

Relocation of the IUPAC Secretariat

From 30 September 1997, all correspondence should be directed to the office of the new Executive Director:

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During October the Oxford Secretariat will be occupied in shipping files to RTP and to the Chemical Heritage Foundation in Philadelphia (see page 161) and in disposal of furniture and equipment.

It has been a very busy presidency up to now and I am convinced that it will remain so until the end of the year. In these days of rapid globalization, we can readily perceive the effects that the high-speed changes taking place around us are having on IUPAC. Yet globalization is not new to IUPAC: looking back over the Union's history, we see that globalization was an important topic as early as 1919 and that it was the driving force behind the creation of IUPAC just after the First World War. Globally accepted standards, codices and nomenclature for chemicals had the same prime importance for academia and industry then as they have now. This being said, however, I have to add that IUPAC's objectives, as set out in our Statutes, give the Union a much broader mandate.

Today, the rapid pace of growth and change in the basic experimental sciences of biology, chemistry and physics is apparent to all. Looking at the information explosion in these areas, our attention is frequently drawn to the crossover between the sciences and to the fact that Nature is—alas—not organized like our universities. Adaptation and flexibility are needed in academia as well as industry.

Moreover, it is our responsibility as scientists to ensure that both government and the public at large are made aware of scientific progress at an early stage. In particular, our task as chemists is to put over the message that chemistry is already very important today and that it will go on to be a key science in the world of tomorrow, with a tremendous outreach into sister sciences, the environment, industry and the economy as well as into our everyday lives.

Achievements

Administration and finances

As you are aware, Dr Mo Williams, who was head of the IUPAC Secretariat from 1968, retired this year at the end of April. You will also be aware that our new Executive Director, Dr John W. Jost, took up his post at Research Triangle Park (RTP), NC, USA, at the beginning of April. The transitional period, during which there will be two Secretariats, will last until September 1997. In October our Oxford office will ship documents to RTP and then close down.

At this point in my report I feel privileged to have the opportunity to express my sincere thanks to Mo Williams for his long and outstanding service, and for his loyalty during his time with IUPAC. He personified stability for a substantial part of IUPAC's existence and



was also the leading authority on all matters relating to IUPAC. At the same time I also want to extend my very best wishes to our new Executive Director, who is building up our new USA Secretariat into a globally active Secretariat, devoting special care to emphasizing activities which will ultimately enhance IUPAC's visibility.

As part of this process, our web site (current Home Page address <http://chemistry.rsc.org/rsc/iupac.htm>) will be further enlarged and made more accessible by setting up a main site at RTP with the domain name of iupac.org. The current site, hosted by the Royal Society of Chemistry, will become our European mirror site. We expect soon thereafter to have also an Asia/Pacific mirror site. It is intended that the site should become the chief channel of communication with the community and especially with those engaged on IUPAC projects.

Our finances are now in good shape, thanks to the work of our Treasurer, as well as to the Finance Committee and the new USA banker taking care of our securities. These have been supplemented by windfall money from Barings Bank. The Executive Committee decided that the Treasurer should set up a new endowment fund to harbour our surprise resources.

Congresses

I would like to pick out just three of the many IUPAC-sponsored conferences that have taken place or are still to take place this biennium.

This year, for the first time since 1967, the IUPAC Congress and General Assembly (GA) have been scheduled to take place in the same city in two successive weeks—'back to back', so to speak. The venue is Geneva, Switzerland, and the two events will be taking

place in the last two weeks of August; the Congress first, then the GA. The same pattern will be repeated in 1999 in Berlin, Germany, after which IUPAC will be able to take proper stock of the new combined event. Holding the two events in successive weeks obviously increases the organizing committees' workload substantially, and I would like to express my thanks to the two organizing bodies in Switzerland and Germany who have taken up the challenge.

In fall 1996 the CHEMRAWN IX Conference took place in Seoul, Republic of Korea, under the heading 'The Role of Advanced Materials in Sustainable Development: Use, Disposal and Recycling of Materials'. Thanks above all to a magnificent effort by the South Korean industry, the event was a great success. Incidentally, this was the third time that IUPAC has had the pleasure of holding a CHEMRAWN Conference in the Asian/West Pacific Rim region: the other two were 'Chemistry and World Food Supplies' in Manila in 1982 and 'Advanced Materials' in Tokyo in 1987.

A third IUPAC workshop on Safety in Chemical Production was organized in April 1997 by our industrial wing COCI, the Committee on Chemistry and Industry. The workshop was held in San Francisco, CA, in conjunction with the American Chemical Society, the US Chemical Manufacturers Association and the US Environmental Protection Agency. The attendance of two 1995 chemistry Nobel laureates generated keen interest. After the first workshop, which was held in Basle, Switzerland (1990), and the second, which was held in Yokohama, Japan (1993), there is still continued interest in holding workshops in other parts of the world.

Nomenclature

I am happy that IUPAC is now able to submit a final list of names and symbols for elements 101–109 to the Council for approval in Geneva in August this year. As you are aware, the naming of the transfermium elements was a lengthy, controversy-ridden process. The three laboratories in Germany, Russia and USA which were involved in the discovery of the elements have been consulted at length and their comments solicited. Their input was most important, given that one of IUPAC's responsibilities is to formulate widely accepted recommendations capable of forming a basis for international communication in chemistry. A press release was issued in February 1997 and the final say rests with the Council. I should also mention that activities have been started to enable IUPAC to put forward proposals for the nomenclature of elements 110–112. The process will be conducted in accordance with our Bylaws and in close collaboration with the discoverers. Once these activities have concluded the final decision will once again be made by the IUPAC Council.

Collaboration with UN and ICSU Bodies

Collaborative efforts with UNESCO, UNIDO and WHO have been substantially intensified during the biennium.

CHEMRAWN IX was organized jointly by our CHEMRAWN Committee and UNESCO, while COCI continued its three-way collaboration with UNIDO and UNESCO. This gives safety experts from the Third World the opportunity to spend a period of approximately one month with IUPAC Company Associates and discuss existing safety measures in a direct hands-on fashion. The visiting safety experts, a substantial number of whom were government specialists, subsequently returned to their home countries. We are thus constructing a progressively expanding network of safety experts in chemical production and also bringing IUPAC into closer contact with the developing world.

All the programmes which IUPAC is undertaking in conjunction with UNESCO are supervised by the International Chemistry Council (ICC), a body comprising four chemistry Nobel laureates from Canada, France, UK and USA, one Japanese industrialist and three developing world representatives from Africa, Asia/Pacific and Latin America. The inaugural meeting took place in Paris in January 1997. The executive part of the programmes is in the hands of IUPAC and UNESCO Officers. The ICC will convene every second year to make a critical assessment of all joint IUPAC/UNESCO activities. We will also be inviting representatives of our Committee on Teaching for Chemistry (CTC) to take part in IUPAC's annual meetings with UNESCO. This is because CTC has been collaborating with UNESCO for quite some time in areas of key interest to the ICC. Furthermore, some of our Commissions have been enlisting UNESCO's help to have larger-scale programmes followed up. Such joint activity also presents an opportunity for us to strengthen our links with the International Organization for Chemical Sciences in Development (IOCD) and the Third World Academy of Sciences (TWAS).

The President of our Division on Chemistry and the Environment is acting as WHO liaison. He is representing our interests at the WHO-led International Forum for Chemical Safety (IFCS) and International Programme for Chemical Safety (IPCS). In the course of his duties, he will be maintaining very close contact with the President of our Division on Chemistry and Human Health. IUPAC together with IUPHAR, IUTOX and the International Life Science Institute (ILSI) constitute the scientific ICSU-NGOs in these UN bodies. IUPAC is currently acting as the group's spokesman.

Collaboration with ICSU executive bodies, a large number of sister unions, ILSI and the ICSU Scientific Committee on Problems of the Environment (SCOPE) has improved substantially in 1996–97.

Chemistry and society

In October 1996 COCI published its first White Book as a contribution from science to the debate on the effects of chlorine and chlorine-containing compounds on the environment. This 'White Book on Chlorine', published as a special issue of the IUPAC journal *Pure and Applied Chemistry*, is an independent and unbiased collection of original articles written by renowned scientists from all over the world, which critically evaluates various aspects of the subject. It has proven to be a success and of interest not only to academic institutions, industry, governmental agencies and environmental organizations, but also to the general public.

The White Book is the first publication of this type and more are set to follow. IUPAC is thus able to use its special position as a science-based, non-governmental, non-industry foundation with a world-wide network of experts from various fields of chemistry and sister disciplines to offer a platform for publications.

State of the Union

Countries and companies

A glance at the world map of National Adhering Organizations (NAOs) and Observer Countries (OCs) shows that while IUPAC is represented in all but a few areas of the Americas, the West Pacific Rim and Europe, it has as yet failed to enlist broad participation from either the strip of countries stretching from Syria to Kazakhstan or the countries of Africa—with the exception of Egypt, the Republic of South Africa and Tunisia. Egypt and South Africa have both been affiliated to IUPAC for quite some time now. This year the Executive Committee will have the pleasure of submitting to the Council in Geneva the membership application of the Union of Yugoslav Chemical Societies as well as requests for upgrading from Pakistan and the Philippines, two of our Observer Countries. Let me add at this juncture that our well accepted voting system is special in that it reflects the countries' actual chemical turnover figures as published by the UN. As a rule, while NAOs with stronger chemical and pharmaceutical industries have a somewhat larger voting share in the Council, they also make a greater financial contribution to IUPAC.

