1984 on DB21 and on the diffractometers D1A, D9 and D10.

The general introduction of CAMAC scalers on the 3-axis spectrometers will be completed for summer 1985.

PREMISES

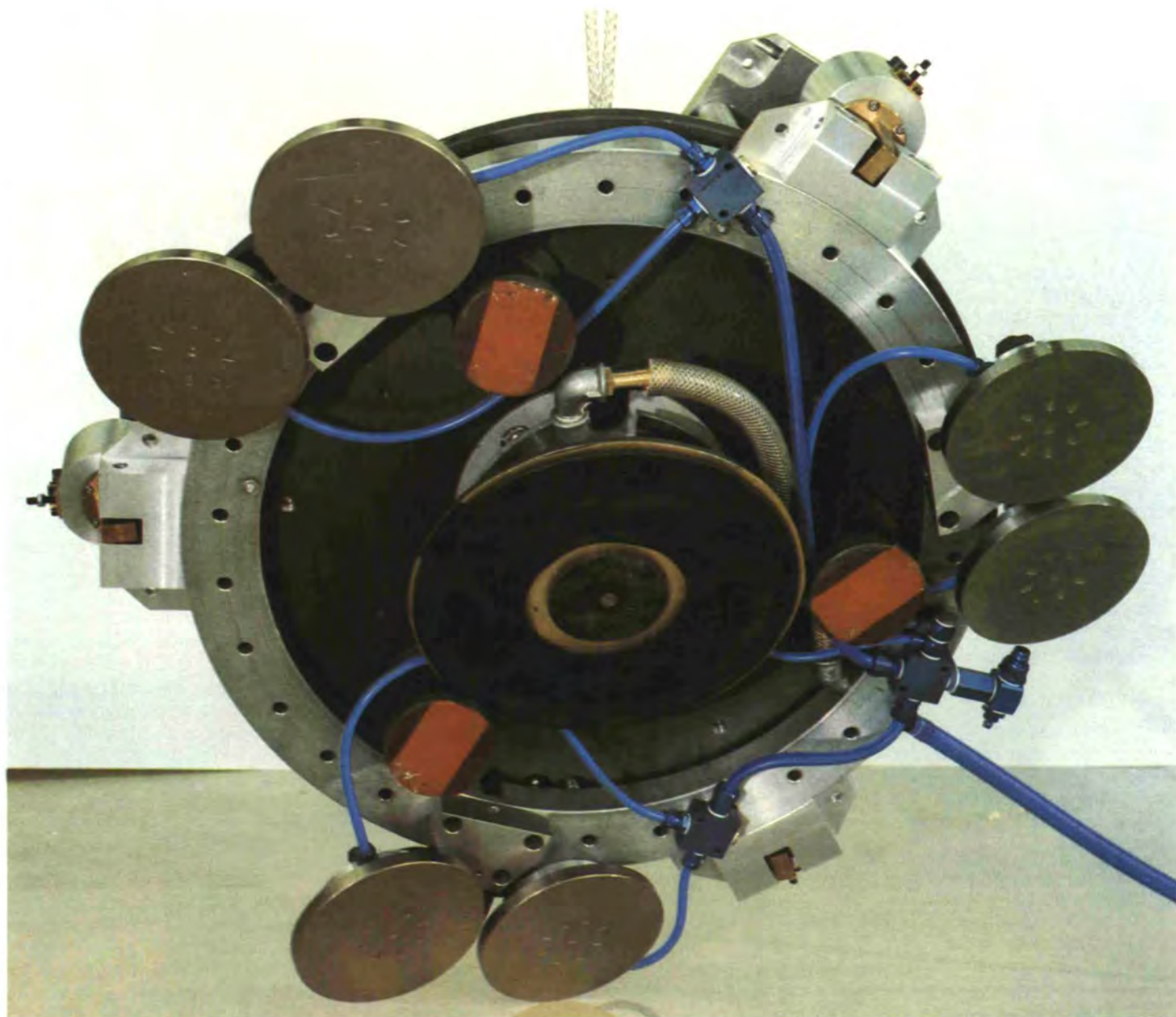
Extension was in progress when this report was prepared. This is to rehouse the small general service group in a more suitable 30 m² laboratory.

The resulting free space will mean that a laboratory of more than 120 m² organised around the development computer mentioned earlier can be allocated to the two groups responsible for the instruments.

The more interesting projects completed include:

- the construction of the diffractometer DB21, financed partly by EMBL, in a very short time,
- the completion, tests on platform and assembly of the new 3-axis instrument IN20,
- the design study for a PRECILEC multiplexer making possible the use of these encoders in a "pseudo-closed" loop to control the motors of diffractometers D9 and D10,

- the completion of a Solar-Camac interface for installation of Camac scalars on the 3-axis spectrometers,
- the restoration and improvement of S18-S20,
- the start-up of a new data acquisition system on D20, permitting kinetic and/or stroboscopic measurements (suitable for the acquisition of 1 to 4000 individual detectors),
- temporary installation of the new diffractometer D2B testing and phasing of new choppers rotating at 30 000 rpm on IN4,
- dismantling of all the instruments at the reactor in preparation for the work scheduled for the first half of 1985.



Standard module (simple version) of an ILL instrument support equipped with inflatable air cushions and stabilizing aerostatic suspension.

3. MULTIDETECTOR DESIGN AND CONSTRUCTION GROUP

(A. OED, J. JACOBÉ)

The ILL plans the new construction of six position sensitive neutron detectors (PSD) for the equipment of several instruments; the prototypes for the spectrometers D20 and DB21 have already been constructed and tested at an earlier stage.

Two small gas detectors with 64×64 cells each which are planned for the instruments D9 and D5 offer the possibility of testing thoroughly new arrangements for detector electrodes and of applying the technical findings to the construction of detectors with large dimensions. On the one hand, the traditional arrangement has to be simplified as far as possible in order to permit a partially mechanical production; on the other hand, an attempt should be made to eliminate entirely the wires used for gas amplification of the signals. The wires will be replaced by a structure of conductors applied to a ceramic or glass substratum.

The technical problems to produce such an electrode structure are almost solved since the procedures already used for the fabrication of integrated circuits can be adopted. The first preliminary experiments to test these two points are encouraging.

Besides this project, other developments using crystal scintillators with a high light output are envisaged: the photons are not detected with photomultipliers but with highly sensitive semi-conductor diodes. Recently commercialized photodiodes of this kind seem to be appropriate to this purpose. Whether it will be possible with this arrangement to produce a large-scale neutron detector with a low sensitivity can only be determined in the light of what the preliminary tests will demonstrate.

In the field of laboratory equipment and production, the group was transferred in 1984 to new premises especially adapted: on the one hand a detector workshop providing for the first time at ILL a dust-free room, making it possible to work in satisfactory conditions on wiring grids, and on the other hand a spacious electronics laboratory in the new building ILL22.

As regards production, the following instruments have been commissioned: IN20, IN11B (45 detectors), D2B (64 detectors), D7 (16 detectors).

The 128 wire multidetector D20 was handed over to the experimentalists after numerous tests on the electrode system; this detector is equipped with electronics permitting high counts; a new type of detector using gadolinium foil has also

been used on the instrument DB21. This detector is extremely sensitive, and further tests are in progress. Interesting results have been obtained on D9 with a small low resolution (2 mm) detector and high efficiency for hot neutrons. For this application, wire reading electronics using a fast microprocessor and a barycentre calculation method has been tested.

In conclusion, various tests have been carried out with a view to simplifying and automating as far as possible the production of wiring grids; also the replacement of printed circuits by ceramic or glass supports.

4. MULTILAYER LABORATORY

(Responsibles: O. SCHÄRPF, W. KAISER, W. JUST, W. GRAF)

The new evaporator ETE with 2 electron guns with a possible power of 15 kW, controlled by 3 quartz monitors, microprocessors and by a PDP11 was installed in April 1983. This apparatus opened up many new possibilities with its large crucibles and complete automation.

At the beginning of 1984 many staff were engaged in the development of multilayer devices. F. Fujara continued with the evaporation of microguides to higher layer numbers which even at the first test produced a bending angle of the neutron beam of 40 degrees over a length of 10 cm. The thickness achieved was 0.2 mm in aluminium layers of 4500 Å and nickel layers of 500 Å. W. Petry, W. Just and Mrs. J. Diehl investigated the problem of defining the entrance and exit faces for the neutrons, the main field of application. W. Just subsequently carried out comprehensive tests on S3B which included chemical polishing and etching, mechanical and electro-polishing followed by the evaporation of new layers on the polished surface of the entrance and exit sides. Electron micrographs were taken. Ultimately a transmission of 47% was achieved. One multilayer was tested for its polarising capabilities, using layers of iron instead of nickel as the reflecting medium and resulting in two separated polarised beams.

In view of the imminent reactor shut-down supermirror production was transferred to the new evaporator and tests continued until the end of the cycle. F. Fujara produced the first non-polarising supermirrors on the new apparatus and overcame the problems of omitted layers. Effort was then expended on the production of polarising supermirrors with silver and iron layers and the associated problems were finally overcome by cooling down the layers before the next one was evaporated.



The ILL stand prepared by the Department Instruments and Methods for the exhibition of the Société Française de Physique in Paris from 11-14 December 1984.

Supermirrors with antireflecting layers presented no problems and production is continuing on S3 with polarizing supermirrors for D7 and on ETE for small polarisers. In total there are now 1400 supermirrors of $100 \times 300 \text{ mm}^2$ and 400 supermirrors of $65 \times 300 \text{ mm}^2$ from ETE and this number is still increasing. This makes it possible to satisfy a considerable proportion of the in-house requirements and some external orders (LLB, Gif-sur-Yvette, France; Tohoku University, Japan; BNL, USA; PTB Braunschweig, Germany; HMI, Berlin, Germany).

Due to the reactor shut-down further development was restricted. At present mirrors are being tested successfully at Würenlingen, Switzerland by W. Just.

O. Schärpf concentrated on the application of supermirrors to D7, both to gain experience in their use and to investigate possible areas of development. D17, the SAS instrument was also used during these studies and at Geesthacht (Germany) the possibility of polarisation analysis on a suitable SAS facility with multidetector was investigated.

The long reactor shut-down will also make it possible to consolidate the experience gained to date with supermirrors. The IAEA conference to be held at Jülich on "Neutron Scattering in the 90s" will be given more information about these devices.

During 1984, however, the group engaged in the evaporation of multilayers suffered from a gradual reduction of staff, which will necessarily also reduce the future effort available for this type of development.

5. SPECIAL INSTRUMENTS

(W. DREXEL)

Practically all S-Instruments and S-Experiments were in routine operation in 1984. Modifications were done either during normal reactor shut-downs or were scheduled for execution during the long shut-down.

Major modifications and improvements are summarized as follows:

S6 — the in-beam NMR spectrometer — will be withdrawn from the H25 neutron guide (an improved version of it is planned to be installed at the reactor at Jülich).

S18 — the neutron interferometer — will be dismantled for rewiring; its motor modules will be given a thorough overhaul.

S20 — neutron topography — was provided with a simple automatic control system; programming work is still underway.

On S21 — the high resolution double crystal spectrometer — test experiments on the *simultaneous* use of neutrons and a γ -ray beam have been performed. Due to exciting results it is planned to construct an automated arm for the γ -spectrometer during the long shut-down. A Ge γ -detector has been acquired for use on S21 and S34.

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For S42 — the Laue diffraction test site — a proposal for a simple control system is under discussion.

S50 — the h/m precision measurement — on completion of preliminary experiments the instrument was returned to Braunschweig for conversion into the definitive apparatus which will be re-installed during the long reactor shut-down. S52 — a neutron life-time experiment — received its detector and data acquisition system and the first test measurements were performed just before the reactor shut-down in September 1984.

Of great importance for S-activities at the ILL will be the installation of a vertical guide tube viewing the vertical cold source and thus supplying very cold neutrons and — in combination with a neutron turbine — ultracold neutrons to "Level D". This VCN-UCN source will open up new fields both in the fundamental and nuclear physics area as well as in condensed matter research. Amongst other instruments it is planned to install a neutron gravity diffractometer and a neutron gravity spectrometer (most of these activities by A. Steyerl, TU Munich).

6. MONOCHROMATORS

(A. FREUND)

Instruments:

D13A: Neutron double-crystal diffractometer on the thermal guide H24.

D13C: Neutron double-crystal instrument on the thermal guide H23.

Li2A : X-ray double-crystal diffractometer.

Li2B : X-ray orientation unit.

Li3 : Gamma-ray diffractometers.

Laboratory for crystal preparation.

STATUS OF THE INSTRUMENTS

D13A served as usual for various types of short experiments, often preliminary to extended studies on other instruments. Examples are: topography, magnetic, studies, reflectivity, transmission and mosaicity of single crystals, strains in metallurgical samples. No major modification was made.

D13C operated satisfactorily and was used for the test and assembly of production monochromators. Because of its high angular and wavelength resolution and of its versatility, some experiments were carried out, for instance on hydrogen in metals and on the thermal expansion of CaF_2 , below room temperature. There were no major modifications necessary. As

in 1983, D13C was transferred to the CENG Siloë reactor after the HFR shut-down, for continuing monochromator preparation.

The reconstruction of the Li 2A X-ray facility is almost completed, and electronics, together with a small computer for data acquisition and instrument control, were purchased. Li2A is a reduced scale version of a neutron triple-axis instrument using the air cushion technique and will serve mainly for the beryllium monochromator production: tests, in-beam plastic deformation and monochromator assembly.

The γ -ray diffraction facility Li3 consists of five independent diffractometers which are installed at two γ -ray sources of 0.0301 and 0.0187 Å wavelengths, respectively. One is dedicated to experiments and is currently used for studies of incommensurate phases, phase transitions, crystal perfection and other problems in solid state physics and materials science. The other beam line is used for the direct control of crystal perfection during growth. Up to now the Bridgman furnace for crystal growth has already produced about 40 Cu single crystals 6 cm in diameter and 15 cm long as starting material for monochromators. The in-beam control proved to be very valuable for optimising growth parameters and yields a considerable gain in time. The cylindrical ingots have a mosaic spread of only a few minutes and are subsequently deformed in a heated press installed on another γ -ray diffractometer. Thus, the increase of mosaic spread with plastic deformation is observed directly. The capacity of the press was increased in order to deform the as-grown ingots without the further cutting into parallelepipeds done before.

This has the second advantage that if the deformation fails to give satisfactory results, the ingot can be reprocessed in the Bridgman furnace without special shaping thus permitting a saving of time and material. An effort was made to improve the computer control of the diffractometers and to reduce the data to a more convenient level.

MONOCHROMATOR PRODUCTION AND DEVELOPMENT

The IN20 Heusler alloy polariser with variable vertical curvature was completed and gave excellent results (cf IN20 report). Also prepared were the focussing graphite monochromator and analyser for IN20 and the vertically focussing Ge Monochromator for D2B ($30 \times 5 \text{ cm}^2$).

The production of material for the composite focussing Cu monochromators for IN20, D20, IN8 and D19B is continuing. Two Cu monochromators were prepared for the KFA Jülich in exchange for Cu as-grown crystals delivered earlier by the Kristall-Labor of the KFA.

The major event in monochromator development was the beginning of a beryllium crystal growth project on a real production scale. Within three years it is planned to grow a total of 180 single crystals > 15 mm in diameter and > 100 mm long equivalent to a monochromator area of 1350 cm^2 at the Pulvermetallurgisches Laboratorium of the Max-Planck-Institut für Metallforschung, Stuttgart, FRG. Major investments, namely a new growth facility and purification devices, were made thanks to the financial participation of six neutron scattering centres: the Hahn-Meitner-Institut, the Institut für Reaktortechnik Würenlingen, Brookhaven National Laboratoire Léon Brillouin. The development of a new mirror furnace and of a zone refining facility for purification of the polycrystalline material prior to crystal growth was completed and both devices should be operational early next year. In parallel, progress has been made with the existing facilities. The cross-section of the crystals was increased from 1 to 2 cm^2 and 8 samples 8 cm long were grown within the last four months. Based on this success, it is hoped to reach a diameter of at least 2 cm with the new furnace.

The in-beam controlled growth of oriented Cu crystals on the γ -ray diffractometer is producing high quality material at a rate of about six ingots per week. The soft mould technique allows this quality to be obtained with only medium purity Cu which proved to give better results at the plastic deformation than high purity material. This Bridgman crystal growth furnace has been developed in collaboration with the crystal laboratory of the CNRS Grenoble.

The ILL facilities for monochromator production are increasingly used by external laboratories. This year we had visitors from Los Alamos, Petten, Stockholm and the CEN-Grenoble. At present the Monochromator Group is composed of one engineer, four technicians and a part-time laboratory assistant.



The Bridgman furnace for in-beam controlled growth of large Cu single crystals on the γ -ray diffraction facility.

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REACTOR OPERATION 1984

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OPERATION OF THE SUB-ASSEMBLIES

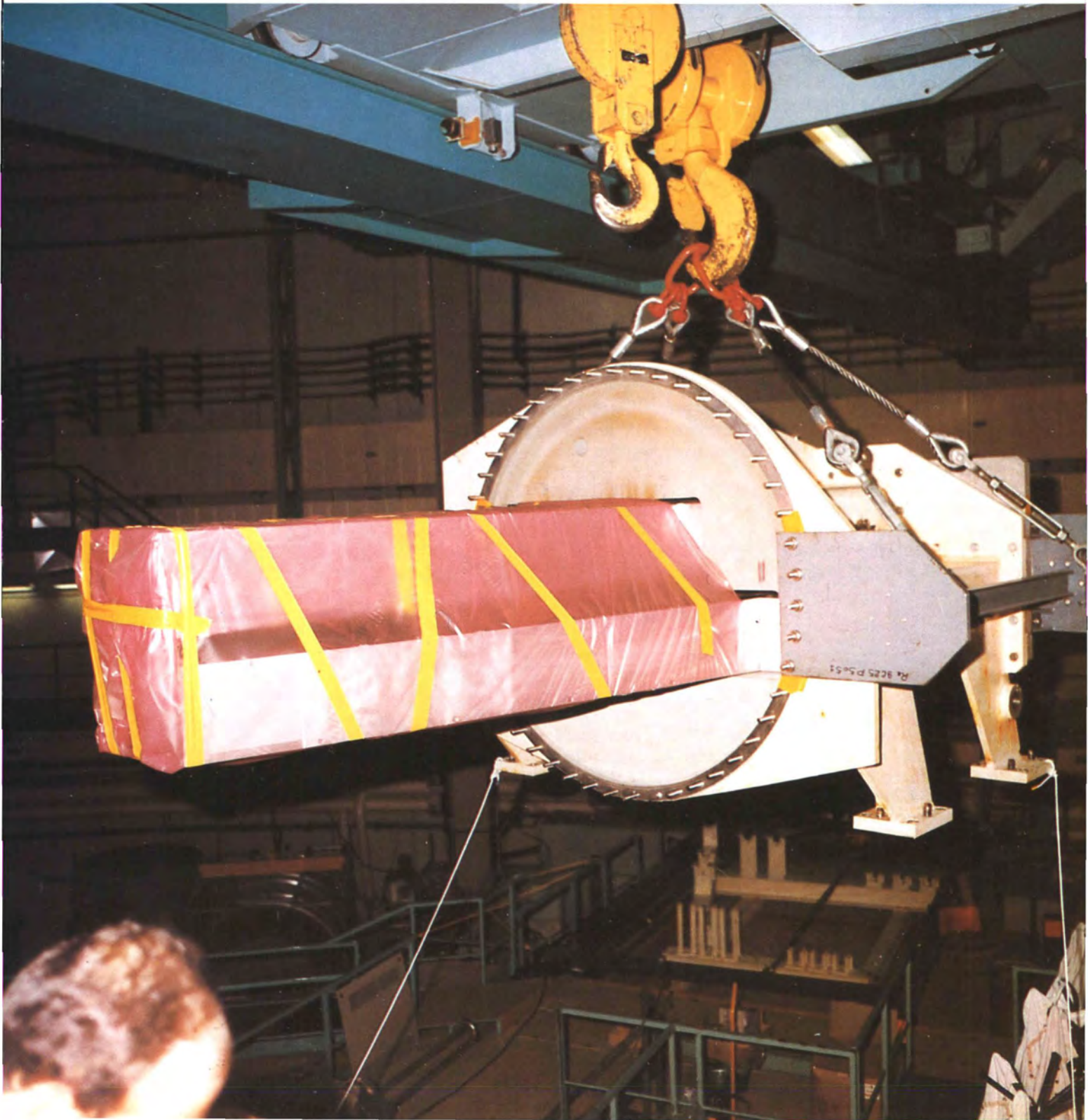
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OTHER WORK

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Removal of the liquid shutter unit of H1/H2 (view of the in-pile part) feeding the neutron guides. ►

REACTOR OPERATION DEPARTMENT



5

Introduction

Reactor operation continued at the usual rhythm during the first nine months of the year, five cycles of 44 days operation being completed.

From 4 October the reactor was shut down to permit the replacement of the beam tube liners which had not yet been changed, the removal of the central part of the heavy water collector in the reactor block, and the replacement of the vertical cold source and of certain major components of the reflector tank.

Einleitung

Der Reaktor lief während der ersten neun Monate des Jahres (5 Zyklen mit je 44 Betriebstagen) im gewohnten Rhythmus. Er wurde am 4. Oktober zur Durchführung der folgenden Arbeiten ausser Betrieb gesetzt :

- Auswechslung der noch nicht ausgetauschten Strahlrohre.
- Entfernung des Zentralteils des Schwerwasserkollektors im Reaktortank.
- Ersatz der vertikalen "Kalten Quelle".
- Ersatz bestimmter wichtiger Teile des Reflektortanks.

Introduction

Le fonctionnement du réacteur s'est poursuivi au rythme habituel durant les neuf premiers mois de l'année où cinq cycles de 44 jours de marche ont été effectués.

A compter du 4 octobre le réacteur a été maintenu à l'arrêt pour procéder au remplacement des doigts de gants des canaux qui n'avaient pas encore été changés, à l'ablation de la partie centrale du collecteur de reprise de l'eau lourde dans le bloc pile, au remplacement de la source froide verticale et de certains composants importants du bidon réflecteur.

