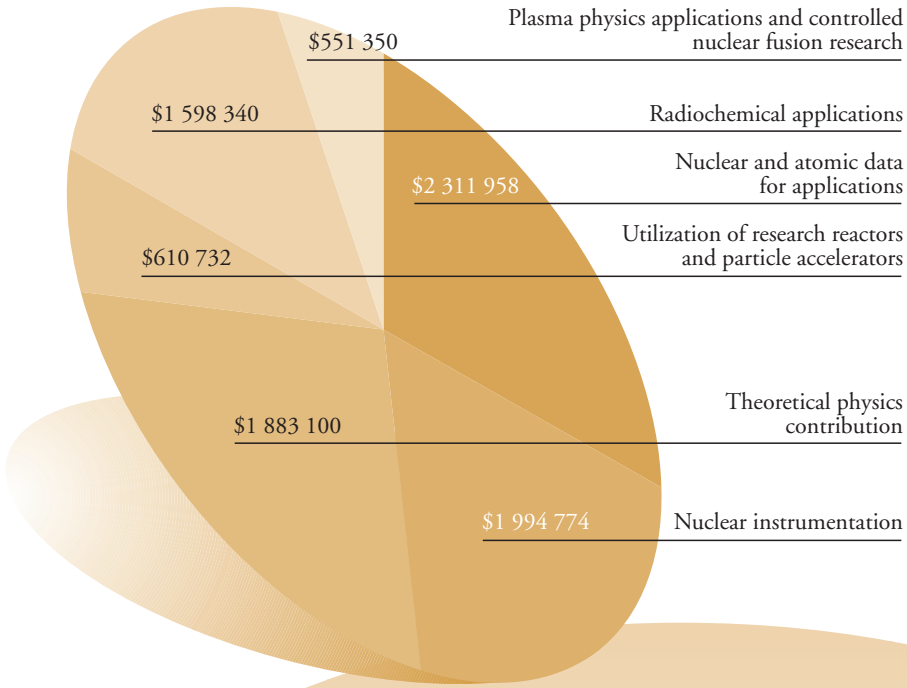
PHYSICAL AND CHEMICAL SCIENCES



Regular budget expenditure:
$8 950 254

Extrabudgetary programme expenditure (not included in chart):
$82 841

Programme objective

To promote application oriented research, development and implementation of techniques and technologies based on nuclear physical and chemical sciences for solving practical problems in the fields of medicine, environment, energy and mineral resources prospecting; to assist in the better utilization of research reactors and accelerators and provide technical help to national analytical laboratories to improve the quality of their analytical measurements.

The activities of the physical and chemical sciences programme focused on advanced areas of nuclear science and on the use of nuclear technology for the benefit of Member States. Version 2 of the Fusion Evaluated Nuclear Data Library (FENDL-2) was completed and made available to users in Member States on the Internet and on CD-ROM. The incorporation of a World Wide Web graphic interface led to the Agency's nuclear database being more user-friendly and resulted in a large increase in the number of nuclear data retrievals and the volume of data retrieved. The Agency's Laboratories at Seibersdorf conducted a worldwide survey of X ray fluorescence (XRF) laboratories and developed a new 'fluorescence/Compton ratio' method and software for XRF applications and analysis. These advances will help Member States conduct rapid, accurate analyses of environmental, industrial and medical samples. One of the results of a

CRP concluded in 1998 was standardization of the production methods of therapeutic radiopharmaceuticals for metastatic bone pain and arthritis. Work also began on the development of such agents for other therapeutic applications. The Agency's 17th Fusion Energy Conference was held in October in Yokohama. And the design of the International Thermonuclear Experimental Reactor was finalized by the collaborating parties and the Final Design Report published.

Nuclear and atomic data for applications

The development of a full World Wide Web user interface to the Agency's comprehensive nuclear and atomic databases was completed. This method of access is now offered in addition to the existing Telnet based on-line nuclear and atomic data retrieval system. Owing to its convenient graphic user interface, more and more users prefer to use the Web environment to retrieve their data. As a result, the number of user retrievals through Telnet decreased in 1998, while the number of Web based data retrievals increased sharply, with users located in 90 Member States.