The participation of single companies—IUPAC is the only scientific union with direct industry participation—is remarkable, and membership of the Company Associate scheme remains astonishingly stable given the conditions which industry has to contend with today. Top of the participating companies table in 1996 was Japan with 46 companies, followed by USA with 23 and Germany with 12. The EU15 have 44 altogether. Comparing financial contributions for 1996, USA is on first place, followed by Japan and Germany. The EU15 are on second place behind USA.

Adapting mission, goals and structures

My predecessors' State of the Union reports discussed the critical remarks voiced against some of IUPAC's activities in considerable depth. Incidentally, some of these criticisms are still the subject of discussion. I would like here to inform you about the actions taken in 1996–97 in response to valuable constructive criticism. I believe that the steps we have taken will result in goals and structures which reflect the tasks facing IUPAC in the next millennium.

Several brainstorming sessions took place during the biennium at which IUPAC Officers, all of whom were very much involved in the organization of the meetings, were able to discuss thoroughly IUPAC's current situation, mission, objectives and future. These always involved well-known chemists from academia and industry, plus representatives from inside and outside IUPAC. An initial meeting was held in Belmont, USA, during June 1996. A subsequent European one-day meeting was organized in London for February 1997 and a third brainstorming workshop for the Asia/Pacific region took place in Singapore during June 1997. All were very fruitful in clarifying IUPAC's mission and goals as it heads into the next millennium as well as in promoting an intensive and rewarding exchange of opinions about the strengths and weaknesses of the Union. The meetings reinforced the need for the changes being discussed in IUPAC. All were extremely valuable, instrumental even, in the formulation of new objectives and activities, and to increasing IUPAC's visibility.

The IUPAC Officers also held an extraordinary meeting with the Divisional Presidents/Vice-Presidents and Section Presidents in Frankfurt, Germany, in March this year. This meeting was an opportunity to go through each Division's restructuring plans. While the creation of the Divisions on Chemistry and the Environment and on Chemistry and Human Health at the last General Assembly represents a major step there are still some desiderata. We need to find ways of integrating both the area of materials and the major scientific activities taking place at the interface between chemistry and biology into IUPAC. With the Divisional Presidents' input, the Frankfurt meeting yielded proposals for solutions which should result in structural changes to eliminate overlap and provide IUPAC with the missing activities and structures. The meeting was also used for a thorough discussion of the Vice-President's Critical Assessment and to some extent for discussion of further proposals for structural change.

These proposals and the Vice-President's Critical Assessment were taken up again at the Executive Committee (EC) meeting at Jerusalem in April 1997. After detailed discussions the EC decided to establish a Strategy Development and Implementation Committee

(SDIC) to define the science policy of the Union and to examine the feasibility of converting the bulk of IUPAC's scientific work to a project-driven/project-financed system with time-limited Commissions, as described in the concept endorsed by the EC. The eleven members of the SDIC were appointed by myself following consultations. The Committee was placed under the chairmanship of Vice-President Joshua Jortner and it met for the first time in June.

Scientific work

I am delighted at the large number of committed volunteers who devote their time and scientific expertise to furthering the IUPAC cause. More than 1000 scientists are actively involved in IUPAC, an achievement which I strongly believe to be cause for congratulation. That this is an enormous strength goes without saying, and we have to safeguard its continuity under the best possible circumstances. It also goes without saying that the limited financial resources available to IUPAC and the small time window available for new scientific endeavours are forcing us to choose our projects carefully.

Future perspectives

As the only purely scientific global chemical organization mandated to undertake this kind of work, it is essential that IUPAC continues with its codification, nomenclature and standardization activities. It has to do so at a much faster pace than in the past and in close association with the professional bodies which are also involved in these activities. They are working rapidly using their excellent skills, and IUPAC should try to find a collaborative basis with them which is not only acceptable to all stakeholders, but which will also enable all parties to benefit from the special advantage which IUPAC derives from being a global, strictly scientific, non-governmental organization.

It is also my belief that collaboration with UN and ICSU bodies has to be intensified and focused. Here IUPAC has a special responsibility, arising from the immense outreach of chemistry into the other sciences and the remarkably close relationship which has existed for quite a long time between chemistry in academia and the now giant chemical and pharmaceutical industry. This relationship has no parallel in physics and has started to emerge in biology only relatively recently with the advent of small biotechnology companies, the first of which was set up in California in 1976. Chemistry is a pervasive part of our everyday lives and one that accompanies us throughout our lives.

For these reasons, IUPAC should also increase its activities in the field of 'Chemistry and Society'. Here again the Union occupies a very special position, main-

taining as it does close contact with all the major stakeholders in innovation, i.e. academia, industry, government and society. We have been successful in strengthening our links with society, and through society with governments as well; nevertheless, I think, there is still a lot of room for improvement.

As always, there are still some issues to be resolved. One is that all of us in IUPAC have to make greater efforts to recruit the best scientists for our activities. This is extremely important to IUPAC since all our collaborators are volunteers. One of the advisors whom I had the pleasure of consulting during my period as Vice-President summed it up by saying that serving IUPAC comes under the heading of *noblesse oblige*.

A second unresolved issue is that we have to be very careful in selecting the activities in which we wish to get involved. We have to make sure that we are resolute in the pursuit of our goals once they are defined and that we come up with the desired result quickly. Let me also add that we have to remain true to our scientific base, unswayed by any pressure of a non-scientific nature, irrespective of whether it comes from academia, industry, governments or society.

Conclusions

Significant progress has been made, but a lot still remains to be done.

I have enjoyed having responsibility for a large number of teams, and I feel privileged to have been able to work with such colleagues as my fellow IUPAC Officers and the Members of the Secretariat, Executive Committee and Bureau as well as to have interacted with the Council, IUPAC's highest body. I am also very pleased to have been given the opportunity to establish contacts with our Divisional Presidents as well as with the Chairmen of CHEMRAWN, COCI, CTC, the Committee for Printed and Electronic Publications (CPEP) and the Committee on Affiliate Membership (CAM). If we look at CAM, it becomes apparent that, although progress has been made, there is still a need for further action. Additionally, CPEP is in need of a new policy on the submission of papers for publication in *Pure and Applied Chemistry*.

Let me close by thanking all members of IUPAC bodies for their efforts and the dedication with which they have worked for our Union over the last biennium in particular, even though I am aware that most of them have been working on IUPAC's behalf for substantially longer. It is due to them, their commitment, flexibility and creativity, that we can look with confidence to the future of IUPAC.

Secretary General's Report

Edwin D. Becker

The IUPAC Statutes give the Secretary General the responsibility for carrying out the business of the Union, keeping its records and administering the Secretariat. There are many aspects of the organization and management of our operations that fall into these categories and that are currently the subject of intense analysis and discussion. Since reports on those activities will largely be included in the presentations by other Officers, I would like to concentrate here primarily on the Secretariat, which is one of the most visible physical manifestations of the Union and which plays a central role in the smooth functioning of IUPAC.

Since the last Council meeting two years ago, there have been major changes in the Secretariat, as you know. Let me review briefly the reasons for those changes, then describe the current status and plans for the new Secretariat in Research Triangle Park, North Carolina, USA (RTP).

Location of the Secretariat. IUPAC first established an independent permanent Secretariat headed by a full time professional staff member in 1968. Since that time the Secretariat has been located in Oxford, UK, under the direction of Dr Maurice (Mo) Williams. Two years ago, when I was elected Secretary General at Guildford, I was well aware of the fact that Mo was scheduled to retire in April 1997, that two other long-time senior staff members had recently retired or were slated to retire by 1998, that the fourth professional staff member was potentially interested in other opportunities, and that one of the supporting secretarial staff would also retire in 1998. I also soon became aware of on-going discussions on possible relocation of the Secretariat; certainly this concatenation of personnel loss suggested that this was an appropriate time to consider such a move. Initially I was opposed to a move. With the awesome responsibility for recruiting several new staff members, I was concerned (as were a number of others) that the disruption of a move would be more than IUPAC (and I as Secretary General) could handle. However, over the next few months I completely changed my views, and ultimately the Executive Committee overwhelmingly came to the conclusion that a move to RTP was desirable. There were three factors that influenced me, and I think, the Executive Committee:

- Prof. Albert Fischli (then Vice-President) convincingly articulated the view that IUPAC, as a global organization, should think globally in terms of all its activities, including future locations of the Secretariat. He pointed out that with modern electronic communications, the Secretariat could be located almost anywhere, yet be in instant contact with ac-



tivities in all countries. In keeping with the pace of modern international research and the activities of multinational companies, he advocated that a move of the Secretariat every 10 years or so should be considered to enhance IUPAC's global image.