REACTOR OPERATION 1984

Cycle 1/84

Operation from 3 January to 18 February.
The reactor cycle was interrupted by two incidents from 18 to 19 January and from 8 to 10 February. The cycle initially planned was extended by 2 days.

Cycle 2/84

Operation from 26 February to 13 April.
This cycle commenced 2 days before the scheduled date to permit an experiment to be carried out at low power (4 MW); the end of the cycle was also delayed by one day to compensate for a shut-down from 27 to 29 February, following an operation incident.

Cycle 3/84

Operation from 24 April to 7 June.
The scheduled dates were respected and the cycle was completed without any notable incident.

Cycle 4/84

Operation from 18 June to 2 August.
The scheduled dates were respected and the cycle was completed without any notable incident.

Cycle 5/84

Operation from 14 August to 4 October.
The cycle was interrupted by several incidents, including the failure of a main pump for the D₂O circuit, which necessitated operation at 70% of nominal power from 23 September to the end of the cycle.

Data for 1984

No. of days originally scheduled	: 220
actual No. of days of operation	: 225
No. of equivalent days of full power	: 216.6
actual operating time as proportion of year	: 61.6
actual operating time in relation to time scheduled	: 98.5
No. of fuel elements used	: 5
No. of fuel elements despatched for processing	: 4
No. of new fuel elements received	: 4
No. of unscheduled shut-downs	: 7
including: brief shut-downs	: 4
shut-downs with Xenon poisoning	: 3

OPERATION OF THE SUB-ASSEMBLIES

REACTOR BLOCK

During the first nine months of the year the work mainly centred on preparations for the work planned for the shut-down, in particular:

- design and construction of the beam tube liners to be changed,
- design and construction of the various remote-controlled cutting machines,
- finalising the procedures for carrying out the replacement of the essential parts within the reactor tank.

Starting on 4 October, the following dismantling work was undertaken:

- fuel element support,
- safety and control rods,
- natural convection and non-return valves,
- support structure and beam tube liners H1/H2,
- beam tube liners H12, IH1, IH3,
- ultra-cold neutron loop for beam tube IH3,
- central chimney of the reflector tank,
- vertical cold source.

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CIRCUITS

The Circuits group prepared and carried out the changeover to demineralised water of the reflector tank, preceded by the emptying and thorough drying of the circuit, which previously contained heavy water.

In addition to the usual maintenance and adjustment operations, the installation should be noted of a by-pass on the main secondary circuit, which makes it possible to avoid the constraints due to the considerable temperature variations with changes in operation.

ELECTRICITY

The reliability of the ILL's electricity supply has been improved by a change in the connection of one of the two 15KV supplies. The two supplies are now fed by two independent sources.

The controls for the ventilation system in the detritiation building have been replaced using programmable control devices.

ELECTRONICS

Planning and design study for the replacement of the measurement electronics associated with the thermodynamic sensors and certain health physics measuring devices. Design study for the replacement of the reactor control panel.

DETRITIATION

Before the shut-down, the detritiation plant processed heavy water from the reactor to lower the tritium level in the heavy water to a figure compatible with satisfactory conditions for intervention work. In October 70 000 Ci of tritium had been removed and the activity of the heavy water reduced to 1.7 Ci/l (0.063 T.Bq/l).

OTHER WORK

DEVELOPMENT OF THE VERTICAL COLD SOURCE

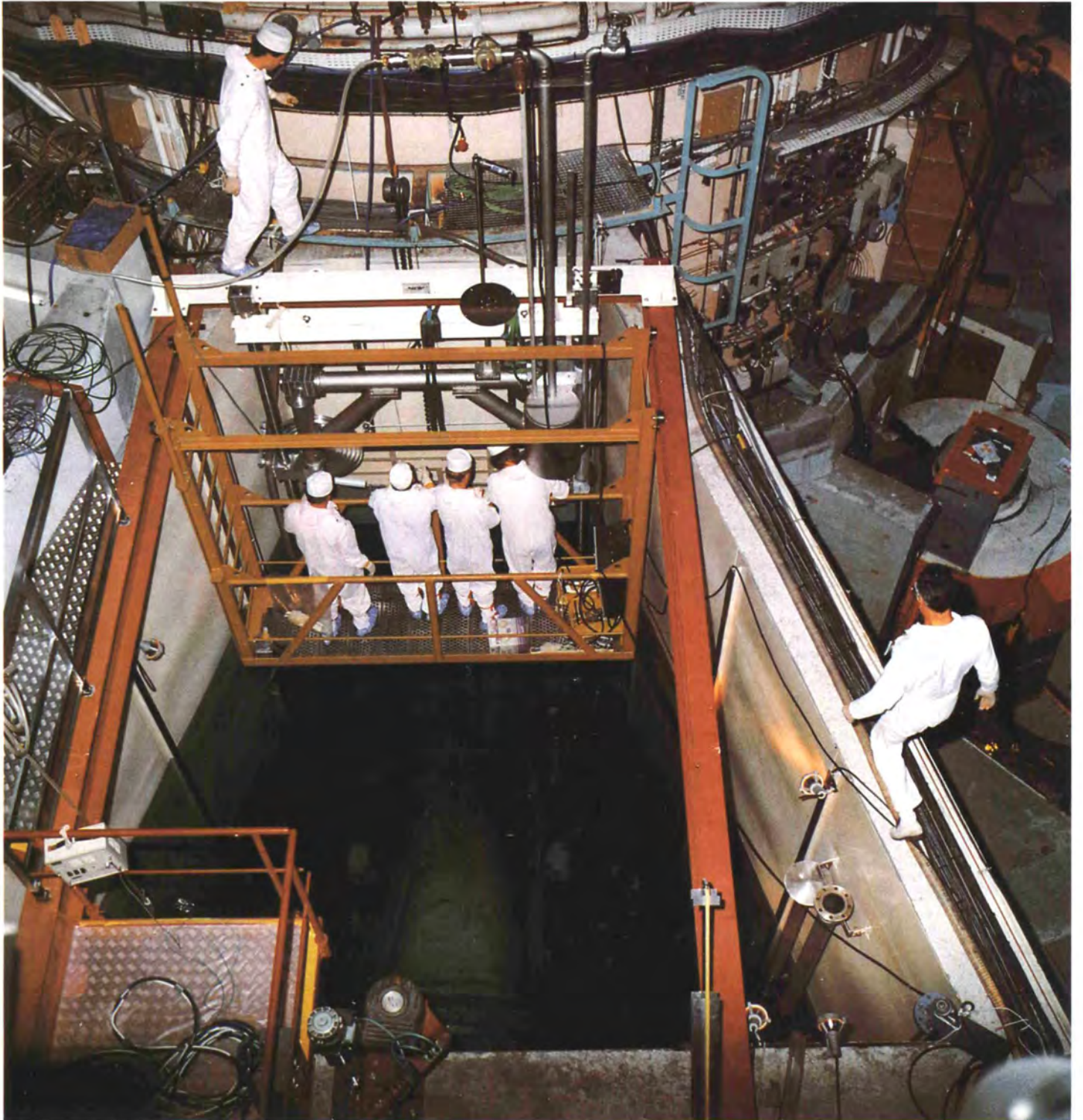
The work associated with the installation of the new vertical cold source has continued:

- acceptance of the in-pile part of the alignment plug of the vertical cold source SFV3,
- development in collaboration with Munich and electro-deposited nickel reflector tests for the vertical guide and the part in the swimming-pool,
- miscellaneous installation work in level D.

The installation of this new source is planned during the current long shut-down.

HORIZONTAL COLD SOURCE (beam tube H5)

The definition work is continuing, and has already resulted in the first invitations to tender and a contract for the in-pile part. The main arrangements for the complete cold source as far as the safety valve are practically decided, and the current phase of issuing the invitation to tender will continue during the early part of 1985.



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AUTOMATION AND DATA SERVICE (SAD)

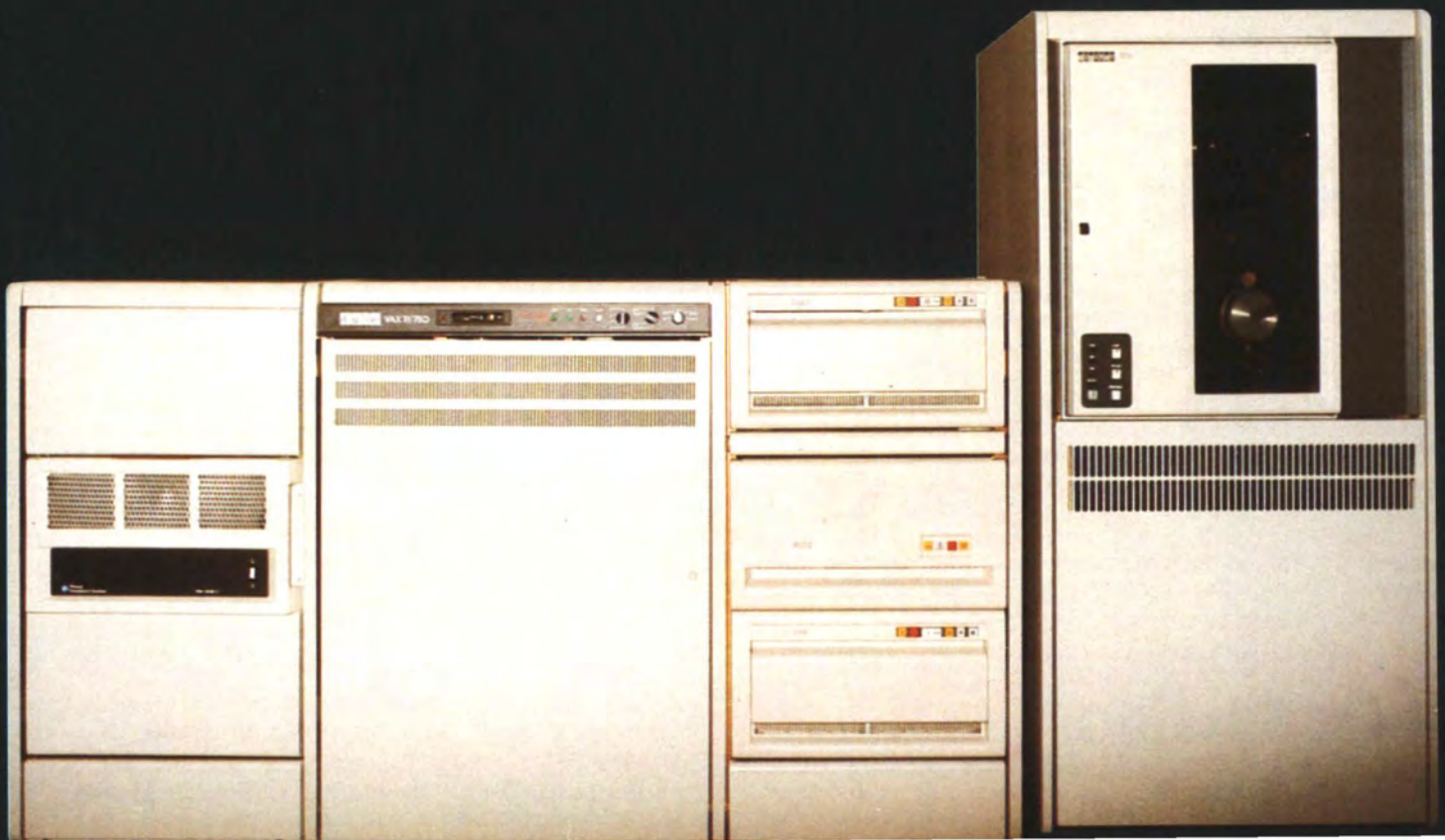
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CENTRAL COMPUTING SERVICE

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The picture shows a new type of computer introduced at the ILL, a VAX 11 1750. It will be used in conjunction with D19, the large PSD diffractometer. The same type of machine will serve also for ILL office automation.

COMPUTING DEPARTMENT



6

Introduction

Whilst the daily routine continued normally, at least up to the reactor shut-down, a number of investment decisions with long-term implications have been taken. ILL and the EMBL outstation will jointly purchase an Evans and Sutherland PS330 Graphics System, which should greatly facilitate the modelling of complex molecular structures. The Management Information Services Group is acquiring a VAX 11/750 which will both permit the OS11 word processing facility to be enhanced and extended to more secretariats, and enable the salaries calculations and personnel statistics to be undertaken in-house. An investigation on the role that could be played by personal computers (of the "professional" rather than "home" variety) is being started, as is a

Einleitung

Während die tägliche Routine, zumindest bis zum Reaktorstillstand, normal ablief, wurde eine Anzahl von Investitionsentscheidungen mit langfristiger Tragweite getroffen. Das ILL und die EMBL-Aussenstelle werden zusammen ein graphisches System Evans and Sutherland PS330 erhalten, was die Darstellung komplexer Molekülstrukturen in Form von Modellen bedeutend erleichtern sollte. Die Büroinformatik-Gruppe kauft eine VAX 11/750, die es erlaubt, die OS11 Textverarbeitung zu verbessern und auf andere Sekretariate auszudehnen, und ausserdem die Gehaltsabrechnungen und Personalstatistiken im Hause vorzunehmen. Die Abteilung prüft im Augenblick die Möglichkeit für eine Anwendung von "personal computers", ebenso wurde eine Studie über ein Ethernet Pilotprojekt im Angriff genommen. In Rahmen des Verbundsystems mit auswärtigen Grossrechnern

Introduction

Pendant la période de routine journalière, tout au moins celle qui a précédé l'arrêt réacteur, il a été décidé un certain nombre de projets d'investissements avec implication à long terme. L'ILL et l'antenne EMBL vont acheter en commun un système graphique Evans et Sutherland PS330, lequel devrait faciliter grandement la modélisation des structures moléculaires complexes. Le groupe "Management Information Services" acquiert un VAX 11/750 qui permettra d'une part, de développer le système de traitement de textes OS11 et ainsi de toucher un plus grand nombre de secrétariats, d'autre part d'effectuer sur place les calculs des salaires et les statistiques du personnel. On a démarré l'étude sur le rôle qui pourrait être joué par les ordinateurs personnels (catégorie « ordinateurs professionnels » de préférence à « ordinateurs domestiques »), ainsi que celle d'un projet pilote de réseau Ethernet. Pour les communications extérieures notre connexion au Transpac (Service de Transmission National Français)

pilot Ethernet study. For external communications our connection to Transpac (French national package switching service) has simplified the problem of remote access to computers, but inter-computer file transfer has still to be resolved.

Particularly in the instrument control area, the arrival of the long reactor shut-down has brought some freedom from the routine of support and maintenance, and this is being put to profitable use. Some staff have been awarded leave of absence to visit related institutes and laboratories. Other are preparing lecture courses for scientists, technicians and anyone else wishing to improve their understanding of computers and computing. Efforts are also being made, as indicated above, to investigate new methods and techniques, but this is somewhat handicapped by lack of investment funds outside the instrument area. At the practical level, the opportunity is being taken to systematically recable the links from the instrument computers.

hat unser Anschluss an Transpac (Französischer National-Übermittlungsdienst) das Problem des Zugangs zu diesen Rechnern vereinfacht, aber das Problem der Übertragung ganzer Datenbanken zwischen diesen Rechnern bleibt noch zu lösen.

Vor allem im Bereich der Instrumentrechner bedeutete die lange Reaktorpause eine gewisse Loslösung von der Routine, was die Unterstützung und Instandhaltung dieser Geräte anlangt. Hier-von profitierte die Abteilung, indem sie einen Teil des Personales vorübergehend an andere Institute und Labors abordnete. Andere Mitarbeiter organisieren Kurse für Wissenschaftler, Techniker und alle diejenigen, welche ihre Kenntnisse über Rechner und Informatik vertiefen wollen. Wie bereits erwähnt, wird viel Mühe auf die Untersuchung neuer Methoden und Techniken verwendet ; leider wird diese teilweise geschmälert durch die im Vergleich zum Instrumentensektor spärlichen Investitionsmittel. Der Reaktorhalt wird ausserdem zur systematischen Neuverkabelung aller Rechneranschlüsse genutzt.

a simplifié le problème de l'accès à des ordinateurs éloignés, mais il reste encore à résoudre le problème du transfert de fichiers entre ordinateurs.

Tout spécialement dans le domaine du contrôle d'instrument, le long arrêt du réacteur a pour conséquence d'apporter un certain degré de liberté dans les activités de routine relatives au support logiciel et à la maintenance et ceci devrait être bénéfique. Une partie du personnel s'est vue autorisée à s'absenter pour visiter des instituts et laboratoires similaires. D'autres préparent des séances d'information pour scientifiques, techniciens et pour quiconque désireux d'améliorer ses connaissances sur les ordinateurs et l'informatique. Des efforts ont également été faits, comme indiqué ci-dessus, pour étudier de nouvelles méthodes et techniques, mais ceci se trouve en quelque sorte handicapé par le manque de fonds d'investissement en dehors du domaine des instruments. Sur un plan pratique, on profite de l'occasion pour recâbler systématiquement tout ce qui est connexion venant des ordinateurs d'instruments.

AUTOMATION AND DATA SERVICE (SAD)

Whilst the current situation as regards instrument computers is, with a few exceptions, satisfactory, a growing cause for concern is that in a few years time we shall have to start the replacement of the many computers acquired during the years 1977-9, when the change-over to autonomous systems largely took place. Current budget lines in this area are insufficient to cover this. A multiannual programme for replacement has been prepared and costed, in a paper submitted to the Steering Committee in December 1983. The same paper discussed purchasing policy and indicated that, with the need for strict standardisation on hardware and software, in order that the limited manpower be used to maximum efficiency, there seems no choice at the present time but to remain with the VAX and PDP-11 ranges.

SOFTWARE A (CRYSTALLOGRAPHIC INSTRUMENTS)

This group is responsible for software for the instruments D1A, D1B, D2B, D3, D4, D5, D9, D10, D15, D16, D19, D20, DB21, LI5, S18.

With the close-down of IN2, operation of the CARINE system, for which the group was responsible, came to an end. Thus all the centralised control systems, with which operations started in 1972, have now been phased out.

Amongst the new instruments D2B, using a PDP 11/24, was brought on-line with few problems. Some testing of DB21 at its provisional position, was also possible. DB21 follows the D19 design, having a PDP 11/24 for data acquisition and a VAX 11/750 (which also serves as the new EMBL central computer) for data reduction. Progress on D20 has been delayed awaiting resolution of the detector problems, but towards the end of the year a decision was taken to acquire a PDP 11/24 for its provisional configuration.

On D19, work has continued on the integration of peak intensities, using the two alternative procedures known as BRAGGVAX (ILL) and PEAKINT (developed by Queen Elizabeth College, London).

Efforts to improve standardisation of the Group's instruments also continue. The results of an exercise involving D3, D4B and D5 will be implemented during the shut-down.

The group is also responsible for general management of the ILL computer network, JUDAS. Instruments which were newly linked in during the year were IN3, IN8, IN10, IN13, D2B, DB21 and the EMBL VAX. Also in the domain of networks, a small Ethernet connection has been set up for evaluation.

The group has for some time been pressing for an examination of the possible uses of personal computers at ILL. This year it became possible to acquire two, a DEC Professional 350 and a Rainbow 100. Their usefulness, both as stand-alone machines and as workstations linked to the network, is being studied.

SOFTWARE B (OTHER NEUTRON SCATTERING INSTRUMENTS)

The group is responsible for the control software and assistance in data treatment for instruments in the THREE-AXIS and VERCORS groups (IN1, IN3, IN8, IN12, IN20, D7, D11, D17, IN4, IN5, IN6, IN10, IN11 and IN13). Until the start of the long shut-down the principal activities of the group were to consolidate the projects and modifications initiated in 1983, detailed tests being limited primarily to the scheduled shut-down periods, since all instruments normally operate under a full workload. In general, little measuring time was lost due to software errors.

Developments for the THREE-AXIS group enabled more reliable recovery from hardware faults (IN8). To resolve problems encountered with the micro-processor controlled counting system, and offer supplementary flexibility, the study of linking a standard CAMAC based counting system to the SOLAR 16/40 computer was completed in conjunction with the electronics group. This was operational in tests at the start of the long shut-down. Close collaboration with the scientists responsible for IN20 permitted basic evaluation of this instrument operating in polarisation analysis mode before the shut-down.

For the VERCORS group inelastic instruments the main effort was expended on improvements to the new control programs for IN4 and IN5, together with development of programs for controlling the new drive electronics for the phase-locked rotating crystals and choppers. On IN6 the principal innovation was the optimisation of temperature control of the notoriously recalcitrant cryostat in conjunction with the ILL standard temperature controller. A number of strategies were tested out using the instrument control computer, and including full coordination of counting and temperature monitoring.

A new implementation of temperature control on IN13 permits temperature-scan measurements to be performed more easily, and provide a basis for new experimental modes. As in the case of IN6, sample cells are only weakly coupled to the cryostats; some results of these tests can subsequently be incorporated in the software of the temperature controller itself.

6

All programs of the small-angle scattering instruments (D11, D17) have been reviewed during the year, and extensions made to recording of cyclic and single-shot time-dependent measurements on both machines. A VAX 11/730 has been acquired as a replacement computer for D11; this has involved software development with an important contribution from the Software A Group to link-up the existing electronics. Collaboration with the Neutron Division at the Rutherford Laboratory gave this project a flying start, and plans for developments in data analysis using the same type of computer for similar experiments in the two centres should be mutually beneficial.

Other instruments still supported by members of the group, and demonstrating progressive improvements (even if sometimes heavily labour intensive) include MACAMAC Systems on D4 and D20; this latter has served as a valuable testbed for very rapid kinetic diffraction measurements. The results of much programming effort for PN1 have been used during the current year for several successful experiments.

SOFTWARE C (NUCLEAR PHYSICS AND SPECIAL INSTRUMENTS)

Amongst the regularly scheduled Nuclear Physics Instruments, PN1, PN2, PN3 (GAMS 1, 2, 3, 4), PN4, PN6, PN8, it has been a year of good reliability, but one notes increasing pressure on support media (especially discs) due to the greater number of event parameters being recorded. It may be necessary to introduce high-capacity Winchester discs more generally.

As a consequence data analysis also becomes more complex. A local data treatment centre (a PDP 11/23 with a wide range of peripherals) is available for operations which do not need the power of the DEC 1091. For example, in the "Listmode" process, which is now widely used, the complete matrices are generated locally, the windowing being done on the 1091.