Since some data users have limited access to the Internet, CD-ROM versions of the main nuclear databases — Computer Index of Neutron Data (CINDA), Compiled Experimental Nuclear Data (EXFOR) and Evaluated Nuclear Reaction Data Files (ENDF) — were prepared in co-operation with other data centres. Since they are completely analogous to the databases accessible on-line, they provide effective, updated off-line retrieval of the specific data needed by a local user. In addition, new releases of the ENDF/B-VI data library and the evaluated photon data library EPDL97 were made available to users as a result of the continuing worldwide co-operation between nuclear reaction data centres.

In order to reduce printing costs, the practice of porting certain data relevant publications to the Web was started. Electronic versions of 6 nuclear data newsletters and 11 data reports have been placed on the Web in HTML or PDF formats. Electronic versions are more convenient for many users and also facilitate the updating of frequently revised information.

Development of the Reference Input Parameter Library (RIPL Starter File) was completed with the aim of producing a tool for the effective evaluation of nuclear data for emerging nuclear applications. The library organizes and preserves the immense knowledge accumulated over the years by the worldwide nuclear physics community in calculations of low energy nuclear reactions. A technical document describing the library was published and the library was made available on the Web and on CD-ROM.

A major international library of nuclear data for fusion applications (FENDL-2), developed under Agency auspices, underwent successful quality assurance tests. In addition, documentation for users was prepared and, as with other databases, the library was made available on the Web and issued on CD-ROM.

A workshop on nuclear reaction data and nuclear reactors was conducted at the International Centre for Theoretical Physics in Trieste. Its primary goal was to facilitate the transfer of know-how on the use of nuclear data in nuclear reactor calculations to scientists and engineers from developing countries. The workshop resulted in more than 300 requests for computer codes being submitted to the Computer Program Services jointly operated by the Agency and the OECD/NEA.

Two new CRPs were initiated. The first addresses X and gamma ray emission data for detector calibration in

NUCLEAR DATA RETRIEVALS

	1994	1995	1996	1997	1998
Volume of data retrieved from the Web (megabytes)	—	—	100	2600	8600
Telnet nuclear data on-line retrievals	3200	4400	5700	7350	2700
CD-ROMs with databases, libraries and files distributed on request	—	—	—	—	205
Off-line retrievals	1950	1550	800	1900	1995

response to needs for improved quality of data in spectroscopy measurements in safeguards, dosimetry and industry. The second one deals with nuclear model parameter testing for nuclear data evaluation in order to provide quality assurance of these evaluation tools for emerging nuclear applications.

Two major numerical databases dealing with atomic and molecular data were completed: one on the chemical erosion of fusion reactor plasma facing materials induced by plasma particle impact; and the other on the total and differential cross-sections for elastic scattering and momentum transfer processes in collisions involving hydrogenic ions, atoms and molecules, and their isotopic variants. These databases can be used by fusion plasma modellers and fusion reactor engineers in predicting the behaviour of large plasma devices.

In response to the needs of several fusion research laboratories, and in collaboration with the Institute for Plasma Physics in Garching, Germany, and the Technical University of Vienna, an atomic database for lithium beam penetration in fusion edge plasmas was completed. This database is already being used in the lithium beam diagnostics of ASDEX, TEXTOR and other tokamak plasmas.

Work on an international database on the thermomechanical properties of irradiated nuclear graphites was initiated using extrabudgetary funds. This database will permanently archive the properties of nuclear graphites in graphite moderated power reactors in order to preserve the information gathered over many years by the nuclear power industry.

Nuclear instrumentation

The Agency provided technical support to Member States to enhance their capacity for the repair and maintenance of nuclear instruments. An evaluation carried out on repair trends found that during the years 1995–1997, Latin American countries repaired 240 items of equipment, with a total value of $1.35 million, using spare parts provided by the Agency at a total cost of only $52 000.