- As I analysed the activities in the Secretariat and put new information together with my long experience as a Commission Chairman and as Chairman of the Committee on Publications, I became convinced that we could and should introduce major changes in the scope, organization and conduct of the Secretariat's activities. While these could probably be accomplished in Oxford, where we would have the benefit of the experience and dedication of several talented staff members who would remain, there would inevitably be compromises in trying to adapt new methods to an existing organization. I also became convinced that, with careful management and the cooperation of the staff in Oxford, a transition to a new location could be effected without the 'absolute chaos' that some had predicted. (So far, this expectation has proved valid, and I am confident that when the move is completed later this year, we will continue to feel only moderate moving pains.)
- We received three offers of rent-free space: in Paris, Frankfurt and RTP. The first two were very attractive, and we are grateful for the generosity of the Maison de la Chimie and Gesellschaft Deutscher Chemiker for inviting IUPAC and for offering assistance beyond the well appointed space. Either would have placed the Secretariat in the centre of a bustling metropolis, with many cultural advantages, but with the significant disadvantage of the high salaries and other costs associated with such cities. RTP, on the other hand, is well outside the high costs of downtown New York, Washington and other cities;

salaries, fringe benefits and living costs there are generally well below those of Frankfurt and Paris. RTP is, however, the centre of a major research hub, with 38 000 people employed in research and light manufacturing in the Research Park itself (which includes research laboratories of several major multinational pharmaceutical and electronics companies). RTP is located at the centre of a triangle formed by three major universities—Duke, University of North Carolina and North Carolina State University—and there are many formal and informal scientific and technical interchanges among the organizations in the RTP area. The advantages of this site proved irresistible.

At RTP we have a 10-year, rent-free lease on a 4000 square foot prefabricated building, provided by the Research Triangle Foundation (RTF), a non-profit organization that serves as the developer of the Research Park. Not only has the RTF furnished the building, but they voluntarily spent over USD 20 000 to redecorate the interior of the building for our use. Since the building provides more than enough space for our near-term needs, we have subleased a portion of the building for five years to the *Journal of Endocrinology* for its editorial office, thus bringing in income that should largely offset utility and other related costs.

A New Executive Director. Recruiting a successor for Mo Williams presented the next challenge. Not only would we lose Mo's expertise, but we also would lose several long-time dedicated staff members and their collective knowledge of the Union. While many of Mo's talents are irreplaceable, we felt that we had an opportunity to recruit an individual with a suitable background and abilities to lead the Secretariat into its next era.

We advertised widely and received about 70 applications from 10 countries. I am very pleased that Dr John Jost has joined us as Executive Director. After conducting research in basic physical chemistry and spectroscopy, Dr Jost spent 22 years with Unocal (a major international oil company) in research management and administration. He has brought to IUPAC a rich mix of managerial talent, hands-on experience in information technology and wide experience in chemistry.

John has begun to organize the office in RTP, while we continue the Oxford office until the end of September. This arrangement has permitted him to continue routine activities with the Oxford staff while he analyses the operations and prepares to recruit at RTP only the staff essential to the projected modes of operation.

Basic Functions of the Secretariat. In addition to the essential functions of the Secretariat related to financial management, record-keeping and general administration, the areas viewed as especially important for the new Secretariat are those relating to communications with IUPAC volunteers, Affiliates and the world-wide

chemistry community. This emphasis on communication makes the Union's electronic communication and publishing activities a central activity of the Secretariat. It is expected that by fall a new site for the IUPAC Home Page will be established in North Carolina with its own domain name. In addition to retaining the current site at the UK Royal Society of Chemistry as a mirror site, we expect to attract other mirror sites in the Asia/Pacific region and Eastern Europe. The Home Page will be developed into a central communication and publication hub for the Union.

Under guidelines developed last year by our Committee on Printed and Electronic Publications (CPEP), preliminary Commission Reports will be disseminated mainly electronically rather than as paper. The electronic version made available for comment will, of course, be clearly identified as preliminary. The electronic format will allow the submission of comments easily and quickly. It is expected that publication of preliminary documents in this fashion will greatly increase the visibility of IUPAC Commission Reports in the chemical community.

In addition, CPEP currently has under review other specific proposals to publish final Commission Reports and Conference Proceedings electronically in conjunction with usual publication in *Pure and Applied Chemistry*. There are also on-going discussions of improvements in the print version of *Chemistry International* with ancillary electronic communications on the IUPAC Home Page. It is planned to begin making *CI* available on the Internet in parallel with the print edition late in 1997 or early in 1998. This should make the content of *CI* more widely available than it is currently and enable it to function better as a method of promoting feedback from the chemical community outside the circle of those directly involved in Union activities.

New Support Role for the Secretariat. With economies brought about by relying on information technology, we should require fewer staff members to carry out strictly administrative activities and can recruit professional staff who will be able to give more attention to the needs of our Commissions in carrying out their projects. As part of the concept adopted by the Executive Committee to emphasize a project-driven structure, we will need a better system to help Commissions develop proposals, recruit candidates to serve on Commissions, track projects and provide progress reports. With the full support of the Executive Committee, John Jost is moving carefully to ensure that our routine administration is being handled well, while he determines the staffing needs for implementing this new role. We believe that in the next two years you will see a dramatically transformed Secretariat, which will be able to provide the kind of support that our Commissions need to initiate, carry out and complete important projects in a timely way and to obtain rapid publication of their reports.

Biennial Report of the Treasurer and Finance Committee

J.M. Ward

As I did for the last Council Meeting, I shall give a report of the first year of the present biennium and one of the previous complete biennium 1994–95. I shall also attempt to estimate the outcome for the present year. Also, as this is my last year as Treasurer, I think I should give you a brief summary of my stewardship during the last six years.

I give below the amounts transferred to the Balance Sheet from the Expenses and Income Accounts, i.e. the 'bottom lines' and the corresponding budget figures for 1996 and the 1994–95 biennium, to the nearest one thousand USD. There is also an estimate for 1997 based on the six-month management accounts and estimates of the costs still to be incurred by the move of the Secretariat to the Research Triangle Park, North Carolina.

	Actual	Budget
1994	149	122
1995	113	(180)
1994–95	262	(58)
1996	634/290	161
1997E	(330)	(161)
1996–97E	304/(40)	0

NB brackets denote a deficit, E denotes an estimate.

1994–95 Biennium. I have given in detail the reasons for the departures from budget for the years 1995 and 1996 in my commentary to those years' accounts in the July issues of *CI*, but let me summarize the principal factors. In 1995 the biggest contributor to the departure from budget was an underspend of USD 161k on the Guildford Assembly, mainly brought about because only 85% of TMs attended and because, contrary to what had been expected, there was broadly no inflationary increase in airfares between 1993 and 1995. Another large contributor was an underspend of USD 62k by the Divisions and Standing Committees. Had the Guildford Assembly cost the budgeted USD 490k and had the Divisions and Standing Committees spent their allocations, the result would have been a modest surplus of USD 30k for the biennium. As it was, a small increase over budget in 1994 of USD 27k led to an overall result for the 1994–95 biennium of USD 262k, markedly higher than the budgeted deficit of USD 58k.

1996–97 Biennium. During 1996, there was an expected addition to the Union's funds from Barings Brothers Bank. 'Office International de Chemie' which was



part of the Union when it was created in 1919, did not close its account with the bank when it ceased operating. This money with substantial accrued interest has been paid to the Union as successor, a sum of USD 344k.

It is now part of the reserves but accountancy rules demand that it should go through the 1996 Income and Expenses account so swelling the 1996 surplus. Even so, the surplus without it is still USD 290k, USD 129k better than budget, a result brought about largely by a Publications surplus of USD 61k over budget and an underspend of USD 30k on the Affiliate Membership Programme, both results due mainly to unexpected resignations of staff with consequent reductions in staff costs. There will be, however, consequent increases in Publications staff costs in 1997. A healthy number of smaller contributions make up the balance.

In attempting an estimate for 1997 a number of unbudgeted items, some large, have to be taken into account. These items although unbudgeted were thoroughly discussed and approved by the Executive Committee and the Bureau, recognizing that our reserves are strong and intended to be used for such eventualities. These items arise from two sources, first, the extra meetings to discuss how best to increase the relevant visibility and appeal of the Union's work to the chemical industry as well as to the rest of the chemical community, and secondly, the move of the Secretariat to the Research Triangle Park, North Carolina, USA. The extra meetings, two of which were with eminent figures from industry and academia in Europe and Asia will cost some USD 30k. Redundancy payments to the Oxford

staff will amount to about USD 130k. Recruiting and appointing the new Executive Director plus staff and other costs resulting from running two offices for five months will amount to about USD 100k. Together with an adjusted figure for the budgeted deficit, the estimated deficit is about USD 380k. But despite earlier concern about the cost of the 1997 Assembly, the eventual cost may be USD 50k below budget, giving a total deficit for the year of USD 330k. If the Barings' money is included in the 1996 surplus there will be a biennial surplus of about USD 304k. If, more realistically, this money is taken out, the result is a deficit of USD 40k. The cost of equipping the new office this year will be about USD 55k, but this being capital it can be taken straight to the Balance Sheet and thus come directly from reserves.

The substantial surplus made in the 1994–95 biennium and the good improvement over budget in 1996 is a continuing indication that we have emerged from the difficult financial position of the early nineties about which I shall have more to say later. Provided that we keep the same careful control of expenses and maintain the real value of our income by keeping subscriptions in line with inflation, it will be possible to keep a balanced budget in the years to come. It is unlikely that the circumstances that gave rise to the recent surpluses will reoccur. The next three General Assemblies are in expensive venues, Geneva, Berlin and Brisbane and the new initiatives which should result from present discussions about the Union will require the maximum of resources.