A special effort is being made on S instruments, as it is recognised that they permit some of the most exciting experiments being done at ILL. Problems can arise with equipment coming from laboratories which do not follow the same standards as ILL, but most scientists do appreciate the benefits of hardware and software maintenance support that can be provided if they align themselves with ILL. The instruments S20, S21, S52 are trail-blazing this approach.

For many years the group has operated a PDP 11/55 as a general purpose local computing centre. Despite the arrival of the DEC 1091, this machine has remained very popular with some visitors, principally because of the range of peripherals

available, and demand remains high. However, the processor is now obsolescent and cannot support latest operating system facilities. It has therefore been decided to upgrade it to a VAX 11/750.

MANAGEMENT INFORMATION SYSTEMS AND OFFICE AUTOMATION

The pilot word processing project, linking 4 workstations to an old PDP 11/40 running the package OS11 continued through 1984. It has generally been well received and there are requests from other secretariats to be connected. Unfortunately the computer has neither the power nor the reliability to support more. This has prevented a real demonstration of the benefits of a centralised system using standard ILL hardware (transfer of documents, access to other computers, etc.). The group has ordered a VAX 11/750 for delivery early in 1985 which will have the capacity to support all the secretariats needing such facilities. In addition, for those who really have nothing to gain from a centralised system, the possibility of introducing autonomous machines matched to their specific needs is under review.

The general management information system (MISSILL) continues to run well, but the PDP 11/34 which operates it is now fully saturated. New users, notably the Medical and Training Sections, will run on the VAX.

For some time the Management has been considering the possibility of bringing in-house those administrative functions (principally salaries and finance) which are currently treated externally under contract, and the group has been assessing appropriate packages which would run on our machines.

In September the contractor announced a reorientation of his policy in the salaries area as from January 1985. ILL was faced with having to rapidly take a decision either to go along with the proposed changes or find an alternative solution. Although time was short, a decision was taken to do the work in-house on the VAX, running a package which is widely used in France (PACHA). With the group's VAX not then available, installation was carried out on the D19 machine, this being rather lightly-loaded during the shut-down. The group was temporarily strengthened to meet the tight schedule.

COMPUTER HARDWARE MAINTENANCE

The quantity of equipment in use continues to increase. Apart from completely new instruments, when an instrument changes

its computer all useable components are kept either as spares or to enhance similar configurations. Additional terminals, more discs for data storage, automation of administrative activities and inter-computer links all lead to a steady growth in the investment stock.

Until now this growth has been handled without significant additional resources being put into the maintenance area. This has been achieved by rigorous standardisation, a continuous review of which equipment should be maintained in-house, and which under contract, and the good fortune that electronics is becoming progressively more reliable and easier to maintain. However it seems likely that the cumulative effect of the investments under the modernisation programme is finally going to tip this delicate balance. It is not evident how a solution can be found within the current budgetary constraints. The long shut-down is providing a welcome opportunity both to do some preventive maintenance and to rationalise the cabling from the instruments. Over the past 14 years new cables and connections were simply added as necessary. For the first time it has been possible to remove the false floor in the area where the cables leave the reactor and completely reorganise the cable runs and junction boxes. The new arrangements should simplify maintenance and modifications in the future.

CENTRAL COMPUTING SERVICE

OPERATION OF THE DEC-1091

The DEC-10 system operated very satisfactorily during 1984 with an availability rate of 98% during scheduled operation, apart from periods of preventive maintenance. As in the past, the system has been operational 24 hours per day with operator cover on Mondays from 5.30 to 21.30, Tuesday to Friday from 6.15 to 20.45, Saturday from 9 to 17.00 and the remainder of the time in self-service mode.

The DEC-10 was heavily used as in the second half of 1983, and statistics show that the demand for interactive mode has increased in comparison with the previous year; this has led to saturation of the machine during the day and to longer response times.

In view of this present saturation, which does not permit all computing requirements to be satisfied within a reasonable time, and with the prospect of new instruments which will be operational after the reactor start-up and which will further increase the computing requirements, we have requested an extension of the central system with effect from 1986 at a cost of the order of 5 MF.

SYSTEM WORK AND COMMUNICATIONS

In the system software field we have adapted and tested new versions of products such as the monitor, the spooling system and some communications products. The software connections with the instrument computers were reviewed and improved at the beginning of the year, but this only provided a partial solution with limited possibilities; with the new version of DECNET planned for the near future the DEC-10 will be homogeneously integrated in the ILL network.

Work is also in progress to simplify access to the various ILL computers via the terminal switching device from the considerable variety of terminals operating at very different speeds; these speeds will be converted on the basis of a two-speed standard 2400 and 9600 bauds.

A number of products of the DECUS library have been installed, and some are being adapted to facilitate for example the editing of documents on the DEC-10.

At the beginning of the year ILL was connected to Transpac and to the various national public networks. This service permits access from a terminal at ILL to external computers or data base systems. It is also possible for scientific visitors back in their home laboratory to have access to the DEC-10 for certain preliminary data processing which it is not possible to carry out during their visit to ILL; such access remains limited and restricted.

This service does not permit the transfer of files between computers, particularly between computers of different types. We are at present awaiting software offering this service via public networks such as Transpac, private networks such as JANET (U.K.) or EARN (introduced by IBM for universities or research laboratories).

GRAPHICS

Following a study of the requirements for a graphic system at ILL, a contract has been placed for an Evans and Sutherland advanced graphic system to be shared with EMBL.

The recent purchase of 2 Tektronix 4112 (reconditioned equipment) should permit certain types of manipulations of monochrome images.

Work has also been carried out on the library of graphic programs to permit the display of different types of vector files on graphic terminals.

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MATHEMATICS

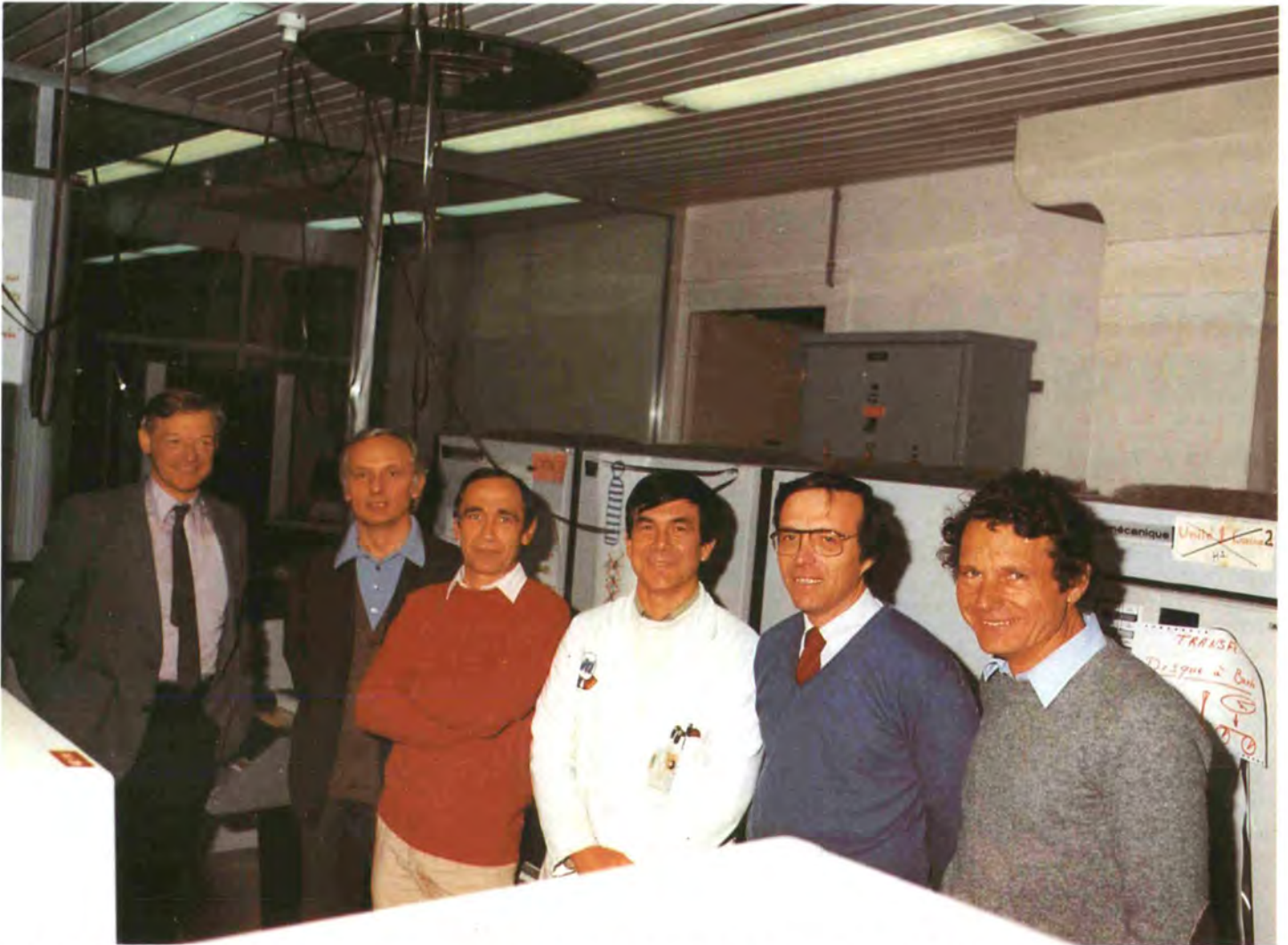
A new very general and readily portable mathematical library has been installed on the DEC-10 and on the D19 VAX; this is more highly developed than the Harwell library and more powerful for minimisation problems, and also incorporates the EISPAC and LINPACK packages; documentation is available for the VAX.

Programs to assist with the documentation of the different mathematical libraries make it possible to set up decision trees to facilitate the choice of the sub-routines in scientific applications.

WORKSHOP, COURSES

In February a workshop was organised by the service on the development of computing in general under various aspects such as the families of scientific computers, languages and networks.

The Automation and Data Service and the Central Computing Service have started organising for scientists a series of general computing courses in the areas which concern them directly in connection with their research. These courses should take place in the first quarter of 1985.



The last part (IN2 link) of the CARINE computer system was taken out of commission in Spring 1984. A souvenir picture was taken to mark the event. From left to right: D. Rimmer, B. Dorner, M. Roure, G. Pastor, A. Barthelemy, W. Kaiser.

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**SAFETY
AND HEALTH PHYSICS GROUP**

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LIBRARY

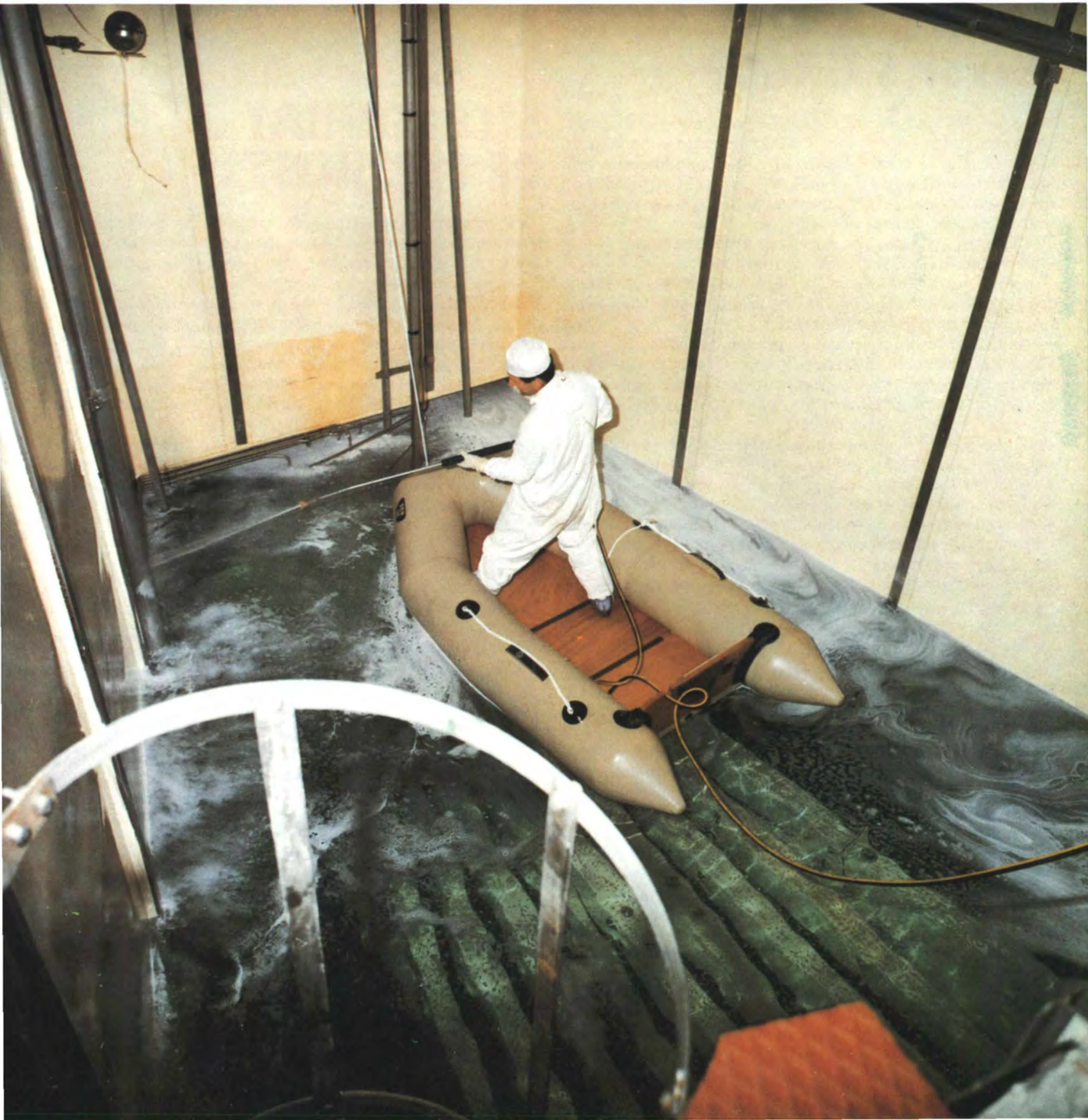
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**SECRETARIAT
OF PHYSICISTS**

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Cleaning of the H1/H2 swimming pool by the radioprotection team. The contours of the guides can be seen under water. ►

OTHER SECTIONS



7

SAFETY AND HEALTH PHYSICS GROUP

The year 1984 has been marked by the preparation of the work connected to the long reactor shut-down, and by the start of this work. The Safety and Health Physics Group has been very much associated with the work concerning the definition of working conditions, the monitoring during the work, decontamination and control of waste.

The following routine controls have been continued:

- the dosimetry of ILL staff and visitors
- supervision and management of radioactive sources which are used either for experiments or for instrument calibration
- inspection of X-ray equipment
- control of radioactive liquid and gaseous waste.

Some experiments have required particular study relating to the operating conditions, to the setting up of the experiment or relating to their requirements for radioactive sources, as in the tritium experiment on D18.

Thoughts have been given to means of electrically monitoring various equipment used at ILL.

The budget for 1984 permitted the following:

- the renewal of the tele-surveillance system
- the renewal of a series of controls of radioactive effluent
- partial renewal of the radioactivity control system during the reactor shut-down.

The renewal was necessary due to the extent of the work on the reactor.

LIBRARY

The price of scientific literature continued to increase and scientific journals now represent 59% of the total library budget (56% in 1983).

• Acquisition of books showed a slight decrease in number (400 including 130 deposited with departments) due in particular to a slowing down in the publication rate of serials. This allowed the binding of 420 volumes of journals. The library has now 8200 books including serials, monographs, and conference proceedings and 8600 reports from other institutes (300 registered this year).

• Reprints were still kept at a very low acquisition level while there was more demand for the use of literature retrieval systems (10 questions from scientists have been treated the last four months, more or less successfully, depending on the field concerned and on the precision possible for the subject).

We can hope that the quieter period of the reactor shut-down

will give some time to investigate improvements in organization and in particular to begin computerization for our books. (Library Budget for 1984: 625 KF).

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).



The radioprotection team cleaning the radioactive part of the removed liquid shutter unit of H1/H2.

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PERSONNEL

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WELFARE

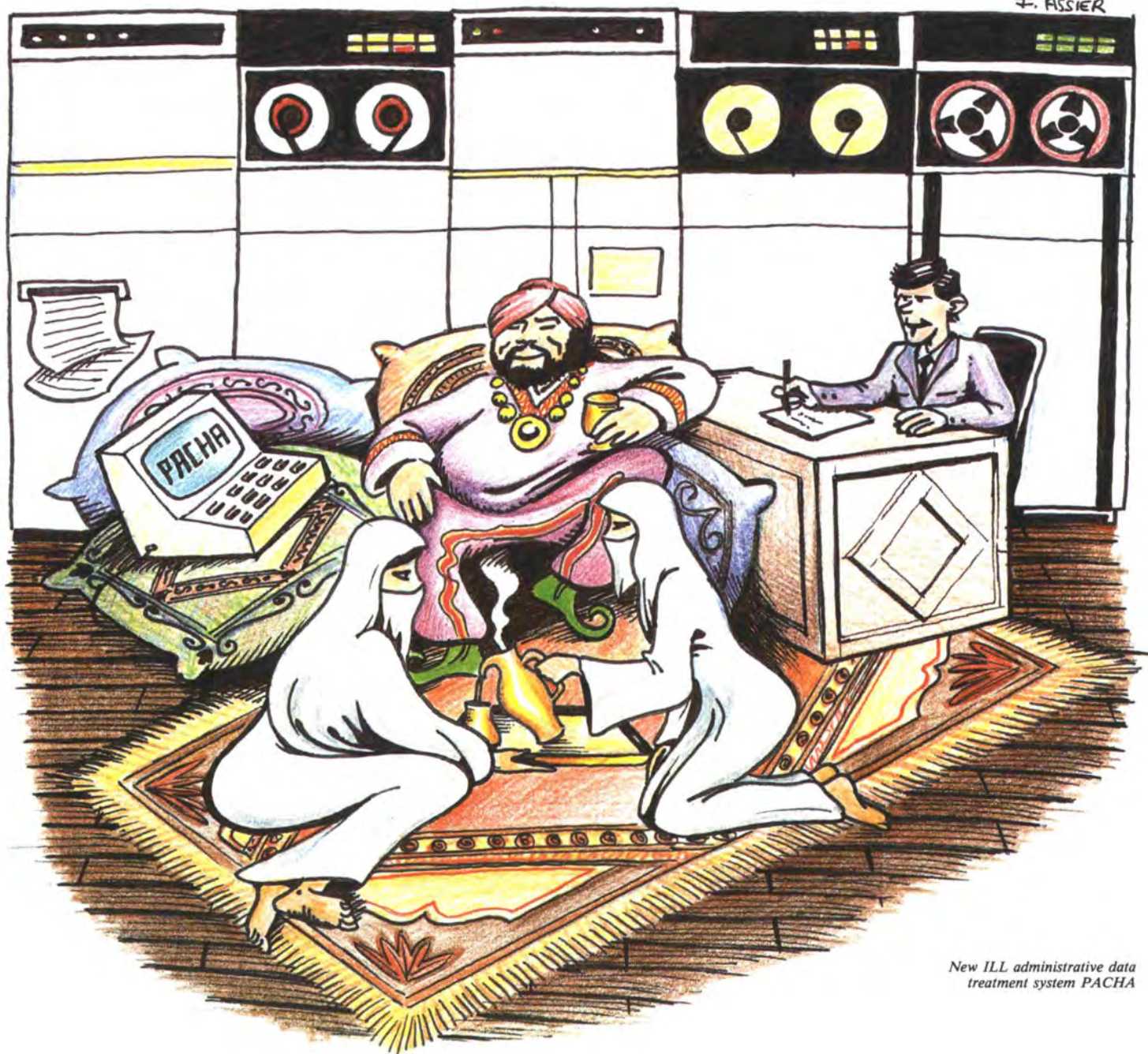
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FINANCE

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ADMINISTRATION DEPARTMENT

F. ASSIER



New ILL administrative data
treatment system PACHA

8

Introduction

The ILL does its best to keep its Administration as small as possible. The work in the personnel, finance, purchasing and welfare areas is done by about 30 staff. For organisational purposes, however, other non-administrative functions are included in the department, such as the works doctor, cafeteria, stores, etc.

The Administration Department (DAF) covers:

- the personnel office for approximately 500 ILL staff
- the finance and purchasing sector
- the fields of training, welfare, schools and ILL flats
- various infrastructure services such as reception, cafeteria, reprography, post, drivers,
- the secretariat of the Steering Committee and its sub-committees,
- the works doctor (regular checks on persons exposed to irradiation risks)

Einleitung

Das ILL ist bestrebt, mit einer möglichst kleinen Verwaltung auszukommen. Die Arbeit in den Bereichen Personal, Finanzen, Einkauf und betriebliche Fürsorge wird von ca. 30 Mitarbeitern erledigt. Organisatorisch sind der Verwaltungsabteilung jedoch noch andere, nicht-administrative Bereiche angegliedert, wie z.B. Betriebsarzt, Cafeteria, Einkaufslager u.a.

Die Verwaltungsabteilung (DAF) umfasst somit

- das Personalbüro für die rund 500 ILL-Angestellten
- den Sektor Finanzen und Einkauf
- die Bereiche berufliche Fortbildung, betriebliche Fürsorge, Schulfragen, Gästewohnungen,
- verschiedene Infrastruktur-Dienste, wie Empfang, Cafeteria, Vielfältigung, Postversand, Fahrbereitschaft
- das Sekretariat des Lenkungsausschusses und seiner Unterausschüsse
- den Werksarzt (laufende Kontrolluntersuchungen der Personen,

Introduction

L'ILL veille à ce que les travaux incombant à l'Administration soient effectués par une équipe relativement réduite. Les domaines Personnel, Finances, Achats ne sont en effet gérés que par une trentaine de personnes. Toutefois, pour des raisons d'organisation, certains autres secteurs, tels que le Médecin du Travail, la Cafétéria et le Magasin sont rattachés à l'Administration.