Seven modular nuclear instruments (quad timing single channel analyser, crate controller, multi-purpose pulse generator, simulated pulse generator, spectroscopy amplifier, single channel analyser, and counter/timer) developed at the Agency's Laboratories at Seibersdorf or under individual Research Contracts/Agreements were evaluated by external experts. The evaluation indicated that these low cost instruments were ideal for education and for application in such fields as nuclear medicine and environmental monitoring.

The Agency's Laboratories at Seibersdorf developed and tested the following:

- Educational kits (including manuals) for training in nuclear electronics, such as the EURO CAN bus controller for real-time applications and a microcontroller training kit;
- A temperature control unit for use in dosimetry;
- A medfly pupae sorter for use in entomology;
- A portable X ray fluorescence (XRF) spectrometer based on a thermoelectrically cooled cadmium telluride (CdZnTe) detector and a portable multichannel analyser.

A new quantitative method based on the 'fluorescence/Compton ratio' concept was developed for laboratory and in-field XRF applications. A dedicated software program was implemented in the laboratory X ray microfluorescence system. In order to improve interpretation of the analytical results, cluster analysis was adopted for classification of the individual particles analysed by an electron microprobe. A worldwide intercomparison survey of XRF laboratories was concluded. The results were evaluated according to the recognized international protocol, which ensured both comparability and proper classification of the participating laboratories.

A Research Co-ordination meeting on the development of computer based troubleshooting tools and instruments was held in Vienna in November. In addition to summarizing recent developments, recommendations were made to develop: a troubleshooting database, including checklists; an in-circuit emulator and analog signal generator; a computer based maintenance and quality control programme; and an expert system for nuclear instrument troubleshooting.

In addition to existing nuclear spectrometry software, gamma ray and alpha particle test spectra were distributed to Member States on diskettes and through the Internet. Several programmes for spectroscopy applications were developed or upgraded. And more than 100 copies of the Agency's nuclear spectrometry software were distributed to Member States.

With the advent of modern notebook computers, the capabilities of portable spectrometry systems have become more powerful and convenient. A workshop was held at the Agency's Laboratories at Seibersdorf to compare the performance of several portable XRF and gamma ray spectrometry systems. The systems under test were classified as portable, hand-held and miniaturized, though it was concluded that they did not contain all of the necessary attributes that would qualify them for use in the field. The report of this workshop will assist Member States in selecting suitable instruments for their specific applications.

Utilization of research reactors and particle accelerators

The WIMS-D thermal reactor physics code is widely used, especially by scientists in developing countries, for research reactors, but the available nuclear data library is based on old information. In order to solve this problem, a new CRP was initiated on updating the WIMS-D Library.

An Advisory Group meeting on the enhancement of research reactor utilization for neutron activation analysis, held in Vienna in June, concluded that neutron activation analysis in its various forms is still a viable and useful technique. There are good prospects in developing countries for long term growth, which can be achieved by the more effective use of existing facilities and with a better end user orientation. It was agreed that neutron activation analysis, which can be carried out with low power research reactors, can contribute to the development of the economy and nuclear infrastructure in many developing countries. For example, it provides a quick method of screening geological samples for minerals which may be commercially useful. Since it also involves a nuclear technique, it stimulates the development of appropriate regulations and procedures for handling radioactive material. Finally, the use of neutron activation analysis requires the training of personnel in sophisticated nuclear techniques, thereby contributing to the technical and scientific 'knowledge base' of the country.

Another Advisory Group meeting in Vienna in July reviewed the technological requirements for proton therapy facilities. At present, most proton therapy centres are not located in hospitals, but in nuclear institutes that are used only partly for therapy. Following the dedication of the world's first hospital based proton therapy centre in 1990, several similar centres are currently under construction and many more are being planned. The typical structure of a hospital based facility was discussed. Many different types of accelerator can be used, with the accelerator system accounting for only about 20% of the cost of all the technical components. The factors influencing the cost of proton therapy centres were also discussed.