Reserves. The recent surpluses and the good returns we have been able to secure from our investments have strengthened our general reserve. In 1996, excluding the Building Fund and the Southern Hemisphere Sinking Fund, it increased in value from USD 2451k to USD 3093k.

It is proposed to use the Barings' money, USD 344k, to found a separate Endowment Fund, the interest from which to be used for special purposes. The capital needed to equip the new Secretariat offices, the 1997 deficit and removal of the Barings' money will reduce the main reserve to USD 2364k but this is still substantially above the target figure for reserves so that there is good opportunity to use the excess for one-off or short-

term endeavours of the type that could emerge from the present discussions about new initiatives.

The several additions made at various times during the year—the decision to use the same investment strategy for the Building Fund as used for the general reserve, the transfer of USD 100k from the cash account to the Building Fund, the conversion of other monies in this account to stocks and shares and the addition of the Barings' money—make it very difficult to deduce a figure for the total performance of the investments during 1996. But if we take the investments which were held for the whole year, some 85% of the final sum, the equity portion gained 24% and the bond portion 4.9%, with a combined gain of 19%. Several bonds matured during the year and only four remained throughout the year. If we assumed the gain on them all was also 4.9%, the combined gain can be calculated as 17%. It should be emphasized that this figure is indicative only.

The Building Fund, which since March 1996 has the same proportion of equities to bonds as the main reserve, an average of 55:45 and to which was added USD 100k in March, gained only 9% in value. This was because the Fund had been held in British equity and bond unit trusts at the beginning of the year and these had to be sold at a loss to buy the dollar mutual funds in order to follow the investment strategy used for the main reserve.

In summary

By carefully controlling expenditure and maintaining the real value of subscriptions, the Union has corrected the imbalance between income and expenditure that led to the dire financial forecasts of 1991 and the subsequent deficits. In addition our reserves are strong and at a level that will enable substantial sums to be spent on short-term initiatives. This strength should not lead Council to neglect the duty to keep the level of subscription income in line with increases in the retail price index, as practised by almost all organizations, companies and shops. It was the failure to do so in the second half of the 1980s that was one of the principal causes of the financial difficulties that are now behind us, and that must remain there.

Income and expenses

At the General Assembly in Hamburg, 1991, I presented, as Chairman of the Finance Committee, a financial forecast for the following four years. Two methods of forecasting were used, one based on projecting regression lines of the results for income and expenses for the preceding four biennia and another based on assumptions about future economic projections. There was satisfactory agreement between the two forecasts which showed that if the past trends continued there would be a cumulative deficit over the next two biennia, i.e. 1992–95, of over one million US-dollars.

The principal reasons for this imbalance between expenses and income were first a failure by Council to agree to keep subscription income at least in line with inflation, and secondly a levelling off after 1985 of contributions from the other main sources of income, investments and publications, an eventuality that the Finance Committee had warned against but which warning had gone unheeded. In 1982–83 subscriptions amounted to 80% of total income, in 1987–88 the proportion had fallen to 55% and had then remained more or less constant.

At its meeting before Council the Bureau agreed to take action and made substantial cuts in budgeted expenses, principally a cut of 12% in the allocation to Divisions, and it recommended an increase in subscriptions of 5% for each of the years 1992 and 1993. Council agreed to the increases.

When I became Treasurer on 1 January 1992 my main concern then was to restore the cuts in the Divisional allocation while maintaining a balanced budget. To do this it was necessary to keep strict control of expenses, and all parts of the Union assisted me in this, and to persuade Council to maintain the real value of our subscriptions. Again, in spite of difficulties in some countries, Council has supported my recommendations.

In 1991 the income and expenses account showed a deficit of USD 162k, which but for a change in accounting convention recommended by the auditors, would have been a deficit of USD 256k. In 1992 the deficit fell to USD 72k. In 1993 the financial measures achieved their purpose and there was a small surplus of USD 23k. In the following year, 1994, there was a further small surplus over budget of USD 27k. There was a further true surplus over budget in 1996 of USD 129k—USD 473k if the Barings windfall was included. Heavy expenses in 1997 will probably result in a biennial deficit of USD 40k.

In summary, the bottom lines of the income and expenses accounts from 1990 to 1996, in thousands of USD, are as follows (an estimate for 1997 is also given).

1990	1991	1992	1993	1994	1995	1996	1997E
12	(162)	(72)	23	149*	113	291	(330)

The biennial figures are

1990–91	1992–93	1994–95	1996–97E
(150)	(49)	262	(40)

N.B. brackets denote a deficit, E denotes an estimate.

*Under the accounting convention now used for a balanced budget, a surplus in the even year is balanced by an equal deficit in the odd (Assembly) year. This accounts for the difference between 149k and the figure of 27k for the difference between actual and budget figures given in the text.

The divisional allocation

Returning to the objective of restoring the cuts made in the Divisional allocation at the Hamburg Council Meeting, although I was able to maintain the Divisional allocation at the 1992 level over the first few years, whereas the allocation to Standing Committees was reduced, the 1994–95 allocation was 18% below the pre-Hamburg value in real terms. Council has continued to agree to subscription increases in line with inflation, and this figure fell to 15% in 1996–98. If the recommendation for a 3% increase in 1998 and 1999 is accepted, the Divisional allocation will have been restored. The details are, in thousands of USD:

	Allocation	Pre-Hamburg allocation, adjusted*
1992–93	301	342
1994–95	301	365
1996–97	331	389
1998–99	420	415

*Adjusted to take account of increases in OECD retail price indices. The OECD figures used are those for the beginning of the years 1992, 1994, 1996 and 1998, the years when the allocations were made. A forecast figure of 3.0% is used for 1997 to give the figure for the beginning of 1998.

Finally, subscription income accounted for 66.5% of total income in the 1995–96 biennium compared with

57% in 1990–91. If the 3% increase in subscriptions is agreed the budgeted income for the biennium 1998–99 will be 69% of total income. As mentioned above, in 1982–83 it was 80%.

The reserves

Although the Union has been in difficulties with its annual income and expenses account, it was not in real financial danger because the reserves were strong. These have remained so and the following summary in thousands of USD shows the value of reserves over the years 1991–1996. The values are book values. The 1996 market values are shown in square brackets.

	General reserve	Building Fund	Southern Hemisphere	Total
1991	2182			2182
1992	2156	319		2475
1993	2082	333		2415
1994	2366	289		2655
1995	2362	303		2665
1996	2520* [2749]	396 [440]	50	2966 [3239]

*Excluding the USD 344k Barings' money.

If the 1991 figure is adjusted for OECD inflation between 1991 and 1996, its value becomes USD 2568k, so it could be said that the general reserve has remained constant in book value; the market value has risen by 7%. Since 1991 the Building Fund and the Southern Hemisphere Sinking Fund have been established—if these are included the book value of the total

reserves is USD 2966, an increase since 1991 of 15%; in market value the total reserves in real terms have increased in value by 26%. Since the Barings' money is a windfall not in any way earned by the Union, I have not included it in the calculations, nevertheless, it is now part of our reserves.

The target value of the general reserve, which is the sum of the last two years' expenses, was USD 2007k at the end of 1996, so that the book value of the general reserve is USD 514k above it; the market value is USD 742k above it. By the end of 1997 these sums will be reduced by the USD 55k needed for capital equipment for the new Secretariat office and by the 1997 deficit which could be as much as USD 330k. On the other hand the market value should be enhanced by capital gains in our holdings of equities and bonds. All in all, there are ample monies for important and urgent short-term initiatives and the Union should take advantage of the opportunity during the next few years.

Conclusion

The finances of the Union are now well under control, both the operational finance and the level of reserves. This latter gives opportunities to undertake special short-term initiatives and these opportunities must not be missed. I hope and trust that Union Members will give my successor the support given to me by keeping careful control of spending and will continue and intensify efforts to increase income. In particular, Council should continue to maintain the real value of national subscription income.

Relocation of IUPAC Archival Material



Dr Mo Williams

Following the transfer of the archival records of the Commission on Atomic Weights and Isotopic Abundances (II.1) to the Chemical Heritage Foundation (CHF)* during 1992, the Executive Committee of IUPAC accepted an invitation from CHF to serve as an archive for other IUPAC documentation.