Le Département Administratif (DAF) comprend donc :

- le Service du Personnel gérant les quelques 500 agents de l'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 (réception, cafétéria, reproduction, chauffeurs),
- le Secrétariat du Comité de Direction et des Sous-Comités,
- le Médecin du Travail (surveillance médicale courante des agents, notamment dans les cas de risques d'irradiation),
- le Bureau de Traductions et la rédaction du "Bulletin".

— the translation office and the internal "ILL Bulletin".

The implementation of the 1984 budget was characterized by the difficulty of keeping expenditure within the total grants approved and of avoiding the need to call on the "reserve" set up by the Associates. In the staff costs budget (in addition to the salary increases totalling 5% in 1984) there was additional expenditure of approximately 2 MF due to the elimination of the upper limits for the calculation of employers' contributions for health insurance.

To resolve these problems, it was necessary to ask the Associates for a number of transfers in the budget. In addition, with effect from summer 1984 it was necessary to impose a freeze in principle on the filling of all posts. When an employee leaves, the question is also very carefully examined whether the post can be left vacant on a temporary or permanent basis, as the ILL is required to reduce the staff complement by a number of posts between now and 1987.

die Bestrahlungsrisiken ausgesetzt sind)

— das Übersetzungsbüro und die Redaktion des "Bulletin".

Die Abwicklung des Haushalts 1984 war durch die Schwierigkeiten gekennzeichnet, die Ausgaben im Rahmen der genehmigten Gesamtzuschüsse zu halten und eine Inanspruchnahme der "Reserve" bei den Gesellschaftern zu vermeiden. Im Personalbudget entstanden (neben den Gehaltserhöhungen um insgesamt 5% in 1984) Mehrausgaben von rd. 2 Mio F durch die Aufhebung der Beitragsbemessungsgrenze für die Arbeitgeberanteile an der Krankenversicherung.

Um diese Probleme zu lösen, mussten bei den Gesellschaftern eine Reihe von Umschichtungen im Budget beantragt werden. Ausserdem musste die Direktion ab Sommer 1984 eine grundsätzliche Stellenbesetzungs-Sperre beschliessen. Ferner wird beim Ausscheiden eines Mitarbeiters sehr sorgfältig geprüft, ob auf eine Wiederbesetzung der Stelle zeitweise oder endgültig verzichtet werden kann, weil das ILL bis 1987 eine Reihe von Stellen einsparen muss.

L'exécution du Budget 1984 a été caractérisée par certaines difficultés à maintenir les dépenses dans le cadre des contributions autorisées et à éviter le recours à la réserve constituée auprès des Associés. Le Budget Frais de Personnel a dû faire face — en plus des augmentations des rémunérations de 5% au total pour 1984 — à des dépenses supplémentaires de l'ordre de 2 millions de F. par suite du déflationnement des cotisations « Employeurs » à la Sécurité Sociale.

Afin de résoudre ces problèmes, la Direction de l'ILL a demandé aux Associés l'autorisation de procéder à un certain nombre de transferts à l'intérieur du Budget. Par ailleurs, la Direction s'est trouvée contrainte de décider à partir de l'été 1984 de stopper toute mesure de recrutement. Elle a décidé enfin d'examiner, en cas de départ d'un agent, si ce poste pouvait rester temporairement ou définitivement vacant puisque l'ILL se trouve dans l'obligation de procéder d'ici 1987 à une série de suppressions de cases.

PERSONNEL

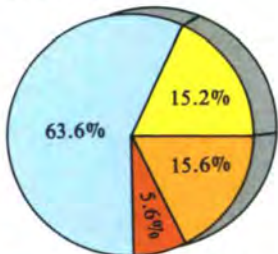
The Personnel Section is responsible for recruitment, salaries, staff management, and administrative aspects of external visits and guest scientists. It also deals with the Social Security and the administrative work for the ILL "Société Mutualiste" (supplementary health insurance).

STAFF

After the increases in 1982 and 1983 due to the incorporation in the staff of employees from external firms working at ILL, staff numbers stabilized in 1984 at an average figure of about 500.

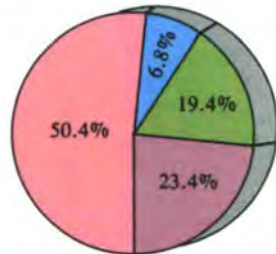
There is still considerable movement among the scientific staff.

1. Nationality



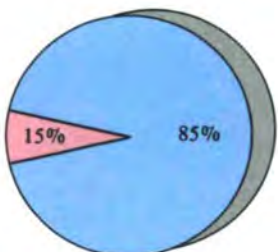
French	318
German	76
British	78
Others	28
Total	500

2. Category of work



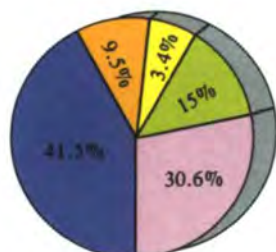
Scientists and thesis students	97
Engineers, technicians, draughtsmen, computing, staff	252
Administration	34
Others (watchkeepers, storemen, cleaners and general services staff)	117
Total	500

3. Sex



Men	425
Women	75

4. Age



Under 25	17
26 to 30	68
31 to 40	171
40 to 50	132
Over 50	112
Average age:	39

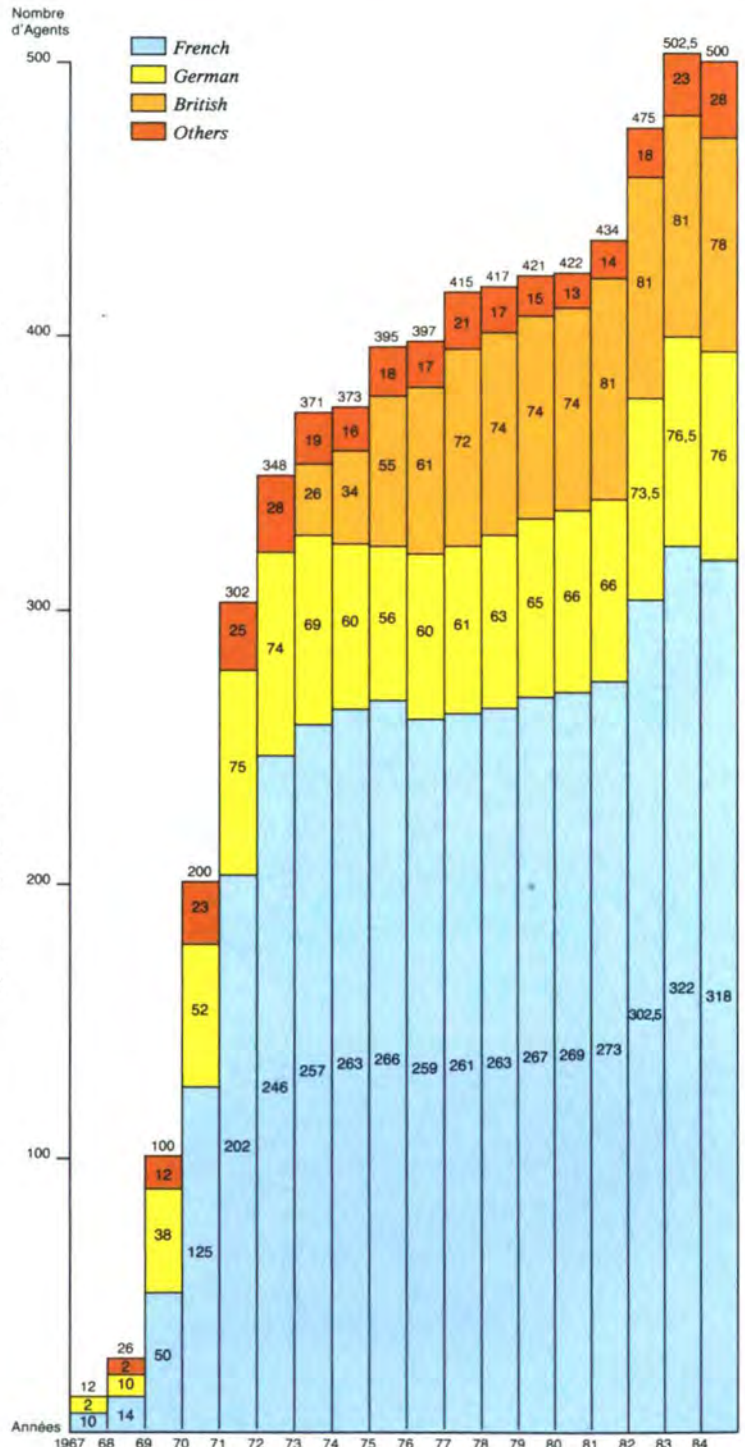


Figure 69: The changes in staff (from the foundation of the I.L.L.) from 1967 to 1984 (by nationality). (The increase in 1982/1983 is due to the incorporation of employees of external firms working at the I.L.L.).

Figure 68: Break-down of staff in 1984 by nationality, staff category, sex and age (average figures over the year).

TABLE 3
Staff changes in 1984

Categories	Position on 31.12.83	Recruitment	Departures	Difference + or -	Position on 31.12.84	Change % col. 4 compared with col. 2
(1)	(2)	(3)	(4)	(5)	(6)	(7)
1. Scientists	77	16	20	-4	73	25.97
2. Engineers	56	—	—	—	56	—
3. Other "Cadres"	9.5	—	—	—	9.5	—
4. Thesis Students	28	6	11	-5	23	39.29
5. Technicians	168	8	3	+5	173	1.79
6. Others	164	2.5	1	+1.5	165.5	0.61
Total	502.5	32.5	35	-2.5	500	6.97

GUEST SCIENTISTS

In 1984 the ILL received a total of 1800 visitors.

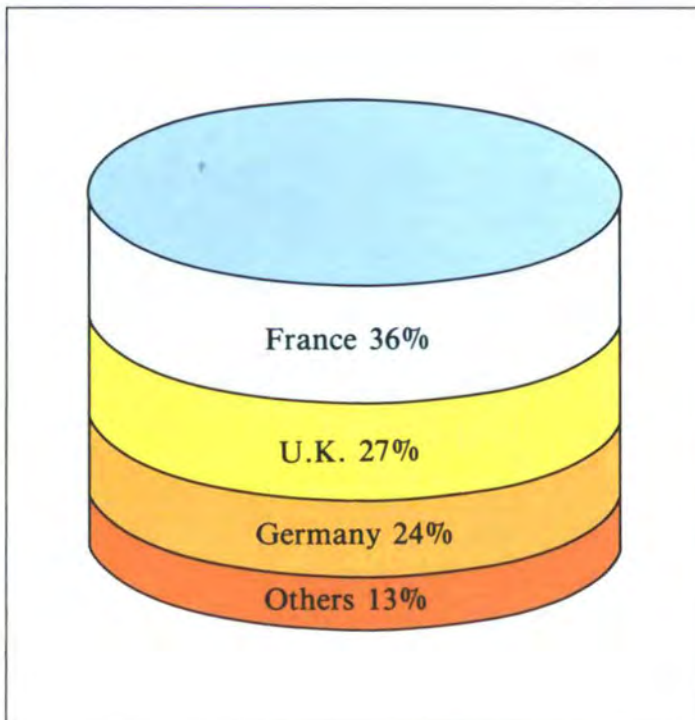


Figure 70: Percentages of guest scientists from the three member countries and other states.



In the framework of the ILL staff training programme a series of lectures were organised under the topic "Research around a large instrument, the ILL". In the picture is B. Maier, second from the left, who gave a lecture on the tasks of the Scientific Coordination and Public Relations Office.

WELFARE + GENERAL SERVICES

The Welfare Section ("Relations Sociales") deals with:

- problems of new arrivals, settling in of families, housing, schools, staff training and
- general services (reception, post, drivers, reprography, cafeteria, etc.).

It also provides administrative support for the medical service and the welfare adviser.

RECEPTION

In 1984, the receptionists assisted approximately 1,500 people: reactor users, members of the Scientific Council and its sub-committees, participants of seminars, workshops, etc.

HOUSING

The ILL currently has 13 furnished flats, which were sublet in turn to 40 guest Scientists or new ILL staff and their families for periods between three weeks and one year.

Loans were granted to staff members under the "0.9%" law on aid for housing (in 1984 17 employees received a total of 0.8 MF, an average of 45.000 Francs per flat).

The loans are repaid over 7 to 10 years or 15 years depending on the sum involved, at a low rate of interest.

EDUCATION

The ILL pays the salaries of teachers to provide lessons for German and British children of staff members in their mother tongue.

Number of children registered at the beginning of term in September 1984:

International Primary School "Houille Blanche"	59 children of English or German mother tongue, including 28 children of ILL staff.
Collège d'Enseignement Secondaire and Lycée des Eaux Claires (Secondary Schools)	49 children of English or German mother tongue, including 14 children of ILL staff and guest scientists.

STAFF TRAINING

French legislation encourages staff training and requires employers to spend approximately 1% of the total pay-roll on this.

There are various types of training courses at ILL:

- French as a foreign language for beginners and advanced pupils: approximately 60 persons (ILL, CNRS, University, CENG) attended classes given by 2 ILL teachers during the school year 1983 to 84.
- English and German: 47 ILL staff attended classes in educational establishments.
- Professional training, i.e. relevant to a particular job: 101 ILL staff attended specialised training (computing, programmable control devices, etc.).
- Courses leading to a degree: 3 staff obtained a degree during the first half of 1984.
- Classes of general interest, at the request of the employee.

In recent years, there has been a significant increase in the number of courses relevant to the particular job, which reflects the constant desire of staff to improve themselves in their professional field.

A training course entitled "Research around a large instrument at ILL", attended by 22 staff members, was organised at the initiative of 3 ILL scientists for the second consecutive year. Those attending the course — new staff and others who have been at ILL for a number of years — become more familiar with the various areas at ILL — scientific, technical, administrative.

MEDICAL SERVICE

ILL and EMBL staff and guest scientists are subject to a close medical surveillance which is much appreciated. Depending on where they work and whether they are exposed to irradiation risks, each individual is required to attend one or two regular medical examinations per year, plus special examinations or analysis at the request of the Works Doctor.

Some figures for 1984:

Staff and long-term guest scientists by working areas:	
"D.A." (normally working in restricted area):	277
"N.D.A." (occasionally working in restricted area):	213
"N.A." (not working in restricted area):	116
Number of medical examinations:	800
Number of blood tests:	1.100
Number of spectrometry examinations:	400

A contract was signed in June 1984 with the La Tronche Hospital by CENG and ILL for the evacuation and treatment at this hospital of injured and contaminated persons, in case this should be necessary.

REPROGRAPHY

278 texts (technical notes, scientific reports, theses, reactor cycle reports, etc.) were handled by the reprography workshop, a total of almost 6,000 documents.

FINANCE

The 1984 normal budget was authorized with expenditure of 225.5 MF. No real growth factor was provided for, except for the staff costs.

The reduction of the number of reactor cycles to five (instead of the six originally planned) permitted a number of savings on fuel elements, electricity, fluids and guests scientists. This sum (6.6 MF) was used to finance:

- additional expenditure in the field of instruments and the Reactor,
- the results of the elimination with effect from 1 January 1984 of the upper limits on the employers' Health Insurance contributions, and increases in the transport and industrial accident contributions,
- certain increases such as the tax on nuclear installations and heating,
- the replacement of the external computerised salary system by an internal one.

At the beginning of October 1984, the reactor was closed down until August 1985, during which period the main reactor beam tubes will be replaced, further work will be carried out on the heavy water collector, and the Vertical Cold Source will be replaced.

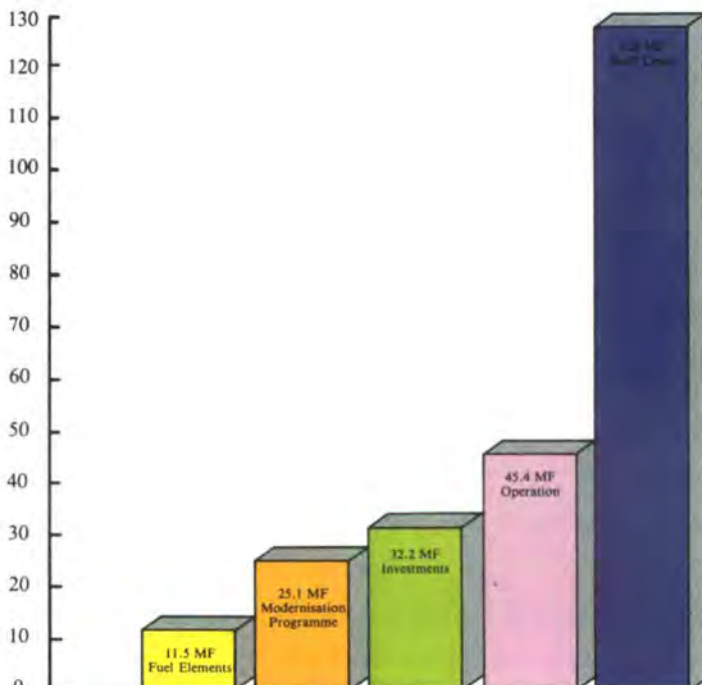


Figure 71: Associates' contributions 1984: 242.6 MF.

The construction of the second neutron guide hall was completed in summer 1984. In 1986 the new Horizontal Cold Source, a cost of which (19 MF) will be covered by the Modernisation Programme Budget, will be installed in this building. The total expenditure for 1984 (Normal Budget and Modernisation Programme) was 249 MF excluding taxes.

TABLE 4
Comparison of expenditure in 1984 and 1983

	1983		1984	
	(× 1000 F)	% of total	(× 1000 F)	% of total
<i>a) Operation</i>				
Consumable materials	13 054	6.4	16 124	7.1
Fuel elements	19 829	9.7	11 478	5.1
Staff costs	116 073	56.8	128 395	56.9
Taxes	936	0.6	1 256	0.7
Long term service and supply contracts	15 595	7.6	18 527	8.2
Other work, supplies and services	9 517	4.6	10 127	4.5
Transport, removal and travel expenses	1 745	0.8	1 801	0.8
Miscellaneous administrative costs	4 088	2.0	5 500	2.4
Total operation	180 837	88.5	193 208	85.7
<i>b) Investments</i>				
Buildings	470	0.2	2 644	1.2
Equipment	6 681	3.3	10 587	4.7
Experimental instruments	12 561	6.1	13 035	5.8
Other investments	3 831	1.9	5 977	2.6
Total investments	23 543	11.5	32 243	14.3
Total expenditure	204 380	100.0	225 451	100.0
<i>c) Income</i>				
ILL's own income	7 472	3.7	7 880	3.5
Grants from Associates	196 908	96.3	217 571	96.5
Total income	204 380	100.0	225 451	100.0

IMPLEMENTATION OF THE 1984 BUDGET

Normal Budget

According to the provisional annual accounts to 31.12.84, the situation as regards expenditure under the Normal Budget is as follows in comparison with 1983 (excluding taxes):

The operation expenditure increased from 180.8 MF the previous year to 193.2 MF (+ 6.8%). If the staff costs and fuel elements are excluded from this comparison, the operation budget remains constant in real terms in comparison with 1983.

Investments increased by 28% in real terms in 1984.

Modernisation Programme Budget

The complete Modernisation Programme as scheduled from 1979 to 1985 was evaluated at 104.2 MF at 1979 prices. At the end of 1984, 82.6% of the aims have been achieved.

The main investments in 1984 were the construction of the second Neutron Guide Hall and the replacement of some of the beam tube liners. The design studies for the new Horizontal Cold Source were continued in 1984, and it will be installed in 1986.

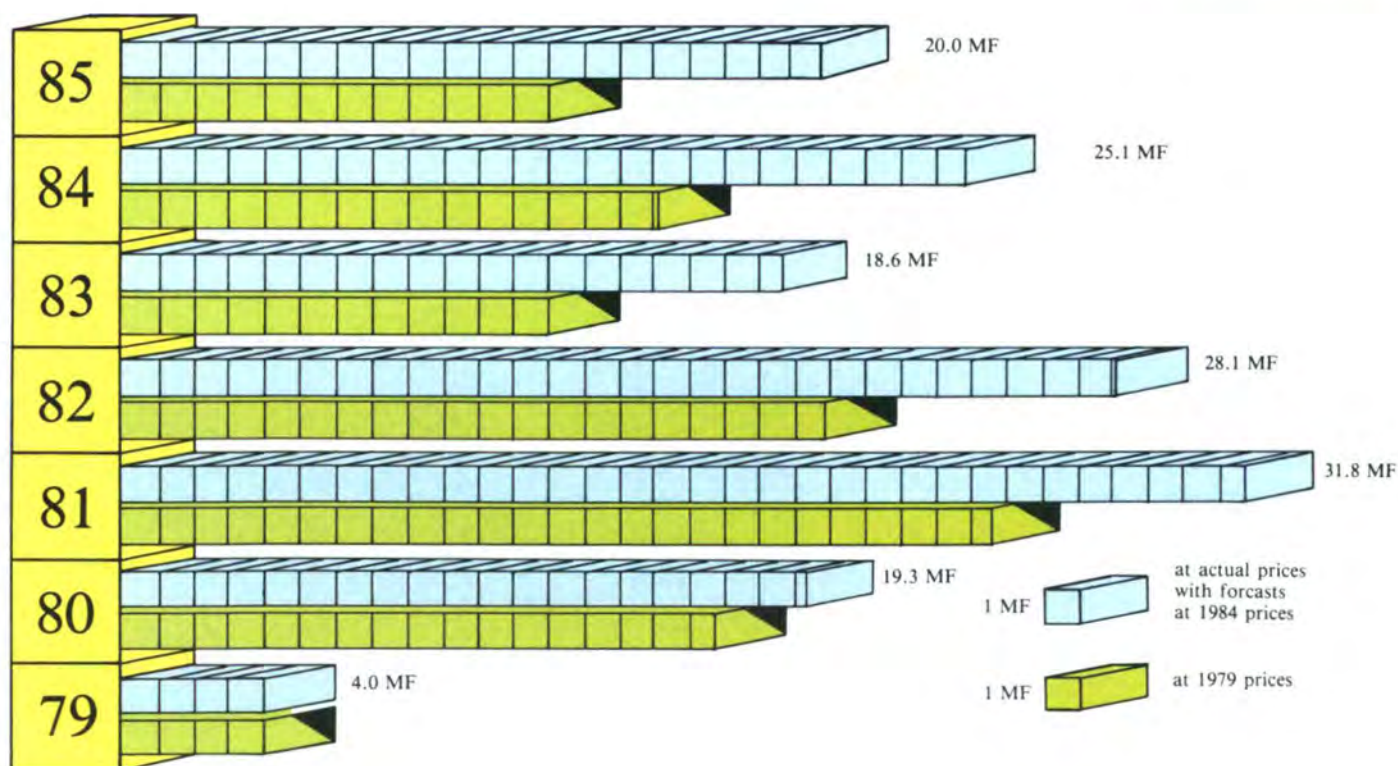
The 1984 instalment of the Modernisation Programme Budget amounts to 25 MF (excluding taxes).