Radiochemical applications

After a gap of nearly 12 years, the Agency organized an international symposium on radiopharmaceuticals, in Lisbon in March–April. The papers presented at the meeting reflected the current developments and future trends in the use of diagnostic and therapeutic agents. The continuing importance of technetium-99m in nuclear medicine and the role of imaging as an important tool in its use were highlighted. Emerging interest in therapeutic radiopharmaceuticals based on beta emitting short lived isotopes such as rhenium-186 and samarium-153 was also recognized. This trend, next in importance only to the use of technetium-99m, seems to be the direction of future developments in radiopharmaceuticals. There was also interest in the development of agents labelled with other established isotopes, especially radioiodine and also indium-111 and gallium-67. The importance of a proper regulatory structure, training and good manufacturing practices for ensuring safety in the regular use of radiopharmaceuticals was also underlined.

A CRP on the optimization of the production and quality control of therapeutic radionuclides and radiopharmaceuticals was concluded. During the course of this CRP, simplified and optimized procedures were developed for the production of the short lived beta emitting isotopes samarium-153, holmium-166 and rhenium-186, including preparation of phosphonate based radiopharmaceuticals for the palliative therapy of metastatic bone pain, and labelled particles for treating certain types of arthritis. These products have been put to regular patient use. The results of the CRP have been published as a technical document.

A new CRP on labelled biomolecules for targeted radiotherapy was initiated. The work will focus on labelling a few selected peptides with rhenium-188, yttrium-90 and samarium-153. Targeted radiotherapy

has several advantages over external beam therapy, including the possibility of selectively delivering higher doses to the tumour and treating multiple metastases. The aim of the CRP is to develop procedures for the preparation of radiolabelled biomolecules such as monoclonal antibodies and peptides.

In a CRP on the development of kits for radioimmunometric assays for tumour markers, progress was made in the local production of the basic reagents needed for total prostate specific antigen (PSA) assay, useful in the early diagnosis of prostate cancer. Purification of the PSA from seminal fluid, preparation of polyclonal and monoclonal anti-PSA antibodies, studies on optimizing antibody coating to solid phase, and standardization of the methodology for enzyme linked immunosorbent assay (ELISA), radioimmunoassay (RIA) and immunoradiometric assay (IRMA) for PSA using external reagents were some of the main achievements.

Implementation of good manufacturing practices and practical regulatory practices for radiopharmaceuticals in many developing Member States is an area that requires support and guidance from the Agency. A draft guidelines document for good radiopharmacy practices in developing countries was prepared and circulated to experts in the field for comments.

An Advisory Group meeting was held in Vienna on the introduction and implementation of quality assurance principles in laboratories using nuclear and nuclear related analytical techniques. A report prepared at the meeting outlined the potential actions that could be taken to implement quality assurance concepts in Agency technical co-operation projects. The report also contains recommendations on the nuclear analytical techniques that can be targeted in a Model Project. The services of consultants were used to prepare training material for another workshop on this subject, and to prepare questionnaires for the selection of the laboratories to participate in the Model Project. These questionnaires were sent out in November.

The Agency's Laboratories at Seibersdorf supported CRPs by: providing supplemental characterization of materials supplied by the US National Institute of Standards and Technology, and characterization of three new air filter samples loaded with Vienna and Prague dust; the preparation, distribution, characterization and certification of reference materials IAEA-391/392/393; the organization and evaluation of intercomparison exercises for reference materials IAEA-085/086 and IAEA-336; the organization of proficiency tests for radionuclide analysis in Member State laboratories; and the co-ordination of the activities of the Analytical Laboratories for Measuring Environmental Radioactivity (ALMERA) network.