As a consequence of the move of the IUPAC Secretariat from Oxford (UK) to Research Triangle Park, North Carolina (USA), which is scheduled to be completed by the end of October 1997, the archives material presently held at Oxford is being sorted into two categories:

1. Current documentation to be sent to RTP
2. All other archival material to be sent to CHF (Philadelphia, USA)

In due course, it is hoped to publish a complete listing



The former First National Bank, Philadelphia, now home of the Chemical Heritage Foundation

of the material relocated at CHF. Meanwhile, the following material was sent to Philadelphia in late 1996:

Bureau: 1940–1948

Commission on Biochemical Nomenclature: 1930–1951, 1966–1970

Publications: 1919–1931, 1968–April 1969

Committee on Teaching of Chemistry: 1968–1969

Finance Committee: 1964–1972

Physical Chemistry Division (I)

—Physical Chemistry Division Committee: March 1964–December 1973

—Commission on Physicochemical Symbols, Terminology, and Units (I.1): 1932–1967, 1970

—Commission on Thermodynamics (I.2): 1936–1950, 1960–1971

—Commission on Electrochemistry (I.3): 1930–1948, April 1962–May 1970

—Commission on Physicochemical Measurements and Standards (I.4): 1919–1941, 1946–1951, 1968–1970

—Commission on Molecular Structure and Spectroscopy (I.5): 1963–1966

—Commission on Colloid and Surface Chemistry (I.6): December 1960–October 1969

Inorganic Chemistry Division (II)

—Commission on Nomenclature of Inorganic Chemistry (II.2): 1919–1971

—Commission on High Temperatures and Refractories (II.3): 1958–1959, 1965–1971

Organic Chemistry Division (III)

—Commission on Nomenclature of Organic Chemistry (III.1): 1919–1955

—Commission on Chemical Plant Taxonomy (III.2): 1968–1973

—Commission on Photochemistry (III.3): 1969

Analytical Chemistry Division (V)

—Analytical Chemistry Division Committee: January 1959–1970

—Commission on Analytical Reactions and Reagents (V.1): 1935–1950, 1964–1966

—Commission on Microchemical Techniques and Trace Analysis (V.2): 1950–1958, 1960–1969

—Commission on Equilibrium Data (V.6): 1967–1971

—Commission on Radiochemistry: 1919–1935

Applied Chemistry Division (VI)

—Applied Chemistry Division Committee: 1919–1944

—Section on Food Chemistry (VI.1): 1919–1946

—Section on Fermentation Industries (VI.2): August 1965–1969

—Section on Oils and Fats (VI.3): 1922–1954, 1958–1970

—Section VI.4: 1919–1936

—Section on Pulp Paper and Board/Reclamation of Solid Wastes: 1959, 1968–1971

—Section on Water Sewage and Industrial Waste (VI.8): June 1969

Clinical Chemistry Section

—Commission on Automation and Clinical Chemical Techniques (VII.1): August 1969

National Adhering Organizations

—Argentina: 1920–1969

—Australia: 1920, 1922

—Belgium: 1925–1971

—Canada: February 1920–May 1969

- Chile, Columbia, Cuba: 1920–1962
- Czechoslovakia: January 1970–July 1971
- Finland, Denmark: 1926–1956
- France: September 1932–July 1969
- Germany: 1922
- Greece: 1920
- Hungary, India, Ireland: July 1930
- Israel: April 1956
- Italy: January 1920–November 1969
- Japan: April 1920–March 1971
- Mexico: 1920
- Netherlands: February 1920
- New Zealand: February 1921
- Poland: June 1919
- Representatives of Portugal, China, Korea, Vietnam: April 1920
- Republic of South Africa: December 1920
- Romania: April 1920
- Spain: April 1920
- Sweden: 1920
- Switzerland: January 1920–May 1971
- Turkey, United Arab Republic: September 1956
- UK: January 1920–May 1971
- USA: January 1920–1971
- USSR (Estonia & Latvia): July 1927–April 1940
- Venezuela, Yugoslavia: April 1920
- Company Associates Scheme:**
- January 1969–December 1969
- Council**
- XXV Council (Cortina D'Ampezzo: July 1969)
- Congresses**
- IX: 1920–1940
- X: 1936–1938

- XI: 1946–1949
- XVI: March 1956–January 1957, July 1957, September–February 1957
- Conferences**
- New York, USA: 1951
- ICSU**
- 1920–1935, 1945–1951, 1964–1965, 1965–1970
- Bulletins: 1955
- General**
- 1919–1945
- Commission Des Constantes Radioactives: 1930–1951
- Ad hoc* Committees—Applied Chemistry, Interdisciplinary Matters: 1969–1971
- Membership of IUPAC Units: 1969
- Machine Documentation in the Chemical Field: 1946–1959
- Coordination Committee: 1966–1969
- Miscellaneous: 1919–1925
- Account Budgets: 1920
- Accounts Banks and Cash: 1935–1943
- Executive Committee Numbers, Miscellaneous, International Circulars: 1932–1950
- IOAch: May 1968
- Joint Commission on Standards, Units and Constants of Radioactivity: 1945–1950
- UN and UNESCO: 1946–1954
- IUPAC and NAO Subscriptions: 1925
- Section on Medicinal Chemistry (III.4): 1969–1970
- Commission on Statutes and Bylaws: 1938–1973
- Correspondence: 1919–1936, 1950–1955, 1968–1969.

*For an account of the origins of CHF, its mission and operating structure, governance, etc., please see *Chem. Intl.* 1995, 17(5) (September), 166–169. CHF is an Associated Organization of IUPAC.

For further information please contact Elizabeth Swan (Director of Library Services) at the Chemical Heritage Foundation, 315 Chestnut Street, Philadelphia, PA 19106-2702, USA. Tel.: +1 (215) 925 2222 ext. 226; E-mail: eswan@chemheritage.org

Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *Pure and Applied Chemistry*.

Methods for the analysis of transient absorbance data
(Technical Report)

Synopsis

Procedures for the generation and collection of transient UV-visible absorbance data are briefly reviewed. Problems associated with signal generation (scattered

light, inhomogeneous distribution of transients, instability of pulsed light sources), signal detection (averaging, filtering) and signal analysis in kinetic and spectrographic flash photolysis are addressed. Methodology for the fitting of model functions to absorbance data that depend on up to three variables (time, wavelength and, e.g. temperature) is discussed.

This report was prepared for publication by Roland Bonneau (LA 348 du CNRS, Université de Bordeaux I, F-33405 Talence Cedex, France), Jakob Wirz (Institut für Physikalische Chemie, Universität Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland) and Andreas D. Zuberbühler (Institut für Anorganische Chemie, Universität Basel, Spitalstrasse 51, CH-4056 Basel, Switzerland) for the Commission on Photochemistry of the Organic Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 979–992.

Molecular characterization of commercial polypropylene with narrow and broad distribution of molar mass (Technical Report)

Synopsis

The molar mass and the molar mass distribution of two commercial grades of isotactic polypropylene, Moplen S30S of Himont Srl and Daplen PT55 of PCD Polymere GmbH, were investigated by 16 laboratories. For Moplen S30S $M_w = 467$ kg/mole $\pm 6.0\%$ (relative standard deviation), $M_n = 83.7$ kg/mole $\pm 9.8\%$ and $M_w/M_n = 5.70 \pm 10.1\%$ were determined by size exclusion chromatography (31 SEC runs), for Daplen PT55 $M_w = 206$ kg/mole $\pm 13.6\%$, $M_n = 61.4$ kg/mole $\pm 13.4\%$ and $M_w/M_n = 3.42 \pm 17.3\%$ were found (38 SEC runs). Light scattering measurements gave $M_w = 445$ kg/mole $\pm 4.1\%$ for Moplen S30S (4 labs) and $M_w = 212$ kg/mole $\pm 10\%$ for Daplen PT55 (3 labs). The intrinsic viscosity in 1,2,4-trichlorobenzene at 140 °C of Moplen S30S $[\eta] = 1.87$ dl/g $\pm 5.4\%$ and of Daplen PT55 $[\eta] = 1.12$ dl/g $\pm 6.7\%$ was measured (nine independent measurements). Samples of the respective lots are available from the authors, Moplen S30S from IM, Daplen PT55 from KL.

This report was prepared for publication by K. Lederer (Institut für Chemie der Kunststoffe, Montanuniversität Leoben, A-8700 Leoben, Austria) and I. Mingozzi (Himont Italia, Centro Ricerche G. Natta, I-44100 Ferrara, Italy) for the Working Party on Molecular Characterization of Commercial Polymers, Commission on Polymer Characterization and Properties, Macromolecular Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 993–1006.

Reference Value Standards and Primary Standards for pH measurements in D₂O and aqueous-organic solvent mixtures: New accessions and assessments (Technical Report)

Synopsis

Recommended Reference Value Standards based on the potassium hydrogen phthalate buffer at various temperatures are reported for pH measurements in various binary solvent mixtures of water with eight organic solvents: methanol, ethanol, 2-propanol, 1,2-ethanediol, 2-methoxyethanol ('methylcellosolve'), acetonitrile, 1,4-dioxane and dimethyl sulfoxide, together with Reference Value Standards based on the potassium deuterium phthalate buffer for pD measurements in D₂O. In addition are reported Primary Standards for pH based on numerous buffers in various binary solvent mixtures of water with methanol, ethanol and dimethyl sulfoxide, together with Primary Standards for pD in D₂O based on the citrate, phosphate and carbonate buffers.

This report was prepared for publication by P. R. Mussini, T Mussini and Sandra Rondinini (Department of Physical Chemistry and Electrochemistry, University of Milan, 20133 Milano, Italy) for the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1007–1014.

Properties and units in the clinical laboratory sciences. II: Kinds-of-property (IUPAC Recommendations 1997)

Synopsis

The document circumscribes the concept 'kind-of-property' (property in a general sense) and lists the kinds-of-property mostly used in the clinical laboratory sciences. The concepts are as defined in the 'Compendium of terminology and nomenclature of properties in clinical laboratory sciences', except for a few that are defined intuitively. Each is given a unique code value and is expressed in different languages for use in the assembly of terms representing individual properties.