The expenditure may be broken down by sections as follows:

TABLE 5
1984 Budget for the Modernisation Programme
(excluding taxes)

	1984 (1000 F)	% of total
<i>a) Operation</i>		
Consumable materials and small equipment	313.0	1.2
Staff costs	4 290.0	17.1
Long-term service and supply contracts	324.0	1.3
Other work, supplies and services from third parties	3 356.0	13.3
Transport, removal and travel expenses	149.0	0.7
Miscellaneous administrative costs	182.0	0.7
Total operation expenditure	8 614.0	34.3
ILL's own income	3 247.0	12.9
Total operation	5 367.0	21.4
<i>b) Investments</i>		
Buildings	3 220.0	12.8
Experimental instruments	16 478.0	65.8
Total investments	19 698.0	78.6
Total expenditure	25 065.0	100.0

Figure 72: The Modernisation Programme.



IMPLEMENTATION OF THE BUDGET (1967 to 1984) AND OUTLOOK FOR 1984 to 1989

The graphs of the ILL Budgets from its foundation in 1967 show the various phases of the Institut's development.

Between 1967 and 1971 there was the construction phase for the buildings, the reactor and its associated installations, followed by the reactor going critical in December 1971, then 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.

In the last few years, the ILL has carried out a major pro-

gramme of reactor renovation and of investments on improved instruments and the new cold source.

In 1986, the reactor will resume its normal operation with 6 cycles a year after the long shut-down from October 1984 to August 1985. This implies the complete financing of the consequences of the increases in the Dollar exchange rate in relation to the Franc under the Fuel Element budget and the coverage of the expenditure resulting from the end of the Modernisation Programme. This hypothesis is shown in the graph as "Option 1+", which has been submitted to the ILL Associates.

The hypothesis of maintaining the budget at a *constant* volume from 1986 would lead the Institut to reduce its operation by one fuel element cycle, close down certain operational instruments, and reduce its staff complement plan.

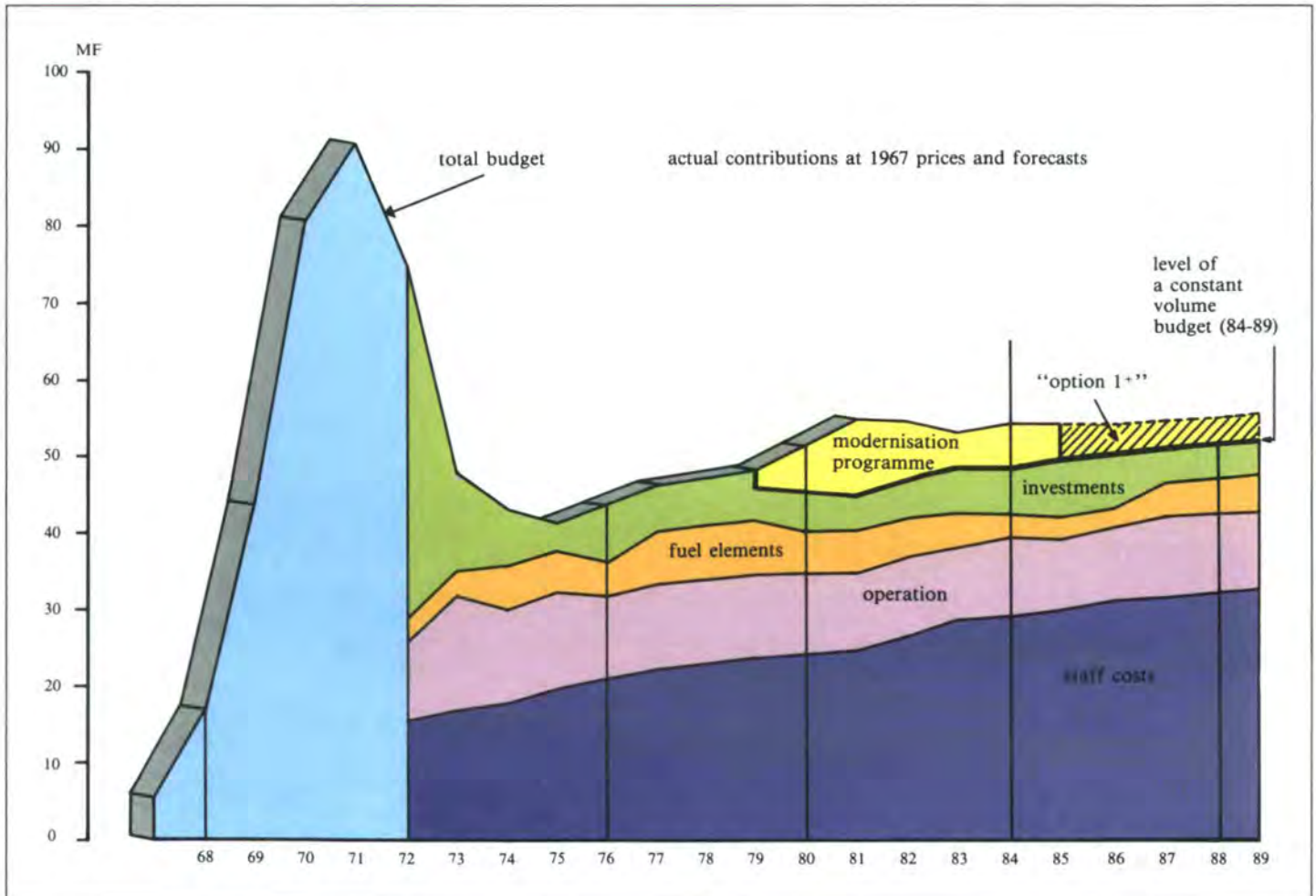


Figure 73: I.L.L. Budgets 1967 to 1989 at 1967 prices.

PURCHASING

The investment programme continued with a number of major purchases in 1984.

Four fuel elements have been ordered, 2 each from CERCA (4 223 KF) and NUKEM (4 390 KF) which will permit reactor operation until the beginning of 1986. Cogema was awarded the contract for Uranium enrichment and conversion of UF₆ to metal at 1 052 KF.

The cell of the new Horizontal Cold Source has been ordered from SICN (797 KF), and consultations for the neutron guide block in nickel are now underway. Invitations to tender for another sub-assembly of the Horizontal Cold Source, the Zircaloy Beam Tube Liner, have been sent out to potential suppliers.

Maintenance work and re-equipment of the Reactor during the long shutdown involves a number of important purchases, such as the replacement of the thermodynamic measuring equipment which has been awarded to Camille Bauer (1 321 KF). The Health Physics system will also be renewed and so far the Beta/Gamma dust and gas detectors have been ordered from Berthold (792 KF).

Other major purchases include the monochromator shielding for D9 which was awarded to SIGRI (952 KF), and twenty high-precision temperature controllers designed by ILL have been ordered from Automatic Systems Laboratories (445 KF) and Duhamel (495 KF).

In the computing area 3 Vax mini-computer systems have been purchased — one from Plessey (589 KF) and the other two from Digital (853 KF and 352 KF respectively). Evans & Sutherland have been awarded an order for a graphics colour system (597 KF).

As in previous years, the ILL ensured that firms in the three member states were invited to tender for all major purchases, and particularly for the components of the Horizontal Cold Source ILL engineers visited the British and German companies involved to discuss technical problems.

TABLE 6
Distribution of ILL's "free" purchases in 1984*

	1984		1983
	MF	%	(for comparison) %
France	7.0	34	60
Germany	7.8	37	21
United Kingdom	2.2	11	8
Other	3.8	18	11
Total	20.8	100	100

* Free purchases means that a free choice of supplier was possible excluding, therefore, the fuel cycle, electricity and small purchases of less than 50 000,- FF.

Since the foundation of the ILL in 1967 the Administration Department has been directed by (right to left): Dr. W. Hasenclever (now Köln) from 1967-1973; Dr. A. Platteneich (now KFA-Jülich) from 1973-1978; Dr. W. Grillo (now GSF-Neuherberg) from 1978-1983; Dr. C. Eitner present head of administration. ►



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- "1/Degeneracy expansion for the Hubbard model".
J. SAMSON, Cornell University.
- "Propagation and scattering of light in powders".
U. FELDERHOF, I.L.L./Aachen.
- "L'effet Hall quantique : propriétés collectives du fluide d'électrons bidimensionnel".
D. HALDANE, University of Southern California.
- "Orbites classiques et niveaux quantiques dans un potentiel nucléaire".
R. ARVIEU, ISN, Grenoble.
- "The electron glass".
J.H. DAVIES, University of Cambridge.
- "Instabilités morphologiques en croissance cristalline".
M. KERZBERG, Xerox, Palo Alto.
- "Quantum dynamics of non integrable systems".
D. GREMPEL, I.L.L.
- "Instabilité 'du premier et second ordre' en injection uni- et bipolaire dans un liquide isolant".
M. ATTEN, Laboratoire d'Electrostatique, CNRS, Grenoble.
- "Fractal dimension of dielectric breakdown".
L. PIETRONERO, Brown-Boveri, Baden, Suisse.
- "Scaling theory and minimum metallic conductivity".
N. MOTT, University of Cambridge.
- "RMN et migration macromoléculaire dans les polymères fondus".
C. COHEN-ADDAD, CERMO, Grenoble.
- "Dynamique sur les fractales".
M.R. RAMMAL, University of Pennsylvania and CNRS, Grenoble.
- "Amas semi-cristallins de charges dans les polymères ioniques".
B. DREYFUS, DRF-CENG
- "Modélisation des verres métalliques par simulation : structure et diffusion atomique".
F. LANCON, DRF-CENG.
- "Differential geometrical approach to dissipation in many-body systems".
U. REINHARDT, Dresden.
- "Equation de Langevin pour le transport d'électrons chauds dans un semi-conducteur".
J.J. NIEZ, LETI-CENG.
- "Transition nématique-isotrope de polymères flexibles".
G. MARET, Max-Planck-Institute CNRS, Grenoble.
- "The structure of simple liquids and non-newtonian behavior".
H.J.M. HANLEY, National Bureau of Standards, Boulder, co., USA.
- "Exactly solvable model of electronic motion in an incommensurable potential".
D. GREMPEL, I.L.L.
- "Un modèle rhéologique des dispersions concentrées".
D. QUEMADA, I.L.L.
- "Rhéologie des dispersions concentrées (II)".
D. QUEMADA, I.L.L.
- "Mécanique statistique des systèmes de neurones".
P. PERETTO, CENG.DRF.
- "Momentum distribution in liquid and solid helium".
R.O. SIMMONS, University of Illinois.
- "Dynamic impurities in ultra pure semiconductors".
L.M. FALICOV, University of California, Berkeley et Lure.
- "Three-body processes in spin polarized hydrogen".
J. WALRAVEN, University of Amsterdam.
- "Non-conservation de la parité en physique (nucléaire notamment)".
B. DESPLANQUES, I.L.L.
- "Transition de phase dans le cas de compétition d'échange et d'anisotropie - Généralisations possibles".
P. BECKER, I.L.L.
- "Fractional quantization of the Hall effect".
V. EMERY, Brookhaven National Laboratory.
- "Recent progress in the theory of metallic magnetism".
T. MORIYA, Institute of Solid State Physics, Tokyo.
- "Domain wall thermodynamics and form factors of non-linear excitations in the easy-plane ferromagnetic chain. Application to $CsNiF_3$ ".
H. FOGEDBY, Aarhus (Denmark).
- "Surface effects in critical phenomena and polymer solutions".
E. EISENRIEGLER, IFF Jülich.
- "Bruit en 1/f dans les conducteurs".
R. RAMMAL, CRTBT/CNRS Grenoble.

- "Stabilité et instabilité en mécanique quantique".
J. BELLISARD, Université de Provence et CNRS, Marseille.
- "Temperature dependence of the Lamb shift".
W. FORD, I.L.L.
- "Les effets de cohérence dans le problème à N impuretés Kondo".
M. LAVAGNA, Laboratoire L. Néel, CNRS, Grenoble.
- "Phase transitions in systems with multibody interactions".
K. PENSON, Freie Universität, Berlin.
- "Conformal covariance and critical phenomena in confined geometries".
T. BURKHARDT, I.L.L. and Temple University, Philadelphia.
- "Dipolar Ising ferromagnets near T_c ".
G.A. GEHRING, Department of Theoretical Physics, Oxford University.
- "Diffusion and absorption in a regular array of traps".
U. FELDERHOF, I.L.L./Aachen.
- "Localisation des phonons".
R. MAYNARD, CNRS, Grenoble.
- "Echelles de temps en intermittence".
M. PAPOULAR, CNRS, Grenoble.
- "On the origin of van der Waals forces".
F. HIRSHFELD, Weizmann Institute and I.L.L.
- COLLEGE 3:**
Fundamental and Nuclear Physics
- "1s Lambshifts"
M. STÖCKLI, GSI Darmstadt.
- "Fission fragment properties in neutron induced fission of the even thorium isotopes."
M.J. TROCHON, Bruyères-le-Châtel.
- "Report on the 'Rencontre de Moriond' workshop on Massive neutrinos in particle and Astrophysics".
K. SCHRECKENBACH, I.L.L.
- "A study of ^{124}Te by neutron capture, nuclear orientation and electron spectroscopy".
D. HAMILTON, University of Sussex.
- "Radioactivity and neutron measurements and standards at the National Physical Laboratory".
P. CHRISTMAS, N.P.L. TEDDINGTON
- "High spin states in the odd-odd nuclei of the rare earth region and the anomalous signature splitting of the $[i_{13/2}]_n [h_{11/2}]_p$ band".
A. PINSTON, RFG/CENG.
- "The contribution of core polarisation to the shell model potential in ^{40}Ca and ^{208}Pb ".
H. NGO, Orsay
- "Metastable superconductors for the detection of neutrinos".
F. VON FEILITZSCH, Technical University, Munich
- "Are protons forever ?"
D. PERKINS, Oxford/CERN.
- "Heavy element research : Review and Preview".
R. CHASMAN, Argonne National Laboratory.
- "Neutron-antineutron oscillations in nuclei".
J.M. RICHARD, I.P.N. Orsay.
- "Fragment angular distribution in heavy ion induced fission reactions and fast fission fractionation".
V. RAMAMURTHY, Trieste.
- "Presentation on Nuclear Physics".
F. GONNENWEIN et al., I.L.L.
- "Capture reactions in rp- and r-processes".
M. WIESCHER, Mainz.
- "Quark structure of the nucleon".
G. RIPKA, CEN Saclay.
- "Measurement and calculation of PEDM in Xe atoms".
I. VOLD, Rutherford - I.L.L.
- "Microscopic approach to the dynamics of fission".
J.F. BERGER, Bruyères-le-Châtel.
- "The distribution of the difference of two Poisson stochastics and its application to n-n experiments".
H. PROSPER, I.L.L.
- "In-beam gamma-ray spectroscopy of light mass Hg isotopes".
S.J. ROBINSON, Vanderbilt University.
- "What do nuclear reactions on ^{26}Al have to do with stellar evolution and the formation of the solar system ?"
H. TRAUTWETTER, Münster.
- "Expérience sur la double décroissance beta sans neutrinos".
M. MENNRATH, Bordeaux.
- "Supersymmetry in nuclei".
(What is it, how and where is it tested and how well does it work ?)
R.F. CASTEN, Brookhaven National Laboratory and University of Köln.
- "Proton life-time experiments in the Fréjus tunnel".
R. BARLOUTAUD, Saclay.

"Fission of highly excited nuclei".
M. FABER, Vienna.

"Parity violation in light nuclei : the $^{19}\text{F}^*$ experiment".
K. ELSENER, Zurich.

"The nucleon optical potential"
P. HODGSON, University of Oxford.

"New techniques in photo fission experiments".
U. KNEISSL, Giessen.

"DIOGENES an instrument for research on light particle accompanied fission".
J. PANNICKE, I.L.L.

"Perturbed supersymmetries in Iridium and Gold Nuclei".
J. CIZEWSKY, Yale University.

"La physique du Toponium".
A. MARTIN, CERN.

"Precise Q_β -measurements for the neutron rich mass chains $^A_{\beta} = 95$ to 98".
F. BLÖNNINGEN, I.L.L.

"Statics and dynamics of the formation of symmetric fission modes in heavy ion collisions".
R. AROUMOGAME, University of Manitoba at Winnipeg.

"Neutron-Antineutron Oscillations".
R.E. MARSHAK, Virginia Polytechnic Institute.

COLLEGE 4:

Structural and Magnetic Excitations

"Diffraction experiments on fast ionic conductors".
H. SCHULZ, MPI, Stuttgart.

"Librational, rotational and vibrational excitations in the solid hydrogens".
A. LAGENDIJK, Amsterdam University.

"Orientational disorder in crystals : a model for the understanding of the structure of glasses".
R. VACHER, USTL, Montpellier.

"Polymorphism in dicarboxylic acid studied by Raman and X-ray scattering".
E.J. SAMUELSEN, Kjeller, (Norway) and Université Paris-Sud, Orsay.

"Magnetic excitations in unusual magnets :
(i) CeAs - a $S=1/2$ f.c.c. antiferromagnet
(ii) Cs Cr Br_2 - a system of dimers".
J. KJÆMS, Risø (Denmark) and L.L.B., Saclay.

"Regions of incommensurability in phase diagrams".
T. JANSSEN, Nijmegen (Netherlands).

"Electron momentum-density measurements in graphite intercalated compounds using synchrotron radiation".
G. LOUPIAS, LURE, Orsay.

"Experimental studies of the effect of a random field on the ordering of Ising magnets".
R.A. COWLEY, Edinburgh University.

"Potassium : charge-density-wave or normal metal".
M. SPRINGFORD, University of Sussex, Brighton.

"Paramagnetic scattering in γ -iron : do it better with time-of-flight".
A.P. MURANI, I.L.L.

"Hydrogen in metals : elastic interaction and phase transitions".
J. PEISL, University of München.

"Hyper-Raman spectroscopy and soft-mode calculations on $\text{KTa}_{1-x}\text{Nb}_x\text{O}_3$ solid solutions".
G. KUGEL, Metz.

"Commensurate and incommensurate structures : simple models and real experiments".
W. SELKE, KFA, Jülich.

"Electron energy-loss spectroscopy".
J.A.C. BLAND, I.L.L.

"Phase separation in liquid $^3\text{He} - ^4\text{He}$ mixtures".
T. BENDA, München University.

"Correlation theory of martensitic transformation b.c.c.-h.c.p. in Zr".
P.A. LINDGARD, Risø (Denmark).

"Phonons, fractons and fractals - A new approach to the thermal properties and lattice excitations of amorphous materials".
H.M. ROSENBERG, University of Oxford.

"Magnetic excitations in the quasi-2D planar magnet $\text{BaM}(\text{XO})_2$ ($M=\text{Co}, \text{Ni}$; $X=\text{P}, \text{As}$).
L. REGNAULT, C.E.N.G.

"Correlations and excitations near structural phase transitions".
G. MEISSNER, Saarbrücken University.

"Proposals for new neutron and synchrotron facilities in the U.S.A."
V. EMERY, G. SHIRANE, Brookhaven National Laboratory.

"Magnetic solitons".
L.J. de JONGH, Kamerlingh Onnes Laboratory, Leiden.

"Bulk magnetic properties and crystal-field excitations of ErAl_2 ".
H. STANLEY, I.L.L.

- "Paramagnetic spin fluctuations in 3d metals and alloys."
Y. ISHIKAWA, Tohoku University (Japan).
- "Excitations in modulated magnetic structures".
J. JENSEN, University of Copenhagen.
- "Studies of condensed matter with KENS spallation neutron sources".
Y. ISHIKAWA, Laboratoire Louis Néel, CNRS, Grenoble.
- "Recent advances in experimental and theoretical superconductivity".
R. ASOKAMANI, International Center for Theoretical Physics, Trieste.
- "Defects in polarisable lattices : vacancies in Zr metal and Li⁺ in KTaO₃".
R.L. MIGONI, Université Dijon.
- "Mixed valence effects in itinerant magnetism".
J. SPALEK, Université Paris-Nord.
- "A simple discrete model for commensurate-incommensurate phase transitions : application to REBe₁₃ and CeSb".
P. BECKER, I.L.L.
- "Magnetic properties of intermetallic Uranium compounds".
P. FRINGS, I.L.L.
- "Presentation of the new neutron guide laboratory in Jülich : cold source, neutron guides and instruments".
K. WERNER, KFA-Jülich.
- "New experimental results for critical phenomena in two-dimensional Ising antiferromagnets".
M. HAGEN, Edinburgh University.
- "Physisorption experiments at HASYLAB".
H.J. LAUTER, I.L.L.
- "High energy resolution X-ray scattering : recent tests at HASYLAB".
B. DORNER, I.L.L.
- COLLEGE 5:
Crystal and Magnetic Structures**
- "Neutron crystallography of membranes ; is it serious ?"
G. ZACCAI, I.L.L.
- "Diffusional broadening of the Mössbauer line in single crystals of FCC metals".
R. RUEBENBAUER, Krakow (Poland)
- "Neutron interferometry in noninertial frames".
T. WROBLEWSKI, I.L.L.
- "Time resolved X-ray scattering studies of field induced nucleation in BaTiO₃".
D.B. McWHAN, Bell Labs. (USA).
- "Relationship between the crystal structures and the superconducting/magnetic properties of rare earth rhodium stannides".
M. MAREZIO, CNRS Grenoble.
- "Anomalous scattering using synchrotron radiation".
D. RAOUX, LURE Orsay.
- "OCCAM - A new language for programming multiprocessors - First impressions".
S.A. WILSON, I.L.L.
- "Competition between magnetism and superconductivity in ReRh₄B₄".
H. MOOK, Oak Ridge.
- "Investigation of antiferromagnetic domains of various kinds by neutron diffraction topography".
J. BARUCHEL, I.L.L.
- "Spin correlation in cubic ferromagnets above T_C".
G. SHIRANE, Brookhaven National Laboratory.
- "Proton-glass dielectric behaviour of the deuterated mixed rubidium ammonium dihydrogen phosphate crystals".
V.H. SCHMIDT, Montana State University.
- "The RETiO₃ perovskites".
J.E. GREEDAN, McMaster University, Ontario.
- "Study of magnetism at surfaces by scattering of neutrons at grazing incidence".
G.P. FELCHER, Argonne.
- "Dipole reorientations in Apatite"
R.A. YOUNG, Atlanta.
- "Neutron crystallography research in Trombay".
R. CHIDAMBARAM, Trombay.
- "The Kondo resonance and volume collapse in cerium materials".
J.W. ALLEN, Xerox Corporation, Palo Alto, California.
- "Neutron diffraction studies of weak antiferromagnetism and anisotropic interactions".
V. PLAKHTI, Leningrad Nuclear Physics Institute.
- "Electron charge and momentum density studies of transition metals".
J.R. SCHNEIDER, HMI Berlin.
- "Low dimensional characteristics of organic superconductors".
D. JEROME, Laboratoire de Physique des Solides, Orsay.