Plasma physics applications and controlled fusion research

At the 17th Fusion Energy Conference, held in Yokohama in October, papers were presented on: magnetic confinement experiments; plasma heating and current drive; International Thermonuclear Exterimental Reactor (ITER) engineering design activities; magnetic confinement theory; inertial fusion energy; innovative concepts; and fusion technology. One of the significant results achieved since the last conference was the realization of significant levels of fusion power — 10.7 MW for 0.4 seconds in the Tokamak Fusion Test Reactor at the Princeton Plasma Physics Laboratory, followed by 16.1 MW for 0.85 seconds in the Joint European Torus in Culham, United Kingdom. These achievements have allowed the experimental observation of significant alpha particle heating. Another key result was obtained in a first experiment with the newly commissioned superconducting Large Helical Device at the Japan Atomic Energy Research Institute, where the predicted theoretical confinement time was reached by the experiment. ITER papers presented: the successful development of large superconducting magnets; high power gyrotrons; the construction of a vacuum vessel sector and divertor; and remote handling equipment.

The sixth Technical Committee meeting on fusion power plant design was held in Culham, the United Kingdom, in March. The meeting reviewed the status of commercial fusion power plant concepts, including technology, material development, economics, environmental aspects, and the safety and socioeconomic aspects of fusion energy. Results were presented on the European Long-Term Fusion Technology Programme, concentrating on four major lines: the European Blanket Project with the main emphasis on water cooled lithium tiles inside stainless steel cases; the helium cooled pebble breeder blanket concept; advanced material studies, including results of the International Fusion Irradiation Facility; and the Safety and Environmental Assessment of Fusion Power within the European Union Framework Programme 5.

Detailed comparisons were presented from Japan on four tokamak reactor studies, one helical reactor study and one laser fusion reactor study. The Engineering Design Options from the US Fusion Reactor Program's studies on the development of spherical tokamaks were assessed on the basis of high performance structural materials such as ferritic steels, vanadium alloys and SiC composites. Optimization criteria for an alternative path to a fusion power plant — the heliac reactor in Germany — were also presented.

A Technical Committee meeting on the steady state operation of tokamaks was held in Hefei, China, in October. Among the topics discussed were: the operation of present long pulse tokamaks, the plans for future steady state tokamaks, advanced magnetic confinement configurations, and hybrid fusion–fission systems. Highlights included the presentation of long pulse experiments in France, Japan and the Russian Federation. Steady state devices are being planned or constructed in China, France, India, Japan and the Republic of Korea. The two hour experiment TRIAM-1M demonstrated good control of plasma position, particle flow and heat control at low plasma density. China will study hybrid fusion–fission systems that use fusion reactor generated neutrons to breed plutonium-239 fuel and to transmute high level wastes from fission reactors.

At a Technical Committee meeting held in Tokyo in October, there was a comprehensive review of present spherical torus experiments, related plasma physics theory, modelling, and future experimental devices. Papers were presented from the spherical tokamak experiments in Japan, the United Kingdom and the USA. The results attained by the START experiment at Culham Laboratory, in the United Kingdom, include good stability, high beta operation and the absence of disruptions. This success has inspired other experiments which are being planned in Brazil (ETE), the Russian Federation (GLOBUS-M), the United Kingdom (Meg Ampere Spherical Tokamak) and the USA (National Spherical Torus Experiment).

At the 13th Technical Committee meeting on research using small fusion devices, held in Shonan Village, Japan, in October, tokamak experiments, compact tori, helical devices, dense plasmas, inertial fusion and theory were discussed. The WT-3 experiment in Japan reported new results on the control of pressure driven $m = 1$ instabilities in a tokamak with significant lower hybrid current drive. The HT-2 experiment (Japan) reported novel results on ohmic breakdown in low resistance vacuum vessels and on vertical displacement event disruptive instabilities in elongated plasmas. The SINP tokamak in India has shown significant improvement in confinement characteristics and the length of time for which plasma current could be sustained. The Large Helical Device experiment provided very impressive results on first plasmas. The magnetic configuration has been measured, compares favourably with the numerical codes and has shown plasma confinement which is much better than expected on the basis of stellarator scaling laws. The performance of reversed field pinches was improved considerably by applying external resonant helical fields. The ADITYA tokamak in India has been modified to enable it to approach the full design parameters and to improve its diagnostic capabilities. First estimations on magnetized targets induced by circular polarized laser light have shown that high energy gain could be reached in powerful Z-pinches combined with sub-nanosecond lasers.