This report was prepared for publication by Desmond Kenny (Our Lady's Hospital for Sick Children, Crumlin, Dublin 12, Ireland) and Henrik Olesen (Department of Clinical Pharmacology, Copenhagen University Hospital, Copenhagen, Denmark) for the Committee on Nomenclature, Properties and Units, Clinical Chemistry Section, Chemistry and Human Health Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1015–1042.

Properties and units in the clinical laboratory sciences. V: Properties and units in thrombosis and haemostasis (Technical Report)

Synopsis

For historical reasons, the elements of properties (terms) used in the nomenclature for properties in thrombosis and haemostasis differ according to 'school' of thought. This hampers communication. In collaboration, the Scientific and Standardization Committee of the International Society on Thrombosis and Haemostasis and the Commission (Committee) of Nomenclature, Properties and Units, previously 'Quantities and Units', have prepared a set of recommended systematic names for properties in that domain. For use in electronic transmission each property has been given a code value. The prefix to the code values has been changed from 'QU' to 'NPU' because of the change of name of the Commission (Committee).

*This report was prepared for publication by M. Blombäck (Department of Clinical Chemistry and Blood Coagulation, Karolinska Hospital, Stockholm, Sweden), R. Dybkaer (Department of Clinical Chemistry, Frederiksberg Hospital, Copenhagen, Denmark), K. Jørgensen (Department of Clinical Biochemistry KB 3011, Copenhagen University Hospital, Copenhagen, Denmark), H. Olesen (Department of Clinical Pharmacology Q 7642, Copenhagen University Hospital, Copenhagen, Denmark) and S. Thorsen (Department of Clinical Biochemistry KB 3011, Copenhagen University Hospital, Copenhagen, Denmark) for the Commission on Nomenclature, Properties and Units, Clinical Chemistry Section, Chemistry and Human Health Division (in collaboration with the Scientific and Standardization Committee of the International Society on Thrombosis and Haemostasis). The full details are to be found in Pure Appl. Chem. 1997, **69**, 1043–1079.*

Properties and units in the clinical laboratory sciences. VI: Properties and units in IOC prohibited drugs (Technical Report)

Synopsis

The term designating a substance being an active ingredient of a drug may be a generic name, a non-proprietary name, a registered trade name, a fantasy name or other. This causes difficulties in the transmission of request and report on such substances to and from the clinical laboratories, and in the collating of this information from different sources. The document comprises a list of properties of drugs of abuse in biological fluids as defined by the International Olympic Committee Medi-

cal Code for use in electronic transmission systems. Standard systematic names are presented with a code value for each. The coding schemes thus prepared are accessible on the Internet from the Commission on Nomenclature, Properties and Units' Home Page address: <http://inet.uni-c.dk/~qukb7642>.

*This report was prepared for publication by H. Olesen (Department of Clinical Pharmacology Q, Copenhagen University Hospital, Copenhagen, Denmark), D. Cowan (Drug Control Centre, London University, King's College, London, UK), I. Bruunshuus (Department of Clinical Pharmacology Q, Copenhagen University Hospital, Copenhagen, Denmark), K. Klempel (Department of Clinical Pharmacology Q, Copenhagen University Hospital, Copenhagen, Denmark) and G. Hill (Department of Clinical Chemistry, Hospital for Sick Children, Toronto, Ontario, Canada) for the Commission on Nomenclature, Properties and Units, Clinical Chemistry Section, Chemistry and Human Health Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 1081–1136.*

Glossary of terms used in computational drug design (IUPAC Recommendations 1997)

Synopsis

Computational drug design is a rapidly growing field which is now a very important component in the discipline of medicinal chemistry. At the same time many medicinal chemists lack significant formal training in this field and may not have a clear understanding of some of the terminology used but need to grasp concepts, follow research results, define problems for, and utilize findings of, computational drug design. In this context the IUPAC Medicinal Chemistry Section Committee felt it would be useful to develop a glossary of terms used in computational drug design for easy reference purposes. Also there is the possibility that in different countries certain terms may not have the same meaning and in such a case there would be value in trying to establish an international definition standard. Accordingly a Working Party of seven experts in the field was assembled who constructed a glossary of some 100 terms. Concise but sufficiently explanatory definitions have been formulated based on a variety of literature sources and selected key references provided.

This report was prepared for publication by H. van de Waterbeemd, Chairman (F. Hoffmann-La Roche, Pharma Research New Technologies, CH-4070 Basel, Switzerland), R.E. Carter (Astra Hässle AB, Computational Chemistry, S-43183 Mölndal, Sweden), G. Grassy (Centre de Biochimie Structurale, Faculté de

Pharmacie, F-34060 Montpellier, France), H. Kubinyi (BASF AG, ZHB/W A30, D-67056 Ludwigshafen, Germany), Y.C. Martin (Abbott Laboratories, Computer-Assisted Molecular Design, Abbott Park, IL 60064-3500, USA), M.S. Tute (University of Canterbury, Kent CT2 7NH, UK) and P. Willett (University of Sheffield, Department of Information Studies, Sheffield S10 2TN, UK) for the Medicinal Chemistry Section of the Chemistry and Human Health Division. The full details are to be found in *Pure Appl. Chem.* 1997, **69**, 1137–1152.

Intrinsic characterization of continuous carbon fibre thermoplastic composites. 3: Fatigue crack growth (Technical Report)

Synopsis

This paper reports some fatigue crack growth results obtained on unidirectional laminates of AS4/PEEK. Crack growth is intralaminar and the study has included the influence of laminate thickness, method of consolidation and level of applied stress level. Presentation of data is by a Paris Law type approach, where crack growth per cycle is plotted against a stress field intensity factor. The measurements have involved four different laboratories and therefore it has been possible to attempt to embrace the likely scatter involved in the collection of fatigue data commensurate when several laboratories conduct seemingly similar measurements.

This report was prepared for publication by D.R. Moore (ICI plc, Wilton, Middlesbrough, Cleveland, UK) and J.C. Seferis (Polymeric Composites Laboratory, University of Washington, Seattle, USA) for the IUPAC Working Party IV.2.1: Structure and Properties of Commercial Polymers of the Macromolecular Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1153–1161.

Guidelines for publication of equations of state. I: Pure fluids (Technical Report)

Synopsis

During recent decades equations of state have become a major tool for the correlation and prediction of thermodynamic properties of fluids. Equations of state can be applied to pure substances as well as to mixtures, and therefore a very large number of publications deal with the development or improvement of equations of state. In order to give authors, editors and reviewers of publications on new equations of state some guidelines and to ensure that future publications will be more profitable for the reader, some criteria for pure fluids are given that ought to be fulfilled by a good manuscript.

This report was prepared for publication by U.K. Deiters (Institut für Physikalische Chemie, Universität zu Köln, D-50939 Köln, Germany) and K.M. de Reuck (Chemical Engineering Department, Imperial College of Science, Technology & Medicine, London SW7 2BY, UK) for the Commission on Thermodynamics of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1237–1249.

Glossary of terms used in bioinorganic chemistry (IUPAC Recommendations 1997)

Synopsis

The glossary contains definitions and (where needed) explanatory notes for about 400 terms used in the multidisciplinary field of bioinorganic chemistry. A need has been recognized for globally acceptable definitions of terms in this field and this glossary was compiled with the objective of fulfilling this need. It is by no means a comprehensive dictionary. The terms selected were those considered essential and/or widely used. The definitions given reflect current usage and complement IUPAC guidelines. Abbreviations and acronyms, frequently used in bioinorganic chemistry, are included.

This report was prepared for publication by M.W.G. de Bolster (Vakgroep Organische en Anorganische Chemie, Faculteit der Scheikunde, Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, The Netherlands) for the Working Party on IUPAC Glossary of Terms Used in Bioinorganic Chemistry of the Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, 69, 1251–1303.

Characterization of SiC powders and the influence of powder properties on sintering (Technical Report)

Synopsis

This report summarizes the characteristics of SiC powders which influence the ability to obtain fully dense (non-porous) ceramics, with good mechanical properties, via the sintering process. Methods for characterizing powder properties, such as particle size, morphology, bulk and surface chemistry, are outlined and specific examples are referenced. The characteristics of typical commercial SiC powders are tabulated.

This report was prepared for publication by G. Schwier and I. Teusel (H.C. Starck GmbH & Co. KG, D-38642 Goslar, Germany) and M.H. Lewis (Centre for Advanced Materials, University of Warwick, Coventry CV4

7AL, UK) for the Commission on High Temperature Materials and Solid State Chemistry of the Inorganic Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 1305–1316.

Chemically modified electrodes: Recommended terminology and definitions (IUPAC Recommendations 1997)

Synopsis

Chemically modified electrodes (CMEs) comprise a relatively modern approach to electrode systems that finds utility in (1) a wide spectrum of basic electrochemical investigations, including the relationship of heterogeneous electron transfer and chemical reactivity to electrode surface chemistry, electrostatic phenomena at electrode surfaces and electron and ionic transport phenomena in polymers, and (2) the design of electrochemical devices and systems for applications in chemical sensing, energy conversion and storage, molecular electronics, electrochromic displays, corrosion protection and electro-organic syntheses. Compared with other electrode concepts in electrochemistry, the distinguishing feature of a CME is that a generally thin film of a selected chemical is bonded or coated onto the electrode surface to endow the electrode with the chemical, electrochemical, optical, electrical, transport and other desirable properties of the film in a rational, chemically designed manner. In this report, the authors have attempted to identify and define the most widely used terminology in the growing field of CMEs and to recommend a particular term in cases where a multiplicity of terms has arisen over the past several years or where previously defined terms have taken on broadened meanings for the special cases of CMEs.