COLLEGE 6:

Liquids, disorder and defects in materials

"Impact of electron energy loss spectroscopy in materials sciences and biological sciences".

C. COLLIEX, Laboratoire de Physique des Solides, Orsay.

"Ion implanted materials : a challenge for solid state studies".

H. BERNAS, Centre de spectroscopie nucléaire et de spectroscopie de masse, Orsay.

"Diffusion in concentrated lattice gases".

K. KEHR, Jülich.

"The structure of simple liquids and non-newtonian behavior".

H.J.M. HANLEY, National Bureau of Standards.

"What can we learn from non-equilibrium molecular dynamics ?"

S. HESS, I.L.L.

"Phonons, fractons and fractals. A new approach to the thermal properties and lattice excitations of amorphous materials".

H.M. ROSENBERG, University of Oxford and I.L.L.

"Quantum evaporation of ^4He ".

A.F.G. WYATT, University of Exeter.

"Recent developments in metallic glasses".

H.J. GUNTHERODT, University of Basel.

"The quantum hall effect".

K. VON KLITZING, Technischen Universität München.

"Low temperature properties of disordered solids".

K. HUNKLINGER, University of Heidelberg.

"Elementary steps of ionic motion in fast ionic conductors".

K. FUNKE, University of Hanover.

"Diffusion of hydrogen in metals".

J. VOLKL, University of München.

COLLEGE 8:

Biochemistry

"Discussion on proposals and on symposium on neutrons in biology".

"Internal dynamics, hydrogen exchange and functional labelling in haemoglobin".

W. ENGLANDER, University of Pennsylvania.

"Halorhodopsin and slow rhodopsin".

W. STOECKENIUS, University of California, San Francisco.

"Protein dynamics observed by nuclear magnetic resonance".

Dr. K. WUTHRICH, ETH - Zürich.

"Site-specific recombination of bacteriophage λ and related phages".

S. NUNES-DUBY, Brown University, Rhode Island and Cell Biology, ETH Zürich.

"Neutron diffraction studies of B.P.T.I., RNase and insulin".

A. WLODAWER, N.B.S., Washington.

"The unwinding of ds DNA by RecA protein (its study by electron microscopy)".

E. DI CAPUA, ETH Zürich.

"Nerve fibres in the visual pathway".

J. SCHOLLES, MRC Cell Biophysics Unit, London.

COLLEGE 9:

Chemistry

"Relaxation phenomena in simple gaseous systems".

F.R.W. MCCOURT, University of Waterloo and Imperial College.

"Fractal structure of polymers and colloidal aggregates".

D.W. SCHAEFER, Sandia National Laboratory, Albuquerque.

"Neutron and X-ray scattering from surfaces and interfaces".

R.K. THOMAS, Oxford University.

"Etude par diffusion Raman des phases plastiques de molécules de symétrie ternaire".

J.L. SAUVAJOL, Université de Lille.

"Phase equilibria in liquid crystalline systems. Oligomers of the p-Oxybenzoate series".

M. BALLAUFF, University of Mainz.

"Electrochemical intercalation reactions".

J.O. BESENHARD, München.

"Recent results in inelastic neutron spectroscopy".

H. JOBIC, CNRS Lyon.

"Structural investigations on electrically conducting polymers".

M. STAMM, KFA Jülich.

"SANS studies of micellar and microemulsion systems".

L. MAJID, University of Tennessee.

"Optical studies of proton tunneling in carboxylic acid crystals".

M. TROMMSDORF, Laboratoire de spectrométrie Physique, Université de Grenoble.

"Etude par spectrométrie infrarouge et Raman de la rotation interne du groupement méthyle CHD_2 dans le toluène et le nitrométhane".

D. CAVAGNAT, ILL - Bordeaux.

"Forces between simple molecules"

E.B. SMITH, Chemistry Department, Oxford.

"Computer simulations on a highly parallel computer (the DAP)".

S. PAWLEY, Edinburgh.

"Orientational disordering and wetting transitions of iron pentacarbonyl ($\text{Fe}(\text{CO})_5$) adsorbed on graphite".

H. TAUB, University of Missouri - Columbia.

"Metal-metal bonding with d-, f- and main group elements".

A. SIMON, Max-Planck Institut, Stuttgart.

"Simulation of solid state chemistry and detonation".

S.F. TREVINO, NBS, Washington.

"Static and dynamic light scattering from colloidal silica dispersion in non-polar solvent at finite concentrations".

A. VRIJ, Utrecht.

"On the temperature dependence of rotational tunnelling".

G. HUGGINS, MPI Stuttgart.

"Solvation forces and molecular layering of liquids at surfaces".

J. ISRAELACHVILI, Canberra (Australia).

"Diffusion of long molecules through molten polymers".

A.R. RENNIE, Universität Mainz;

"Influence of the antileprosy drug, DDS, on model membrane systems".

K. USHA-DENITZ, Bhabha Atomic Research Centre, Bombay.

"Determination of the chain form factor of Urethane Elastomers in the isotropic and unidirectional stretched state".

K. HAHN, BASF, Ludwigshafen.

"An apparatus for the investigation of polymer coil deformation in a shear gradient by SANS".

P. LINDNER, I.L.L.

"Spectroscopy of adsorbed species and model compounds" (The 1984 Waddington Memorial Lecture).

J. HOWARD, University of Durham.

"A square commensurate 2-dimensional solid of CD_4 physisorbed on a $\text{MgO}(100)$ - surface".

B.⁴ CROSET, Groupe de Physique des Solides, Université Paris VII.

OTHERS

"Atténuation des ultrasons dans H^3 -A associée avec les textures".

K. MAKI, Kyoto University.

"Information sur le TRANSPAC".

O. TILLIER, I.L.L.

"Méthodes et outils de développement des systèmes informatiques".

M. GREVAZ, I.L.L.

"Comment s'étale une goutte".

P.G. DE GENNES, Collège de France

I.L.L. WORKSHOPS AND CONFERENCES

WORKSHOPS ORGANIZED BY THE I.L.L. IN 1984

- Workshop on "Reactor Based Fundamental Physics", (organized by B. Desplanques, F. Gönnerwein, W. Mampe)
Journal de Physique-Colloques, Vol. 45, C3 (1984) I.L.L. 7-9 November, 1983
- Workshop on "Sample Environments in Neutron and X-Ray Experiments", (organized by C. Vettier, A. Wright, B. Maier)
Revue de Physique Appliquée, Vol. 19, pp. 643-833 (1984) I.L.L. 13-15 February, 1984
- Workshop on "Semiclassical Methods in Nuclear Physics", (organized by R.W. Hasse, R. Arvieu, P. Schuck)
Journal de Physique-Colloques, Vol. 45, C6 (1984) Grenoble, France 5-8 March, 1984

Workshop on "Water". Structure and Dynamics of Water and Aqueous Solutions : Anomalies and their Possible Implications in Biology, (organized by P. Chieux, A.J. Dianoux, B. Maier, J. Teixeira, G. Zaccari)
Journal de Physique-Colloques, Vol. 45, C7 (1984) I.L.L. 16-18 April, 1984

Workshop on "High Resolution Neutron Powder Diffraction", (organized by A.W. Hewat, B. Maier, J. Pannetier) (not to be published) I.L.L. 1-3 August, 1984

WORKSHOPS SPONSORED BY THE I.L.L. IN 1984

NATO Advanced Study Institute, "Glass Current Issues", (organized by J. Dupuy, A.F. Wright, J.P. Causse) Tenerife, Spain 2-3 April, 1984
Martinus Nijhoff, pub., The Netherlands

THESES

The experimental work of which was carried out at I.L.L.

- Johann BARTEL Dissertation zur Erlangung des Doktorgrades der Naturwissenschaften, Universität Regensburg 1984. Semiclassische Berechnung Mittlerer Kerneigenschaften mit Hilfe der Partiellen h-Resummationsmethode.
- Christiane DEVAUX Thèse de Doctorat ès Sciences Université des Sciences et Techniques de Lille, Octobre 1983. Analyse Structurale de l'Adenovirus Humain.
- Paul FRINGS Doctor in de Wiskunde en Natuurwetenschappen aan de Universiteit van Amsterdam, September 1984. Magnetic Properties of Intermetallic Uranium Compounds.
- Peter GERFACH Dissertation zur Erlangung des Grades eines Doktors der Naturwissenschaften der Fakultät für Physik der Eberhard-Karls-Universität zu Tübingen, September 1984. Mittlere Ordnung und Unordnung in der orientierungsfehlgeordneten Phase von Hexachloräthan.
- David GREGSON Thesis for the degree of Doctor of Philosophy, University of Bristol, March 1983. Deformation Density Studies by X-Ray Neutron Diffraction.
- Christopher Ian JEWELL Thesis for the degree of Doctor of Philosophy, University of Lancaster, January 1983. The Interaction of Ultra-Cold Neutrons with Super-fluid ^4He and a New Possible Super Thermal Ultra-Cold Neutron Source.

Colette LARTIGUE Thèse de Doctorat ès Sciences Physiques Université Pierre et Marie Curie Juillet 1984. Contribution à l'Etude des Hydrures des Composés Intermetalliques de Type LaNi_5 : Localisation et Dynamique de l'Hydrogène.

Uwe QUADE Dissertation der Fakultät für Physik der Ludwig-Maximilians-Universität München 10. August 1983. Messung der Ausbeuten der leichten ^{223}U Spaltprodukte aus der Reaktion $^{223}\text{U}(n_{th}, f)$ mit einer Ionisationskammer.

Andreas RUMPF Dissertation zur Erlangung des Doktorgrades der Naturwissenschaften der Abteilung Physik der Universität Dortmund, 15. November 1984. Interferometric der Ausbreitung thermischer Neutronen im Bewegten Medium.

Klaus SCHRECKENBACH Habilitationsschrift für das Fach Experimentelle Physik im Fachbereich Physik der Technischen Universität München, Grenoble, November 1984. Beiträge hochauflösender Elektronenspektroskopie zur Atom-, Kern- und Neutrinophysik.

Thomas WROBLEWSKI Dissertation zur Erlangung des Doktorgrades der Naturwissenschaften der Abteilung Physik der Universität Dortmund, Oktober 1983. Neutroneninterferometrie in nichtinertialen Systemen.

EXPERIMENTS CARRIED OUT AT THE I.L.L.

The following is the list of experiments performed at the I.L.L. up to Oct. 1984 for which experimental reports were received before Jan, 17th 1985. For a detailed study of the results, please refer to: "1984. I.L.L. Experimental Reports and Theory College Activities" (Part 1 College 3 to 5. Part 2 College 6 to 9.) (Reports marked with * are not available for publication).

COLLEGE 3: FUNDAMENTAL AND NUCLEAR PHYSICS

- 3-01-144 Nuclear charge distribution for thermal neutron induced fission of ^{239}Pu . PN 1
SCHMITT C., CLERC H.G., MUETTERER M., THEOBALD J.P. (Darmstadt).
GUESSOUS A., BOCQUET J.P., NIFENECKER H., RISTORI C. (CEN-Grenoble).

BRISOT R., FAUST H.R., GOENNENWEIN F., PANNICKE J. (ILL), ENGELHARDT D. (Karlsruhe).

3-01-145 Cold fragmentation in thermal neutron induced fission of ^{239}Pu . PN 1
CLERC H.G., KOCZON P., SCHMITT C., THEOBALD J.P. (Darmstadt).
BRISOT R., GOENNENWEIN F., FAUST H.R. (ILL).

3-01-157 Isomer ratios of ^{97}Y and ^{98}Y in the fission of ^{235}U and lifetimes of some prompt transitions in fission products PN 1
DENSCHLAG H.O., DITZ W., GUETTLER U., HOERNER S., SOHNIUS B., STUMPF P. (Mainz), FAUST H.R. (ILL).

3-01-158	Qbeta-measurements of neutron-rich isotopes in the mass region $103 < A < 110$ using the mass separator LOHENGRIN. MUENNICH F., KEYSER U., PAHLMANN B. SCHREIBER F. (Braunschweig). WEIKARD H., FAUST H.R., PFEIFFER B. (ILL).	PN 1	3-02-258	The level structure of ^{130}I . MARTYNOV V., KHAZOV YU. (Leningrad). SCHRECKENBACH K., BOERNER H. HOYLER F., KERR S. (ILL).	PN 2 PN 3
3-01-160	Development of ionization chambers. OED A., GELTENBORT P. GOENNENWEIN F. (ILL) STUETZ B. (Tuebingen).	PN 1	3-02-261	Investigation of inter- and intraband transitions of the O_2^+ , 2_1^+ , O_3^+ bands in ^{156}Gd . HOYLER F., SCHRECKENBACH K., BOERNER H.G. (ILL)	PN 3 PN 2
3-01-161	Nuclear charge identification of fission fragments from fast pulse shapes from a surface barrier detector FINCH E.C., DELANEY C.F.G. HENARI F.Z. (Dublin).	PN 1	3-02-262	SEE 3-02-249	
3-01-162	Bragg curves for fission fragments. STUETZ B. (Tuebingen). OED A., GELTENBORT P., GOENNENWEIN F. (ILL).	PN 1	3-02-264	Internal conversion electron spectroscopy of ^{126}Te . HAMILTON D., SUBBER A. (Sussex). SCHRECKENBACH K. (ILL).	PN 2
3-01-163	Fractional yields and isomeric ratios in ^{233}U (nth, F). DENSCHLAG H.O., DITZ W., GUETTLER U. LIETZ C., SOHNUS B., STUMPF P. (Mainz), FAUST H.R. (ILL).	PN 1	3-02-267	SEE 3-02-289	
3-01-166	Study of the beta-decay of long-lived isomeric states of odd-Z nuclei in the mass region $A \approx 100$. MUENNICH F., KEYSER U., PAHLMANN B. SCHREIBER F. (Braunschweig). WEIKARD H., FAUST H.R., PFEIFFER B. (ILL).	PN 1	3-02-273	Neutron capture cross section of the O^- isomer in ^{152}Eu . EGIDY T.V., HUNGERFORD P. SCHMIDT H.H. (Muenchen). HOYLER F. (ILL), PETROV Y.V. (Leningrad)	PN 4
3-01-168	Measurements of the nuclear charge distribution of fission products with high efficiency. CLEMENTE M., HANSCH W., LORENZ H. QUADE U., RUDOLPH K., WEIDL I. (Muenchen). BRISSOT R., FAUST H. (ILL).	PN 1	3-02-276	Internal conversion electrons in presence of a K vacancy. SCHRECKENBACH K. (ILL).	PN 2
3-02-204	A detailed investigation of the structure of the odd mass Dy isotopes. EGIDY T.V., HUNGERFORD P. SCHMIDT H.H., BALODIS M. PROKOFJEV I.P. (Muenchen). BOERNER H.G., KERR S.A., SCHRECKENBACH K. HOYLER F., COLVIN G. (ILL).	PN 3 PN 4	3-02-279	Excited levels of ^{241}Pu from neutron-capture gamma-ray and conversion-electron measurements. WHITE D. (Monmouth), HOFF R. (Livermore). BOERNER H., HOYLER F., COLVIN G. SCHRECKENBACH K. (ILL).	PN 2 PN 3 PN 4
3-02-222	Monoenergetic positrons from the decay of ^{152}Eu . COLVIN G., SCHRECKENBACH K. (ILL). GELLETLY W. (Manchester).	PN 2	3-02-280	Some tests for a dynamical supersymmetry using double neutron capture in ^{191}Ir . COLVIN G., BOERNER H.G. GELTENBORT P., HOYLER F. SCHRECKENBACH K. (ILL). CIZEWSKI J. (Yale Univ.).	PN 2 PN 3 PN 4
3-02-241	Instrumental neutron activation analysis of hercynian granites, Western French Alps. OLIVER R.A. (ILL), VITTOZ P. (Grenoble).	PN 4	3-02-281	Conversion electrons in the $^{103}\text{Rh}(n, \gamma)^{104}\text{Rh}$ reaction. MCMAHON T.D. (Ascot). CHALHOUB O. (London). COLVIN G. (ILL).	PN 2
3-02-242	Investigation of the low-lying states in ^{94}Nb . BOGDANOVIC M., DRITSA S. (Beograd). BOERNER H., KERR S., HOYLER F. SCHRECKENBACH K., COLVIN G. (ILL).	PN 3 PN 4 PN 2	3-02-282	Study of nuclear levels in ^{192}Ir . COLVIN G., SCHRECKENBACH K. (ILL). KALANGA M., KERN J. (Pribourg). EGIDY T.V. (Muenchen).	PN 2
3-02-244	Study of the levels in ^{140}La produced in the $^{139}\text{La}(n, \gamma)^{140}\text{La}$ reaction. SCHRECKENBACH K., COLVIN G. (ILL). STOJANOVIC M., SIMIC J. (Beograd).	PN 2	3-02-283	Study of EO transitions in ^{195}Pt and tests of multi J supersymmetries. CASTEN R.F. (Koeln/BNL).	PN 2
3-02-249	Some tests for a dynamical supersymmetry using double neutron capture in ^{193}Ir . COLVIN G., BOERNER H.G., HOYLER F. SCHRECKENBACH K., GELTENBORT P. KERR S. (ILL), CIZEWSKI J. (Yale Univ.).	PN 2 PN 3 PN 4	3-02-284	Detailed study of ^{102}Ru and tests of gamma softness-mean gamma relationships in the IBA. CASTEN R.F. (Koeln/BNL).	PN 3
3-02-250	Determination of vibrational states in ^{231}Th -measurement of EO admixtures in some transitions of ^{231}Th . BOERNER H.G. (ILL), HOFF R.W. (Livermore).	PN 3	3-02-288	Investigation of ^{172}Er by double neutron capture. HOYLER F., GELTENBORT P. (ILL).	PN 4
3-02-256	Instrumental neutron activation analysis of eight international geochemical standards. VITTOZ P. (Grenoble), OLIVER R.A. (ILL).	PN 4	3-02-289	Absolute measurement of the cumulated beta spectrum of ^{235}U fission products. SCHRECKENBACH K., COLVIN G. (ILL). FEILITZSCH F.V. (Muenchen). GELLETLY W. (Manchester).	PN 2
			3-02-290	Thermal neutron capture in ^{86}Sr and ^{87}Sr . KRUSCHE B., WINTER C., LIEB K.P. (Goettingen). EGIDY T.V., SCHMIDT H.H. (Muenchen). HOYLER F. (ILL).	PN 3
			3-02-291	An initial program of absolute gamma spectroscopy at high energies using a two-flat crystal spectrometer. KESSLER E., GREENE G., DESLATTES R. (Washington).	PN 3