*This report was prepared for publication by R.A. Durst (Analytical Chemistry Laboratories, Cornell University, Geneva, NY 14456, USA), A.J. Bäumner (Institute for Technical Biochemistry, University of Stuttgart, D-70569 Stuttgart, Germany), R.W. Murray and R.P. Buck (Department of Chemistry, University of North Carolina, Chapel Hill, NC 27514, USA) and C.P. Andrieux (Laboratoire d'Électrochimie Moléculaire, Université de Paris 7, 75251 Paris Cedex 05, France) for the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 1317–1323.*

Consistency of pH standard values with the corresponding thermodynamic acid dissociation constants (Technical Report)

Synopsis

With the simplest possible assumptions on the ion activity coefficients, namely a Debye–Hückel approach, pH values of eleven standard buffer solutions have been calculated from the corresponding thermodynamic acidity constants, $K_{(I \rightarrow 0)}$, and compared to the electrometrically assigned pH(S) values (by Harned cell method). Agreement is within ± 0.01 in the temperature range 10–40 °C for all standards, except carbonate. The results for the phthalate, acetate, phosphate and carbonate systems at 25 °C indicate that this consistency is improved if specific ion interactions are taken into account, according to the Pitzer theory.

*This report was prepared for publication by M. Filomena Camoes and M.J. Guiomar Lito (Centro de Electroquímica e Cinética da Universidade de Lisboa, 1294 Lisboa Codex, Portugal), M. Isabel A. Ferra (Universidade da Beira Interior, 6200 Covilhã, Portugal) and Arthur K. Covington (Department of Chemistry, University of Newcastle, Newcastle-upon-Tyne, NE1 7RU, UK) for the Commission on Electroanalytical Chemistry of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 1325–1333.*

Chirality in synthetic agrochemicals: Bioactivity and safety consideration (Technical Report)

Synopsis

Most synthetic agrochemicals with chiral structures are marketed as racemates even though the desired biological activity may be derived from only one enantiopure isomer. However, some synthetic agrochemicals such as pyrethroid insecticides, aryloxypropanoate herbicides and triazole fungicides are marketed as the most biologically active enantiopure isomer. Numerous reports describing the relative biological activities, preparations and analyses of enantiopure agrochemicals are available. Some examples of how different enantiomers in racemates are selectively metabolized have also been reported. When agrochemicals have chiral structures, efforts should be made to define the mode of action, elucidate metabolic pathways and to define the human and environmental toxicity of each enantiopure isomer. If there are large differences in the biological activities of individual enantiomers in racemates, it is desirable to develop and use only the enantiopure isomer with the highest

sought-after biological activities.

*This report was prepared for publication by N. Kurihara (Radioisotope Research Center, Kyoto University, Kyoto 606-01, Japan), J. Miyamoto (Sumitomo Chemical Co. Ltd, Osaka 541, Japan), G.D. Paulson (US Department of Agriculture, ARS, Fargo, ND 58105, USA), B. Zeeh (BASF AG, Agricultural Research Station, D-67114 Limburgerhof, Germany), M.W. Skidmore (Zeneca Agrochemicals, Jealotts Hill, Bracknell, Berks., RG42 6EY, UK), R.M. Hollingworth (Pesticide Research Center, Michigan State University, East Lansing, MI 48824, USA) and H.A. Kuiper (State University for Quality Control of Agricultural Products, Rikult-Dlo Wageningen, The Netherlands) for the Commission on Agrochemicals and the Environment of the Chemistry and the Environment Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 1335–1348.*

Pesticide fate in tropical soils (Technical Report)

Synopsis

Pesticide use is an important component of agricultural and non-agricultural pest control in tropical areas. However, the fate of pesticides in tropical soils is not as well understood as that for soils from temperate regions. Tropical soils defy easy generalizations, but they are typically very old soils characterized by year-round uniformity of temperature regime. Although only a few studies have directly compared pesticide fate in tropical and temperate soils, there is no evidence that pesticides degrade more slowly under tropical conditions. Laboratory studies in which soils have been held under standardized conditions reveal that pesticide degradation rate and pathway are comparable between tropical and temperate soils. However, field investigations of tropical pesticide soil fate indicate that dissipation occurs more rapidly, in some cases much more rapidly, than for pesticides used under similar temperate conditions. The most prominent mechanisms for this acceleration in pesticide dissipation appear to be related to the effect of tropical climates, and would include increased volatility and enhanced chemical and microbial degradation rates on an annualized basis.

This report was prepared for publication by K.D. Racke (DowElanco, Indianapolis, IN, USA), M.W. Skidmore (Zeneca Agrochemicals, Bracknell, Berkshire, UK), D.J. Hamilton (Resources Sciences Centre, Indooroopilly, Queensland 4068, Australia), J.B. Unsworth (Rhône-Poulenc, Ongar, Essex, UK), J. Miyamoto (Sumitomo

*Chemical Company, Osaka 541, Japan) and S.Z. Cohen (Environmental and Turf Services, Wheaton, MD, USA) for the Commission on Agrochemicals and the Environment of the Chemistry and the Environment Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 1349–1371.*

Optimum use of available residue data in the estimation of dietary intake of pesticides (Technical Report)

Synopsis

Prediction of pesticide residue intake in human diets is vital for approving the use of pesticides and for gaining official acceptance of pesticide residue levels which occur in food commodities in international trade. Estimates for pesticide residue levels likely to be present in food as consumed are derived from supervised pesticide residue trials, residue monitoring, pesticide metabolism and food processing studies. The results of properly conducted total diet studies should generally displace other estimates, but they do not cover all pesticides and, in particular, are not available for a pesticide at its initial registration. Information was compiled on the range of residues occurring in a set of supervised residue trials with identical application rate, number of applications and pre-harvest interval, but at different sites with various crop varieties, operators, equipment and cultural practices. Eighteen recommendations are provided for estimating the level of pesticide residues likely to be present in food as consumed.

*This report was prepared for publication by D.J. Hamilton (Resources Sciences Centre, Indooroopilly, Queensland 4068, Australia), P.T. Holland (Horticulture and Food Research Institute of New Zealand Ltd, Hamilton, New Zealand), B. Ohlin (National Food Administration, Uppsala, Sweden), W.J. Murray (Pest Management Regulatory Agency, Health Canada, Ottawa, Canada), A. Ambrus (Plant Health and Soil Conservation Centre, Budapest, Hungary), G.C. de Baptista (Departamento de Entomologia, Universidade de São Paulo, Brazil) and J. Kovacicová (Institute of Preventive and Clinical Medicine, Bratislava, Slovakia) for the Commission on Agrochemicals and the Environment of the Chemistry and the Environment Division. The full details are to be found in Pure Appl. Chem. 1997, **69**, 1373–1410.*

Pure and Applied Chemistry (PAC) is the official journal of IUPAC. It publishes the main invited lectures of symposia sponsored by the Union; the recommendations of its Commissions on nomenclature, symbols and units, and technical reports on standardization, recommended procedures, collaborative studies and data compilations. Summaries of the most recent IUPAC recommendations on nomenclature and symbols, and technical reports appearing in PAC are published in *Chemistry International* in the section Recent Reports. In this section we take a brief look at symposia and lectures published in recent issues of PAC.

Lectures from Symposia

The April 1997 issue of *Pure and Applied Chemistry* (Vol. 69, no. 4) contains the texts of lectures from three symposia: the International Symposium of Sweeteners, held in Jerusalem, Israel, on 14–20 July 1996; the 16th IUPAC Symposium on Photochemistry, held in Helsinki, Finland, on 21–26 July 1996; and the International Conference on Chemical Physics on the Border of the 21st Century, held in Moscow, Russia, on 16–19 April 1996.

Sweeteners

The International Symposium on Sweeteners was held under the auspices of IUPAC, the Hebrew University of Jerusalem and the Israel Academy of Sciences. The programme included plenary and contributory lectures from many areas of natural and synthetic sweeteners, structure–activity relationships of sweeteners, mechanism of gustation, health aspects of sweeteners, side effects of commercial sweeteners, use of sweeteners in foods, sensory characteristics of sweeteners, neuro-physiological, inborn and acquired aspects of sweetness, sweeteners in weight control and diabetes and legislation of commercial sweeteners.

Prof. HRH Princess Chulabhorn Mahidol was the guest of honour at the Symposium and, at a ceremony prior to the lectures, she was presented with an Honorary Fellowship by the Hebrew University of Jerusalem. Her presentation, entitled 'Natural products for the improvement of the quality of life', covered work on the utility of some Thai plants as a source of food, including toxicological studies of stevioside and chemical investigations of cassava (*Manihot esculenta* Crantz). Her full text, plus that of the nine other plenary lectures to the conference, is presented in *Pure & Applied Chemistry*, **69**(4), 655–727.

Photochemistry

The plenary and invited lectures to the 16th IUPAC Symposium on Photochemistry [**69**(4), 729–856] as in previous years, covered a wide range of topics, including theoretical chemistry, biological chemistry, chemis-

try in the solid state, energy transfer and fast reaction kinetics. In particular, many examples were presented of the reactions of short-lived intermediates, such as biradicals, which exemplified their synthetic utility.