3-03-179	Test of the applicability of the high temperature ion source of PN6 for the study of neutron-rich rare-earth elements. (Part II) PFEIFFER B. (ILL),MUENZEL J. (Giessen). MONNAND E.,PINSTON J.A.,SCHUSSLER F. (CEN-G)	PN 6	3-13- 66	Systematic study of (n, α) and (n,f) reactions. WAGEMANS C.,D'HONDT P. (Mol). SCHILLEBEECKX (Gent). EMSALLEM A. (Lyon),BRISOT R. (ILL).	H22D
3-06- 22	Level schemes of neutron-rich A=99 nuclei. Part II : Beta decay of ^{99}Zr and of the ground state of ^{99}Nb . PFEIFFER B. (ILL). MONNAND E.,PINSTON J.A. (CEN-G). LAWIN H. (Juelich),MUENZEL J. (Giessen).	PN 6	3-13- 67	Nanosecond lifetime measurements in thermal neutron capture. ANDREJTSCHIEFF W.,PETKOV P. PROTOCHRISTOW C. (Sofia). HAMILTON W.D. (Brighton),MORE B.R. (ILL).	S34
*3-06- 36	Gamma-ray coincidence and correlation measurements in ^{98}Rb . HAMILTON D. (Sussex).	PN 6	3-13-68	SEE 3-13 63	
3-06- 58	β -measurements of neutron-rich Cs- and Ba-isotopes with mass number A=146 and above using the mass separator OSTIS. MUENNICH F.,GRAEFENSTEDT M. KEYSER U.,PAHLMANN B. (Braunschweig). PFEIFFER B.,WEIKARD H. (ILL).	PN 6	4-01-243	Elastic shear constants of polyethylene. BUCHENAU U.,STAMM M. (Juelich). NUECKER N. (Karlsruhe).	IN 6
3-06- 65	SEE 3-06- 58		*4-01-244	Lattice dynamics of trans-polyacetylene. PEPY G. (CEN-Saclay). ROSTA L.,HOLCZER K. (Budapest).	IN 8
3-08- 1	Mass and energy distribution of fission fragments in $^{249}\text{Cf}(n,f)$. AKER E.,ENGELHARDT D. (Karlsruhe). BRISOT R.,GELTENBORT P. GOENNENWEIN F.,OED A. (ILL). GINDLER J.,WILKINS B. (Argonne). BARREAU G.,LEROUX B. (Bordeaux). NIPENECKER H.,PERRIN P.,RISTORI C. (CEN-Grenoble).	PN 8	4-01-254	Molecular dynamics in imidazole. LINK K.H. (Darmstadt). GRIMM H.(Juelich),DORNER B.(ILL).	IN 3
3-08- 6	Mass and energy distribution of fission fragments from the $^{245}\text{Cm}(n,f)$ reaction. KOCZON P.,MUTTERER M. THEOBALD J.P. (Darmstadt). MOORE M.S. (Los Alamos). GOENNENWEIN F.,GELTENBORT P. OED A.,PANNICKE J. (ILL).	PN 8	4-01-256	Lattice dynamics of graphite. MAGERL A.,LAUTER H.J. (ILL). ZABEL H. (Urbana).	IN 8
3-13- 13	SEE 3-13- 56		4-01-257	Phonon softening in Nb_3Ga . (Nb_3Sn) PINTSCHOVIVUS L.,REICHARDT W. (Karlsruhe).	IN 8
3-13- 42	Directional correlation in ^{144}Nd . HAMILTON D. (Sussex). SNELLING M. (ILL).	H22F	4-01-274	Phonon dispersion in the CeNi intermediate valence compounds. GIGNOUX D.,GIVORD F.,LEMAIRE R. (CNRS,Grenoble),HENNION B. (LLB). ISHIKAWA Y. (Sendai).	IN 8
3-13- 44	Directional correlation measurements on ^{168}Er . HAMILTON D. (Sussex). SNELLING M.,MORE B. (ILL).	H22F	4-02-158	Magnetic excitations and correlations in $(\text{CD}_3)_4\text{NMnBr}_3$. VISSER D (Oxford),PAUL D.MCK. (ILL).	IN 2
*3-13- 45	Measurement of the magnetic moments of excited states populated in neutron capture. HAMILTON D.(Sussex),SNELLING M.(ILL).	H22F	4-02-158	Magnetic ordering in $(\text{CH}_3)_4\text{NMnBr}_3$. VISSER D. (Oxford),ZIEBECK K.R.A. (ILL).	D15
3-13- 47	Dual polarized beams by reflection on perfect crystals. FORTE M. (Ispra). BOEUF A.(Ispra & ILL),ZEYEN C.(ILL).	S21	4-02-188	Dynamics of the incommensurate phase of NaNO_2 . DURAND D.,DENOYER F. (Orsay). LAMBERT M.,BERNARD L. (LLB, Saclay). CURRAT R.,MEZEI F. (ILL).	IN11
3-13- 56	Multiparameter measurement of light charged particle associated fission on $^{239}\text{Pu} + n$. THEOBALD J.P.,MUTTERER M. KOCZON P.,WEINGAERTNER K. (Darmstadt). GOENNENWEIN F.,PANNICKE J. (ILL).	H22E/S51	4-02-191	Inelastic study of the Kohn anomaly in the quasi-one dimensional conductor $\text{K}_0,3\text{MoO}_3$. POUGET J.P. (Orsay). ESCRIBE-FILIPPINI C.,MARCUS J. SCHLENKER C. (CNRS,Grenoble).	IN 2 IN 3
*3-13- 60	The level structure of ^{126}Te . HAMILTON D. (Sussex). MORE B. (ILL).	S34	4-02-195	Soft zone boundary phonons in the layered tetrafluoroaluminate KAlF_4 . BULO A.,GIBAUD A., NOUET J.,ROUSSEAU M. (Le Mans). HENNION B.(LLB, Saclay),BOUILLOT J.(ILL)	IN 3
*3-13- 61	Directional correlation measurements in ^{158}Gd . HAMILTON D. (Sussex). MORE B. (ILL).	S34	4-02-198	Study of the modulated structure of quartz : inelastic neutron scattering. VALLADE M.,BACHHEIMER J.B.,BERGE B., DOLINO G., (Grenoble). ZEYEN C.M.E.,(ILL)	IN 3
3-13- 63	Prompt gamma activation analysis of geological materials. OLIVER R.A.,HOYLER F. (ILL). KERR S.A. (Surrey). VITTOZ P.,VIVIER G.,BUFFET G. (Grenoble).	H22F	4-02-199	Soft modes and martensitic transformations in $\text{Ti}_5\text{O}_{14}\text{Fe}_3$ characterized by inelastic neutron scattering. MOINE P.,ALLAIN J. (Poitiers). RENKER B. (Karlsruhe).	IN 8
3-13- 68			4-02-206	Dynamics of incommensurate phases of biphenyl under pressure. CAILLEAU H.,MESSAGE J.C. (Rennes). MOUSSA F.,BUGAUT F. (LLB,Saclay). VETTER C. (ILL).	IN12

COLLEGE 4: STRUCTURAL AND MAGNETIC EXCITATIONS

4-02-207	The influence of pressure on the dynamics of pretransitional effects in p-terphenyl. CAILLEAU H., BAUDOUR J.L. DELUGEARD Y., TOUDIC B. (Rennes). VETTER C. (ILL).	D15	4 03 335	Antiferro quadrupolar ordering and Kondo effect in CeB6. EFFANTIN J.M., ROSSAT MIGNOD J. KASUYA T. (CEN-Grenoble). VETTER C. (ILL).	IN12
4-02-213	Symmetry of incommensurate phases of biphenyl. CAILLEAU H., MESSEGER J.C. (Rennes). ZEYEN C. (ILL).	D10	4-03-341	Magnetic excitations in plutonium antimonide. LANDER G.H. (Argonne). ROSSAT-MIGNOD J., SPIRLET J.C. VOGT O. (CEN-Grenoble). STIRLING W.G. (ILL).	IN 8
4-02-219	Structure of domain walls in DKDP. COWLEY R.A., GIBBONS P.D. HIGGINS S.A. (Edinburgh).	IN 3	4-03-344	The energy width of the central component in CsNiF3 in an external field at low q. STEINER M., KAKURAI K. (Berlin). MEZEI F. (ILL).	IN 5
4-02-221	Inelastic study of the low frequency excitation in the incommensurate phase of Rb0.3MoO3. POUGET J.P. (Orsay). FILIPPINI C. (C.N.R.S.-Grenoble).	IN12	4-03- TES	Magnetic cross-over behaviour in CsFeBr3. VISSER D. (Oxford). STEIGENBERGER U., DORNER B. (ILL).	IN 3
4-03-262	Magnetic excitations in a palladium 5% iron alloy. MITCHELL P.W., COWLEY R.A. (Edinburgh), PAUL D.MCK. (ILL).	IN 8	4-04- 77	Polarization analysis of n-scattering from spin-waves in EuS. BOHN H.G., MALETTA H. (Juelich). WAGNER V. (Braunschweig).	IN 8
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5-32-192	Magnetic field dependence of the antiferromagnetic structure of neodymium. FORGAN E.M. (Birmingham). MCEWEN K.A.,BOUILLLOT J. (ILL). STANLEY H.B. (Southampton).	D 2	5-33-136	Polarisation analysis of the magnetic diffuse scattering of FeCrCa ₃ (GeO ₄) ₃ . BRUECKEL T.,PRANDL W. (Tuebingen). SCHAERPF O. (ILL).	D 7
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5-32-196	The effect of hydrostatic pressure on the magnet structure of the pseudo 1-D ferromagnet RbFeCl ₃ . HARRISON A.,VISSER D.,DAY P. (Oxford),VETTIER C. (ILL).	D15	5-34-103	Form factor of Ce and correlations in CeMg by polarization analysis. GALERA R.M.,PIERRE J. (CNRS,Grenoble).	D 7
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5-33- 76	Magnetization density in manganese orthosilicate Mn ₂ SiO ₄ . FUESS H.,LOTTERMOSER W. (Frankfurt).	D 3	5-43- 5	Neutron interferometry in noninertial frames. BONSE U. (Dortmund),WROBLEWSKI T. (ILL).	D18
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5-33-100	Magnetic ordering in a semimagnetic semiconductor. STEIGENBERGER U.,SCHAERPF O. (ILL). LEBECH B. (Riso),KEPA H. (Warsaw).	D 7	5-43- 7	Static versus time-dependent absorption in neutron interferometry. RAUCH H.,SUMMHAMMER J. (Wien).	D18
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6-01- 81	IN 8	Scattering of liquid hydrogen at intermediate energies. LANGEL W. (ILL).	6-06- 42 Propagating collective modes in molten alkali halides. MCGREEVY R. ,HOWE M. MITCHELL E.W.J. (Oxford). IN 4
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6-03-124	D 4	Liquid semiconductors and the Mott transition. ENDERBY J.E. ,BARNES A. (Bristol).	6-06- 44 The temperature dependence of the structure of molten alkaline earth halides. MCGREEVY R. ,MITCHELL E.W.J. DAY S.E. (Oxford). D 1B
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6-03-127	D 4	Liquid semiconductors and the Mott transition. ENDERBY J.E. ,BARNES A. (Bristol).	6-07- 55 Structural properties of Cl ⁻ ions in aqueous solutions. NEILSON G.W. ,ENDERBY J.E. SALMON P. (Bristol). D 4
6-04- 21	D 5	Polarized neutron studies of amorphous ferromagnetic alloys. WILLIAMS D.E.G. (Loughborough).	6-07- 59 Dynamics of aqueous solutions. ENDERBY J.E. ,SALMON P. (Bristol). IN10
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6-05- 73	D 2	Structural properties of liquids containing carbon : benzene. NEILSON G.W. ,CUMMINGS S. (Bristol).	6-07- 70 Understanding of crystallisation in a glass-forming electrolyte : role of the glass elements. DUPUY J. ,AOUIZERAT ,JAL J.F. (UCB, Lyon),CHIEUX P. (ILL). D 2 D11
6-05- 75	D 4	Structural changes in supercooled water with temperature variation. BELLISSENT-FUNEL M.C. ,TEIXEIRA J. (LLB, Saclay),BOSIO L. (Paris). DORE J. (Canterbury).	6-07- 71 Hydration of complex ions in aqueous solution : NaClO ₄ in heavy water. LUCK W.A.P. ,SCHIOBERG D. (Marburg). NEILSON G.W. (Bristol). D 4
6-05- 77	D 2	Polar group hydration using isotopic substitution : acetamide. FINNEY J.L. ,TURNER J. (London). NEILSON G.W. ,CUMMINGS S. (Bristol).	6-07- 76 Dynamics of aqueous solutions. ENDERBY J.E. ,SALMON P. (Bristol). HOWELLS W.S. (Rutherford). IN10
6-05- 78	D 4	Structure factor of benzene, hexa- fluorobenzene and its 1:1 mixture. BERTAGNOLLI H. ,BARTSCH E. (Wuerzburg).	6-07- 78 Vibrational frequency spectrum in ZnCl ₂ aqueous solutions by incoherent inelastic neutron scattering. BELLISSENT-FUNEL M.C. (LLB, Saclay). FONTANA M.P. (Parma). MAISANO G. ,MIGLIARDO P. (Messina). IN 4
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6-06- 27	IN 6	The separation of acoustic and optic modes in molten CsCl by isotopic substitution. MCGREEVY R. ,MITCHELL E.W.J. MARGACA F.M.A. (Oxford).	6-08-105 Small angle neutron scattering by a superionic conductor glass of the system AgPO ₃ -AgI. TACHEZ M. ,MERCIER R. ,MALUGANI J.P. (Besancon). D17
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6-08-112	The structure of new fluoride glasses "M ₁₁ M ₁₁ M ₁₁ F ₇ ". LE BAIL A. ,JACOBONI C. (Le Mans). CHIEUX P. (ILL).	D 4	6-12- 24	SANS studies of cement pore size development and variations with conditions of preparation. ALLEN A.J. ,PEARSON D. ,WINDSOR C.G. (Harwell).	D11
6-08-125	Low angle scattering studies of metallic amorphous alloys. RODMACQ B. ,CHAMBEROD A. (CEN-Grenoble).	D17	6-12-25	SEE 6-12-4	
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6-08-127	Substitution of Se by Te in Ce-As-Se ternary chalcogenide glasses ; consequences for medium range order and phase separation. JANOT C. (ILL),GEORGE B. (Nancy). PARANT J.P. (Marcoussis).	D11 D 2	6-12- 29 5-21-237	Structure determination of Bi ₁₂ PbO ₁₉ and Bi ₈ Pb ₅ O ₁₇ . BEECH F. ,STEELE B.C.H. ,KILNER J. MURRAY A.D. (London).	D 1A
6-08-128	Nucleation and crystallisation in aluminium based amorphous alloys. DUBOIS J.M. ,DEHGHAN K. (Nancy).	D 1B	6-12- 33	Anisotropy in small angle neutron scattering in metallic glasses. YAVARI A.R. ,JOUJOU J.C. ,BIJAOUI D. MARET M. (Grenoble).	D11
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6-08-142	a-Si ₈₅ : H ₁₅ short range order. CHENAVAS-PAULE A. (LETI,Grenoble). MENELLE A. ,BELLISSENT R. (LLB,Saclay).	D 4	6-12- 39	SEE 6-12- 26	
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6-08-145	Structure and hydrogen mobility in spun and sputtered (Cu ₅₀ Ti ₅₀)H amorphous alloys. RODMACQ B. ,CHAMBEROD A. (CEN-Grenoble).	D 1B IN 6 D17	6-12- 41	A study of the temperature dependent anisotropic scattering from silicon single crystals at low Q. KINDER S. ,PIKE B.C. ,STEWART R.J. (Reading).	D17
6-12- 4 6-12- 25	A study of oxygen precipitation in silicon. KINDER S. ,PIKE B.C. ,STEWART R.J. (Reading).	D11	6-12- 43	A study of crack growth and propagation in a PWR steel. MESSOLORAS S. ,STEWART R.J. (Reading).	D11
6-12- 6	The effects of electron irradiation on the precipitates in a nimonic PE16 superalloy. HULL S. ,MESSOLORAS S. ,STEWART R.J. (Reading).	D11	6-12- 44	Short range order in non-stoichiometric Ni-Cr alloys. CERRI A. ,KLAIBER F. ,KOSTORZ G. SCHOENFELD B. ,ZAUNE U. (Zurich).	D10 D11
6-12- 8	Small angle scattering from oriented latent nuclear tracks. ALBRECHT D. ,ARMBRUSTER P. ,SPOHR R. (Darmstadt). SCHAUPERT K. (Giessen).	D17	6-12- 45	Decomposition of Ni-Ti alloys. KOSTORZ G. ,CERRI A. ,SCHMELTZER R. ZAUNE U. (Zurich).	D11
6-12- 14	Effect of an applied elastic stress on the unmixing of Al-Zn single crystals. LIVET F. ,GUYOT P. ,BLOCH D. (ENSEEG,Grenoble).	D17	6-12- 46	SAS study of the thermal embrittlement behaviour of iron-base glasses. GEORGE B. (Nancy),JANOT C. (ILL).	D11
6-12- 18	Voids and crack nucleation in fatigued copper single crystals. CERRI A. ,KOSTORZ G. ,SCHMELTZER (Zurich). KETTUNEN P.O. ,KUOKKALA V.T. LEPISTO T. (Tampere).	D11	6-12- 53	Investigation of time-scaling properties during formation and reversion of GP-zones in AlZnMg. BERNOLE M. ,BLASCHKO O. ,FRATZL P. (Vienna).	D 7
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			6-13- 2	⁸ Li spin-lattice relaxation in liquid binary alloys of Li with Ge and Si and in pure liquid Li at very high temperatures. VAN DER MAREL C. ,HEITJANS P. ACKERMANN H. ,BADER B.	S 6

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6-13- 3	Nuclear spin relaxation in a Li-borate S 6 glass. SCHIRMER A. ,HEITJANS P. ACKERMANN H. ,BADER B. FREILAENDER P. ,STOECKMANN H.J. (Marburg/ILL). PETERSON N.L. ,THOMAS M.P. (Argonne).		6-14- 48	Diffusion processes in the superionic conductor Li3N. PETRY W. (ILL),BADER B. (Heidelberg).	IN13
6-14- 1	Local H(D)-vibrations in isotope mixtures of VHxDy. RICHTER D. ,HEMPELMANN R. LAESSER R. (KFA-Juelich).	IN1 B	6-14- 51	SEE 6-14- 35	
6-14- 3	Neutron powder diffraction study of PuDx. FOURNIER J.M. (CEN-Grenoble). BOEUF A. ,CACIUFFO R. (ILL). REBIZANT J. (Karlsruhe).	D 2	6-14- 53	Elementary jump process for fast diffusion of Co in beta-Zr single crystals. VOGL G. ,PLOTTMANN T. (Berlin). PETRY W. (ILL).	IN10
6-14- 5	Measurement of optical dispersion curves for PdD0.8+x. ROSS D.K. ,MCKERGOW M.W. GILBERD P.W. (Birmingham). CARLILE C.S. (Rutherford). BLASCHKO O. ,FRATZL P. (Wien).	IN 8	6-14- 54	Test of non-hopping channel-diffusion model by quasielastic scattering from a single crystal of alpha Ag2Se. FUNKE K. ,EWALD J.P. (Hannover).	IN12
6-14- 24	Pressure-dependent H distribution between tetrahedral and octahedral sites in VHx (0.05<x<0.5). WIPF H. (Darmstadt). MAGERL A. ,VETTER C. ,LAUTER H.J. (ILL),HEMPELMANN K. (Juelich).	IN 1	6-14- 56	Proton mobility in electrochemical and chemical alpha and beta PbO2 at low temperatures. BOHER P. ,GAVARRI J.R. ,GARNIER P. (Chatenay-Malabry),DIANOUX A.J. (ILL).	IN 5
6-14- 25	Local diffusion of hydrogen in NbOxHy (x = 0.011, y = 0.01). WIPF H. (Darmstadt). RICHTER D. (Juelich). MAGERL A. ,ANDERSON I. (ILL).	IN13	6-14- 57	Hydrogen in amorphous Pd80Si20. RODMACQ B. ,CHAMBEROD A. (CEN-Grenoble),NAUDON A. (Poitiers).	D11
6-14- 26	Low-temperature hydrogen tunneling in NbOxHy (x,y = 0.002). WIPF H. (Darmstadt). NEUMAIER K. (Garching),MAGERL A. (ILL).	IN12	6-14- 61	Hydrogen delocalisation in NbOxHx, x = 0.001. MAGERL A. (ILL). NEUMAIER K. ,WIPF H. (Darmstadt).	IN 6
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6-14- 29	Quasielastic scattering due to Ag+ ion diffusion in RbAg4I5. FUNKE K. ,EWALD J.P. (Hannover).	IN13	6-14- 63	Site occupancy in YHx. ANDERSON I.S. (ILL). ROSS D.K. ,BONNET J.E. ,GILBERD P. (Birmingham).	IN 1
6-14- 30	Hydrogen diffusion in amorphous Pd0.8Si0.2. RICHTER D. ,HEMPELMANN R. DRIESEN G. ,KIRCHHEIM R. (KFA-Juelich).	IN10	6-14- 65	Measurement of temperature dependence of diffuse elastic scattering from Pd/D. ROSS D.K. ,MCKERGOW M.W. (Birmingham). ANDERSON I.S. (ILL).	D10
6-14- 34	Diffuse quasi-elastic scattering from ZrO2 stabilised with Y2O3. HUTCHINGS M.T. (Harwell). HAYES W. ,OSBORN R. (Oxford). CLAUSEN K. (Riso).	IN12	6-14- 66	Investigation of localized jump motion in alpha YHx. ANDERSON I. (ILL). ROSS D.K. , BONNET J.R. , MCKERGOW M.W. (Birmingham)	IN13
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6-14- 43	Silicium-germanium interdiffusion and structural relaxation in composi- tionally modulated amorphous films. JANOT C. ,ROTH M. (ILL). PIECUCH M. ,MARCHAL G. (Nancy). CHAMBEROD A. (CEN-Grenoble).	D17	7-01-214	Polarised neutron diffuse scattering by iron rich FeV alloys. PARETTE G. ,MIREBEAU I. (LLB, Saclay).	D 7
6-14- 46	Solid state protonic conductors. DANIEL M.F. ,LASSEGUES J.C. , DESBAT B. (Bordeaux)	IN10 IN6	7-01-244	Magnetic short range order in a Y-Gd dilute alloy. CAUDRON R. ,SAFA H. (ONERA).	D 7
			7-01-247	Nuclear and magnetic short range order in single crystal Fe0.9V0.1. LEFEBVRE S. (CECM, Vitry). BLEY F.(ILL),MIREBEAU I.(LLB, Saclay).	D10
			7-03-241	High temperature elastic diffuse neutron scattering study of TiCx. NOVION C.H. DE ,LANDESMAN J.P. LORENZELLI N. (CEN-Fontenay). CHRISTENSEN A.N. (Aarhus).	D 7

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7-03-258	Elastic diffuse neutron scattering study of TiNO.82, (Nb0.8Ti0.2)NO.7 and Nb(CO.3NO.4). NOVION C.H. DE ,LANDESMAN J.P. (CEN-Pontenay),CHRISTENSEN A.N. (Aarhus).	D 7	8-04- 76	Light-induced proton dynamics of chlorophyll systems. FURRER A. ,STOCKLI A. MUEHLETHALER K. (Wuerenlingen). HEIDEMANN A. ,LANGEL W. (ILL).	IN 5
7-06-150	Diffuse scattering from YD0.17. ROSS D.K. ,MCKERGOW M. (Birmingham). BONNET J.E. (Paris),ANDERSON I.S. (ILL).	D 7	8-05-106	The distribution of ions in the lipid-water interface. BUELDT G. ,HENTSCHEL M.P. (Berlin).	D16
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AMOUREUX J.P.	84AM208	BENDALL P.J.	84BE136	BRAGANZA L.F.	84WO329
	84SA1087	BENOIT A.	84LA348	BRAID I.J.	84HO1004
ANDERSON I.S.	84BA6T	BENTLEY G.A.	84BE146	BRANT S.	84TO335
	84AN7T		84MA148	BRAU A.	84BR105
	84AN361	BERGE B.	84RO177	BRETT N.H.	84BR222
	84ME362		84BE364	BRISSOT R.	84MH102
ARMBRUSTER P.	84AL200		84DO138		84EG117
ASGHAR M.	84AS256	BERGEVIN F. de	84DO210		84OE153
	84DJ260	BERNERON M.	84BA237		84DJ260
	84EM1010	BERNOLE M.	84PO1012		84SC332
ASTRUC J.M.	84HO1T	BERNOTAT H.	84BE285		84DH377
	84HO369	BERTAGNOLLI H.	84BL374	BROS J.P.	84BL378
AUVRAY L.	84AU1083	BERTHET-COLOMINAS C.	84RE130	BROWN P.J.	84HE290
AVENIER M.	84AV1031	BESNARD M.	84BE206		84BR167
	84AV1052	BIERSACK J.P.	84CH299		84BR204
BACHHEIMER J.P.	84DO138		84DE372		84BR233
	84DO210	BERTHET-COLOMINAS C.	84LA152		84MA239
	84BA237	BESNARD M.	84BL394		84BR308
BACON G.E.	84BA1096	BEWERSDORF G.	84FI1015		84LA360
BACON P.J.	84BA1096	BIERSACK J.P.	84FI1016	BROWN R.E.	84BR400
BADER B.	84VA120	BINDER K.	84EW207	BROWN W.P.	84BO184
	84HE1097	BINNS M.J.	84LI1088		84LI1088
	84BA1098		84BI1105		84BI1105
	84HE1099	BLACHOT J.	84NE1106	BROWNE J.D.	84IR1084
BADEWEK G.	84SC28T	BLANSHARD J.M.V.	84BL378	BRUECKEL TH.	84BR264
BAFFIER N.	84AL202	BLASCHKO O.	84BL380	BRUECKNER S.	84AL1057
	84AL203	BLETRY J.	84BL374	BRUNEL M.	84PO1012
BAGIEU G.	84AV1052	BLEY F.	84BL278	BUCHENAU U.	84BU373
BAKER C.A.	84PE151		84CE212	BUELDT G.	84BU1023
BALDO-CEOLIN M.	84BA1053	BLIN A.H.	84CE248	BULOU A.	84LA1041
BARANOV V.I.	84SP366	BLISS D.V.	84BL249	BURKE S.K.	84PA221
BARLA K.	84BA403	BLOENNIGEN F.	84LE250	BURLET P.	84RO1109
BARNABEU J.	84NO334	BOCQUET J.F.	84BL254	BURNETT S.M.	84PE151
BARREAU G.	84MH102	BOCQUET J.P.	84KU338	BUSSIÈRE A.	84LI185
	84EG117		84BL394	BYRNE J.	84PE151
	84HO131	BOERNER H.G.	84CH371		84HE228
	84KR176		84DJ260	CABANE B.	84HE1051
	84EG191		84SC332		84CA201
	84TO335		84MH102		84KE272
BARRETT S.A.	84FI192		84EG117		84KE390
BARTHELEMY A.	84BA15T		84HO131	CACIUFFO R.	84AB31T
BARTHELEMY J.F.	84BA6T	BOEUF A.	84KR176		84BO142
BARTL H.	84JO1070		84EG191		84TA196
BARTSCHER W.	84BA337		84GA292		84BO320
BARUCHEL J.	84DR1095		84LA293	CAILLEAU H.	84BA337
BASTIDE J.	84BA1020		84TO335	CANDAU S.	84RE1002
BASTIE P.	84BA101		84AB31T	CAPELLMANN H.	84BA1020
			84BO142	CAPPONI J.J.	84BR308
			84TA196	CARTER A.J.	84PO1012
			84BO320		84WA1009
			84BA337	CASTETS C.	84HI1055
			84HE290		84CA4G

CATLOW C.R.A.	84BE136	COWLAM N.	84CO1008	DORNER B.	84BE20T
CATTERALL R.	84GL301	COWLEY R.A.	84MI341		84KA116
CAUDRON R.	84AB195	CRESPI H.L.	84JU252		84GR193
CAVAGNAT D.	84CA137		84MI1024		84DO347
CAVAIGNAC J.F.	84AV1031	CRETTEZ J.M.	84PA309		84SH351
	84AV1052	CRICO S.	84AB31T	DOUCET J.	84DO409
CAVENETT B.C.	84FY158	CROUCH-BAKER S.	84CR1059	DRAPERI A.	84DR288
CEBULA D.J.	84CE1040	CROWLEY T.L.	84CO1026	DREELE R.B.V.	84GL301
	84MA1112	CUMMINS P.G.	84MU1067	DRILLAT A.	84DR1095
CENEDESE P.	84CE212	CURRAT R.	84CU215	DUBBERS D.	84BO183
	84CE246		84DU259		84BO396
	84CE248		84CU363	DUGGAN M.	84AL103
	84BL249	CUSACK S.	84EN149	DUNSTETTER F.	84BE211
	84LE250		84CU1022	DUPLESSIX R.	84CA201
CHAGNON R.	84ZE284	D'HONDT P.	84DH377		84BA1020
CHAIX-PLUCHERY O.	84CH247		84EM1010	DUPONT W.	84SO342
	84CH257	DACHS H.	84LE32T	DUPUIS A.	84DU107
CHAMBEROD A.	84RO344	DAM J.	84CO213	DURAND D.	84DU259
CHAMPAGNON B.	84DU356	DAMAY P.	84DA300	DURVILLE F.	84DU356
CHAPLOT S.L.	84CH1034		84GL301	DUVAL E.	84DU356
CHAPPERT J.	84VI398		84LE302	EDDY M.M.	84CH1078
CHARLIER M.	84CH223	DANIEL H.	84EG117	EGELSTAFF P.A.	84EG317
CHARVOLIN J.	84HE291		84KR176	EGIDY T.V.	84MH102
CHATER R.	84GA1042	DAVIES H.A.	84CO1008		84EG117
CHATTOPADHYAY T.K.	84CH287	DAY P.	84FY158		84HO131
	84CH1027		84DA265		84KR176
	84CH1063	DE PAPE R.	84PO127		84EG191
CHAUVIN J.	84LI185		84CO240	EICHHORN G.	84KU321
CHEETHAM A.K.	84CH1078	DEGIORGIO V.	84CO267	EISENBERG H.	84ZA330
CHEN S.H.	84TE322	DEGOVICS G.	84LA381	EMSALLEM A.	84DH377
CHENEVAS-PAULE A.	84BE108	DELANEY C.F.G.	84DE1092		84EM1010
CHENG V.K.	84FI1015		84DE1093	ENGELHARDT D.	84OE153
	84FI1016	DELAPALME A.	84LA360		84SC332
CHEVALIER J.	84ZE367	DELLEY B.	84DE209	ENGELMAN D.M.	84TR147
CHEVREAU N.	84SO1006	DEMAZEAU G.	84SO1006		84EN149
CHHOR K.	84CH371	DENOYER F.	84DU259		84MO1021
CHIEUX P.	84CH33G	DEPINNA S.	84FY158	ENNACIRI A.	84EN243
	84RO110	DEPORTES J.	84BR167	EREMETS M.I.	84ST115
	84BO124		84BR308	ERNST G.	84BL374
	84TO135		84BR400	ERNST R.R.	84ME362
	84CH182	DERAMAN M.	84DE333	ESCRIBE-FILIPPINI C.	84JA157
	84BE206	DESLATTES R.D.	84DE1050	ESTRADE-SZWARCKOPF	84CO262
	84BL278	DESPLANQUES B.	84DE186	H.	84CO326
	84CH299		84DE245	ETHERINGTON G.	84MA123
	84DA300		84DE275	EVANS D.J.	84EV106
	84GL301		84DE298	EVANS R.	84CO121
CHIEUX P.	84LE302	DESRE P.	84NO386	EWEN B.	84EW207
	84CH304	DEVAUX C.	84BL278	FAIRCHILD R.G.	84GA292
CHRISTENSEN A.N.	84CH143	DIANOUX A.J.	84DE372	FALAISE J.C.	84FA3T
	84CH1005		84EN149	FALCH S.	84ST1104
	84CH1091		84LA152	FARGES J.P.	84BR105
CIOSMAK D.	84CH257		84MA161	FARRINGTON G.C.	84TH128
CLARK S.A.	84PE151		84BE205		84TH231
CLAUSEN K.	84HU1011		84CO262	FAUST H.R.	84FA12T
	84CL1037		84BE273		84MH102
	84CL1058		84TE322		84SC332
	84HU1066		84BE324		84KE395
CLERC H.G.	84SC332		84PO325		84TO335
CLOUGH S.	84CL197		84CO326	FAWCETT E.	84FA194
	84CL313		84LA370	FEDER D.	84FA194
COCKCROFT J.K.	84CO392		84CH371	FEIL D.	84CO213
COHEN-ADDAD C.	84CO384		84BU373	FEILITZSCH F.V.	84SC187
COLLET C.	84CH33G		84DO409		84CO188
COLLOMB A.	84OB109	DICKENS M.H.	84HU1011		84SC388
COLVIN G.G.	84CO125	DICKENS M.J.	84TO270		84SC387
	84CO188	DICKENS P.G.	84CR1059	FELD R.	84CO213
	84SC388	DISDIER F.	84ZE284	FELSCH J.	84SC219
CONARD J.	84CO262	DJEBARA M.	84DJ260	FENDER B.E.F.	84PO129
	84CO326	DODGSON K.	84HI1061		84BE136
CONVERT P.	84CH33G	DOERR K.	84HE1099		84FI192
	84BO124	DOLINO G.	84DO138		84FI355
COPESTAKE A.P.	84CO121		84DO210	FIELD I.	84MA1112
COPPENS P.	84CO213		84BA237	FILHOL A.	84FI8T
COQUET E.	84PA309	DOLLING G.	84PO402		84BR105
CORNELIUS C.A.	84PA221	DONIACH S.	84RE354		84FI139
CORTI M.	84CO267	DORE J.C.	84RO110		84SC140
COSGROVE T.	84CO1026		84TO135		84BE285
COTTON J.P.	84AU1083		84DE333	FINCH E.C.	84DE1092
COULOMB J.P.	84BE164		84DO1102		84DE1093
COURBION G.	84CO240	DORMANN J.L.	84FI289	FINCH J.T.	84BE146
					84BE364

FINK D.	84F11015	GILLON B.	84DE209	HAYTER J.B.	84EW207
	84F11016	GIORGI A.L.	84PA221		84RI218
FINNEY J.L.	84KU338	GIVORD D.	84BR167		84HA235
	84F11081		84BR308		84CO267
FIORANI D.	84FI289		84BR400		84HA331
FIORINI P.	84AB31T	GLACHANT A.	84BE164		84ZE367
FISCHER E.W.	84F11089	GLAUNSINGER W.S.	84GL301	HAZELL R.G.	84CH1091
FISHMAN S.	84PR238	GODDARD R.	84CO213	HEATHMAN D.	84HE16G
	84PR316	GODFRIN H.	84FR307		84HE17G
	84GR359		84LA404		84HE19G
FITCH A.N.	84PO129	GOENNENWEIN F.	84FA12T		84HE21G
	84F1192		84OE153		84HE22G
	84FI355		84GO172		84HE23G
	84DU356		84SC332	HECK B.	84RU111
FLOUQUET J.	84LA348	GOERLITZ C.	84RU111	HECKEL B.	84PE151
FONTANA M.P.	84BE273	GOGOL E.	84TR147		84HE228
	84BE324	GOLUB R.	84PE151		84HE1051
	84FO325		84GO1111	HEGER G.	84RE130
FORSYTH J.B.	84BR233	GONGADZE G.M.	84SE365		84MU150
FORTE M.	84HE228	GONZALEZ M.	84BR222		84HE279
	84HE1051	GOODWIN J.W.	84CE1040	HEIDEMANN A.	84BA6T
FOUASSIER M.	84LA152	GRAEFENSTEDT M.	84PA261		84AN7T
FOULON M.	84AM208		84KE395		84MA24T
FOURET R.	84LE263	GRASSE D.	84GR193		84LA25T
FOURNIER J.M.	84BO320	GRASSI H.	84BR105		84CA137
	84BA337	GRAY G.W.	84RI218		84PR175
FOURQUET J.L.	84FO127	GREEN K.	84PE151		84CL197
FRANCO H.	84FR307		84HE228		84VO271
FRASE K.G.	84TH128		84HE1051		84NE283
FRATZL P.	84BL374	GREENE G.L.	84HE228		84CL313
FREEDMAN S.J.	84BO183		84DE1050		84AN361
	84BO396		84HE1051		84WI379
FREILAENDER P.	84VA120	GREENWOOD G.	84FI8T	HEITJANS P.	84VA120
	84HE1097	GREMPEL D.R.	84PR238		84ST1090
	84BA1098		84PR316		84HE1097
	84HE1099		84GR359		84BA1098
FREUND A.	84BO142	GRIFFITHS R.K.	84BA1096		84HE1099
	84BA403	GUDKOV A.T.	84SE365	HELLNER E.	84MU150
FREUND A.K.	84FR399	GUENET J.M.	84SA1054		84CO213
FREUND F.	84CH247	GUENTHERODT H.J.	84SU122	HEMPELMANN R.	84FR227
FREYLAND W.	84LA1007		84SU305	HENDRIKX Y.	84HE291
FREYSSINET J.M.	84FR226	GUESSOUS A.	84SC332	HENNION B.	84HE113
FRICK B.	84FR1075H	GUKASOV A.G.	84OK349		84HE165
FRUCHART D.	84FR227		84GU350		84MO1018
FRULLANI S.	84FR295	HAELG W.	84ME362	HENNION M.	84HE113
FUESS H.	84JO1028	HAESSLIN H.W.	84AL202		84HE165
	84TE1045		84AL203	HENRY J.Y.	84RE312
	84JO1070		84HA1030	HENRY Y.	84BO311
	84KL1076		84RI1085	HERDEGEN N.	84HE314
FUJARA F.	84SC28T	HAGEN M.	84HA336	HERINO R.	84BA403
	84OK349	HAGENMULLER P.	84SO1006	HERZ J.	84BE1038
	84GU350	HAHN A.A.	84SC187	HESS S.	84EV106
	84BL374		84SC387		84HE118
	84BA1098	HAHN K.	84HA216		84HE132
FUNKE K.	84HO1014		84FI1089		84HE314
FURRER A.	84ME362	HALL P.L.	84TU134		84HE319
FYNE P.J.	84FY158	HAMWI A.	84BO142		84HE383
GABEL D.	84GA292	HANLEY H.J.M.	84EV106	HEWAT A.W.	84AL103
	84LA293		84HE314		84HA173
GABELMANN H.	84KR393	HANSON R.C.	84GL301		84MU178
GABRYS B.	84GA1039	HARKEMA S.	84CO213		84ME230
GAEHLER R.	84KA1049	HARRIS I.R.	84IR1084		84LA266
GALERA R.M.	84PI220	HART R.	84AV1031		84HE290
GANAZZOLI F.	84AL1057	HASCHKE J.M.	84BA337		84GH357
GARDNER P.P.	84CO1008	HASELDEN D.A.	84AD1003		84TH358
GASPARD J.P.	84CE246		84AD1086	HEYDE K.	84MH102
GAUME F.	84DU356	HASSE R.W.	84HA216	HIGGINS J.S.	84BL380
GAUNE-ESCARD M.	84HE290		84HA253		84WA1009
GAVARRI J.R.	84GA1042		84BL254		84GA1039
GEICK R.	84KU321	HATHAWAY B.J.	84ST255		84HI1055
GEISSE C.	84BL394		84AS256		84AL1057
GELTENBORT P.	84OE153		84AL103		84HI1061
GENET F.	84GA1042		84HA173		84MU1067
GEORGE B.	84JA268	HAWKINS R.K.	84EG317	HILDEBRANDT G.	84LE32T
GERLACH P.	84GE224	HAYES M.H.B.	84TU134	HILLER B.	84BL254
GEURTS J.	84KU321	HAYES W.	84HU1011	HIPPERT F.	84HE113
GHOSE S.	84GH357		84CL1037		84HE165
GIBAUD A.	84LA1041		84CL1058	HIRTE J.	84HI376
GIEREN A.	84SC140	HAYOUN M.	84HU1066	HODEAU J.L.	84HO1032
GILBOY W.B.	84CO125		84HA331	HOECH A.	84HO1014
			84ZE367		

HOFF R.W.	84HO131	KEYSER U.	84PA261	LEFEBVRE J.	84LE263
	84EG191		84KE395		84MO1018
HOFFMAN H.	84HO1046		84KE397		84SA1087
	84TH1047	KIESE G.	84VA120	LEFEBVRE S.	84CE212
HOFFMANN Helmut	84HO1T		84HE1097		84CE248
	84HO2T		84BA1098		84BL249
	84HO10T		84HE1099		84LE250
	84HO11T	KILVINGTON A.I.	84PE151	LEFEBVRE Y.	84LE9T
	84HO251	KJEMS J.K.	84HU1011		84LE30T
	84HO368		84CL1058	LEHMANN M.S.	84LE32T
	84HO369	KLEBE G.	84KL1076		84CH143
HOFMEYR C.	84EG117	KLEIN A.G.	84KL1056		84ME154
	84TO335	KLEMT E.	84BO183		84CO213
	84MA24T		84BO396		84LE229
HOLM C.	84LA348	KOANG D.H.	84AV1031		84OL276
HOLTZBERG F.	84HO1068		84AV1052		84LE327
HORN S.	84BO396	KOBRAS K.H.	84BE339		84CO384
HORNIG L.	84CL197	KOETZLE T.F.	84CO213	LEHNER N.	84RE130
HORSEWILL A.H.	84CA137	KOLLMAR A.	84BO375		84MU150
HORSEWILL A.J.	84HO179	KOSICHKIN Y.V.	84ST115		84KU321
HOU M.K.	84HO340	KOSTNER G.M.	84LA381		84HI376
	84HO1004	KOUCHKOVSKY R.de	84CH304	LEWIT-BENTLEY A.	84BE146
HOWARD J.	84TO135	KRATZ K.L.	84PF225		84RO177
HOWE A.	84HO1044		84KR393		84BE364
HOWELLS W.S.	84FR226	KRUEGER C.	84CO213	LHERSONNEAU G.	84ME385
HUNGERFORD P.	84MH102	KRUEGER E.	84KA353	LIAUD P.	84BO184
	84EG117	KRUMLINDE J.	84PF225		84LI185
	84EG191	KRUSCHE B.	84EG117	LICHTENBEIT J.H.	84CL313
HUTCHINGS M.T.	84FY158		84KR176	LIEB K.P.	84EG117
	84HU1011	KUGLER J.	84FI1089		84KR176
	84CL1037	KUHS W.F.	84KU155	LIEKE W.	84HO1068
	84CL1058		84HE279	LINDNER P.	84LI281
	84HU1066		84KU338	LIPPERT W.	84BL394
IBEL K.	84HO251	KULLMANN W.	84KU321	LISOWSKI P.	84BO184
IDRISSI A.	84AV1052	LAARIF A.	84LA266	LITCHINSKY D.	84EG317
IRVINE S.J.C.	84IR1084		84TH358	LIVAGE J.	84AL202
ISALGUE A.	84OB109	LAGGNER P.	84LA381		84AL203
ISHIKAWA M.	84LA169	LAMPARTER P.	84LA1007	LIVET F.	84LI1043
JACROT B.	84EN149		84ST1100	LIVINGSTON F.M.	84LI1088
	84DE372		84ST1103		84BI1105
JANNOT B.	84JA157	LANDER G.H.	84ST1104		84NE1106
JANOT C.	84JA180		84LA169	LOEWENHAUPT M.	84HO1068
	84JA268		84SM343	LONNGI P.A.DE	84EG317
	84JA269		84LA360	LOUGHEED R.W.	84HO131
	84JA294		84RO1109		84EG191
	84JA296	LANGEL W.	84LA18T	LUCAS B.W.	84LU1110
JEFFREY G.C.	84CE1040		84LA280	LUCAS O.	84PO127
JOBIC H.	84LA152	LANGEN G.	84LA310	LUCAZEAU G.	84CH371
	84JO234	LANGER J.A.	84MO1021	LUCHELLI E.	84AL1057
	84LA258	LAPIN S.G.	84ST115	LYLE I.G.	84MU1067
	84JO382	LARSEN F.K.	84ME154	MA K.T.	84GA1039
	84JO1035		84CO213	MACDONALD J.E.	84CL1037
	84JO1094	LARSSON B.	84GA292		84HU1066
JOENSSON S.	84FR399		84LA293	MACKENZIE G.A.	84SH351
JOHANSEN H.	84CO213	LARTIGUE C.	84LA370	MACKLIN W.J.	84BA1079
JOHNSON S.M.	84BR308	LASCOMBE J.	84CA137	MACONNACHIE A.	84MA1029
	84BR400	LASSAILLY Y.	84LA348		84MA1064
JORAT L.	84AM208	LASSEGUES J.C.	84CA137	MAGERL A.	84MA24T
JOSWIG W.	84JO1028		84LA152		84MA114
	84JO1070		84RI1001		84ZA160
JOUBERT J.C.	84OB109	LAST J.	84BO183		84MA161
JUBB J.S.	84JU252		84BO396		84PO242
JUNG G.	84BE339	LATRACH A.	84ME230		84NE283
KAFFRELL N.	84ME385	LAUNAY J.M.	84LA1041		84WI379
KAHN R.	84BE273	LAUTER H.J.	84BA159	MAGNANI M.	84AB31T
	84BE324		84SI162	MAISANO G.	84BE273
KAKURAI K.	84KA116		84SI171		84BE324
KALMAN A.	84CO384		84LA258		84FO325
KALUS J.	84HO251		84FR307	MAMPE W.	84PE151
	84SH351		84RA323		84BO184
	84HO1046		84LA404		84AG190
	84TH1047	LAVAL J.Y.	84LA1041	MAN P.P.	84PO127
	84KA1049	LAWIN H.	84ME385	MANES L.	84TA196
KAMBOUR R.P.	84MA1029	LEADBETTER A.J.	84RI218		84BO320
KEARLEY G.J.	84CO392	LECHNER R.E.	84RE1002		84BA337
KEKICHEFF P.	84KE272		84HO1014	MANGIN P.	84TE119
	84KE390		84TO1082		84MA181
KELLER A.	84SA1054	LECLERCQ F.	84DA300		84MA236
KERR S.A.	84EG117		84LE302		84MA239
KESSLER E.G.	84DE1050				84RO344

MARCHAL G.	84TE119	MORSE J.	84PE151	PAUL D.MCK.	84PA221
	84MA236		84MO1048		84DA265
	84MA239	MOSES J.D.	84BO184		84HA336
	84JA268	MOUGEY J.	84FR295	PAWLEY G.S.	84SH351
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