The conference concluded with the presentation of the Porter Award to Prof. Noboru Mataga of the Institute of Laser Technology, Osaka, Japan. His lecture presented results from picosecond and femtosecond laser spectroscopy studies on photoinduced transfer phenomena in solutions. Such studies have aided the development of exciplex chemistry. Topics covered included the excited dipolar solute–solvent interactions, solvent and driving force effects on the electronic and geometrical structures of inter- and intra-molecular exciplex systems, energy gap dependencies of charge separation in the fluorescence quenching reactions and charge recombination of product loose ion pairs, non-Marcus type energy gap dependence of charge recombination of compact ion pairs formed by excitation of ground state charge transfer complexes, photoinduced electron transfer coupled with proton transfer or proton shift in benzophenone-amine and some hydrogen bonding exciplex systems, and extensions of exciplex studies to photosynthetic reaction centre models.

Chemical physics

The International Conference on Chemical Physics on the Border of the 21st Century was held under the auspices of the Physical Chemistry Division in conjunction with the Russian Academy of Sciences, Moscow State University. The four plenary lectures are presented [**69**(4), 857–904], including that of the Conference Editor, Alexander E. Shilov of the Emanuel Institute of Biochemical Physics, Russian Academy of Sciences. Prof. Shilov discussed the contribution of N. N. Semenov, the 1956 joint winner of the Nobel Prize for Chemistry, to 20th century chemistry, not only of his discovery of branching chain reactions and the development of the general theory of chain reactions and thermal explosions, but also of his prediction that biology is likely to play a crucial role in future chemistry.

The other three plenary lectures dealt with: the role of

chemical physics in the science of catalysis and design of new catalytic technologies; non-traditional pathways of solid-phase astrochemical reactions; and the thermodynamics of extreme states of matter. The paper on chemical physics and catalysis was the last scientific communication by Prof. K.I. Zamaraev (immediate Past-President of IUPAC) before his untimely death in June 1996.

Solubility phenomena

The May 1997, **69**(5), issue of *Pure and Applied Chemistry* contains the texts of the plenary and specially invited lectures presented at the 7th International Symposium on Solubility Phenomena, held in Leoben, Austria, on 22–25 July 1996. The symposium was held under the auspices of the IUPAC Commission on Solubility Data, in conjunction with the University of Leoben. Nine lectures are published: Experimental studies in high temperature aqueous chemistry at Oak Ridge National Laboratory; Phase changes and chemical reactions in solid aqueous solutions; Mechanisms of crystallization and transformation of calcium carbonates; Improvement of polymer solubility—influence of shear and of pressure; Solubilities of the common L- α -amino acids as a function of temperature and solution pH; Solubility data in physicochemical data collections and databanks; Use of semi-empirical electrolyte theories for modelling of solution chemical data; Solubility data requirements and new experimental methods in atmospheric aerosol research; and Thermodynamic databases and equilibrium calculations in metallurgical processes.

Excitonic processes

The June 1997, **69**(6), issue of *Pure and Applied Chemistry* contains the texts of nine of the invited lectures presented at EXCON '96, the 2nd International Conference on Excitonic Processes in Condensed Matter, held in Kurort Gohrisch, Saxonia, Germany, on 14–17 August

1996. As Conference Editor, Michael Schreiber of the Institut für Physik, Technische Universität Chemnitz, points out, 65 years after the first papers on excitons by Frenkel, research on excitons has now developed into a truly multidisciplinary field. Excitons play a key role in excitation and energy transfer processes in many molecules, molecular aggregates and crystals, as well as in macromolecular and biological systems.

Included is a selective personal perspective on exciton research, presented by R.S. Knox of the Department of Physics and Astronomy and Rochester Theory Center for Optical Science and Engineering, University of Rochester, New York state. Exciton studies have progressed through many stages that correspond to those in atomic studies, including electronic structure, interactions with other particles, determination of oscillator strengths and ionization rates, bonding into excitonic molecules, condensation and thermal equilibration. Driven by huge advances in computation and experimental techniques, exciton research has essentially evolved from a study of structures to a study of dynamics, Prof. Knox told delegates. 'After 65 years, the exciton survives as neither a museum piece for textbooks nor a purely spectrographic detail. It continues to challenge both theorists and experimentalists, it has attained considerable technological significance, and it participates decisively at the very beginning of earth's food chain', he concludes.

The other published lectures include: Dynamics and instabilities of an exciton in the phonon field and the correlated absorption–emission spectra; Excitons in semiconductor nanostructures with disorder; Spin splittings in nanostructures without inversion symmetry; Hawking process in solids—quantum generation of phonon bursts by a strongly excited mode; Non-linear phenomena in organic multilayers; Photosynthetic light-harvesting; Relaxation processes and self-trapping of excitons in rare gas solids; and Parity-broken and -unbroken self-trapped excitons in alkali halides.

News

Measurement technologies in atmospheric chemistry

A workshop and short course on 'Instrumentation and Measurement Methodologies in Atmospheric Chemistry' was conducted during the two weeks 4–15 November 1996 at the Laboratory of Environmental Analytical Chemistry of the Federal University of Bahia, in Salva-

dor (Bahia), Brazil. The course was organized and coordinated by Prof. Tania Tavares, Head of the Laboratory and a Titular Member of the IUPAC Commission VI.2, Atmospheric Chemistry. Several other members of the Commission also took part by serving as lecturers and/or demonstrators.

The objective of the workshop was to broaden theo-



Prof. Tania Tavares in Brazil

retical and practical knowledge in atmospheric measurement techniques among professionals of different scientific backgrounds in Third World countries, especially those that are to some extent connected with WMO Global Atmospheric Watch (GAW) stations. The syllabus included morning lectures and afternoon laboratory practice, as well as a field measurement campaign at the site of the Brazilian GAW station. Subjects taught included the behaviour and reactions of atmospheric constituents, gas phase, particulate and liquid phase sampling and measurement techniques, spectroscopy, chromatography, fundamentals of quality assurance and control, and meteorological concepts required for data interpretation.

This was the first course of its kind, which offered laboratory instruction in addition to lectures. The course was open to anyone who had a good command of English and who was engaged in work related to chemical analysis of components in the air. Twenty-six persons from eight different countries attended: Argentina, Brazil (four different states), Chile, Costa Rica, Indonesia, Kenya, Mexico, Puerto Rico. The lecturers, who were either analytical or atmospheric chemists, aside from two meteorologists, came from Brazil, Croatia, Germany, The Netherlands and the USA.

Sponsors of the workshop, in addition to IUPAC's Chemistry of the Environment Division, included the American Geophysical Union (AGU), the Atmospheric Chemistry and Environment Education Committee of the International Global Atmospheric Chemistry Programme (IGAG), the Inter American Institute for Global Change Research (IAI) and the Global Change System for Analysis, Research and Training (START).

Judging from the comments of the participants, the workshop has been highly successful and fully met all the objectives. Prof. Tavares is to be thanked for a very substantial effort that made this project a success.

Peter Warneck
Chairman, Commission VI.2, Atmospheric
Chemistry

CHEMRAWN in Montevideo

Prof. Patrick Moyna of the University of Montevideo writes:

As a result of extensive discussion in the CHEMRAWN Committee and with all the Chemical Societies in Latin America, there is considerable support for a CHEMRAWN-style conference to be held in Montevideo. The conference, proposed for 15–20 March 1998 under the title 'Chemical Studies Applied to Environmental Evaluations', will be aimed at improving the evaluation and understanding of changes to the environment and the implementation of sensible measures to conserve it. Montevideo is at the heart of the recently established Mercosur economic region (which includes Argentina, Brazil, Paraguay and Uruguay, and will shortly be extended to include Bolivia; there is an initial association with Chile and negotiations have begun with Peru, Ecuador, Columbia and Venezuela).

The conference goals are to enable experts in Latin America to analyse the present situation and to exchange experiences and help foster use of best practices and to prepare recommendations for future work, establish monitoring networks and build up the concepts and practice of quality assurance and control. Emphasis will be placed on the need for collaboration between government, environmental agencies, industry and academic institutions.

Support from and collaboration with other relevant IUPAC Divisions and also UNESCO, IOCD and RAQAL are considered essential for the success of the conference.

For further information, please contact: Prof. Patrick Moyna, Facultad de Quimica, University of Montevideo, CP 11800 Montevideo, Uruguay. Tel.: +598 2 94 1884. Fax: +598 2 94 1906.

COSPAR scientific assembly

The 32nd COSPAR (Committee on Space Research established by the International Council of Scientific Unions) Scientific Assembly is scheduled to be held on 12–19 July 1998 in Nagoya, Japan. The programme is intended to cover around 80 meetings and symposia, on topics including:

- The Earth's surface, meteorology and climate
- The Earth–Moon system, planets and small bodies of the Solar System
- The upper atmospheres of the Earth and planets, including reference atmospheres
- Space plasmas in the Solar System, including planetary magnetospheres
- Research in Astrophysics



- Life sciences as related to space
- Materials sciences in space
- Fundamental physics in space
- Satellite dynamics
- Scientific ballooning
- Space born geophysical data for global change studies
- Science and engineering aspects for Solar System exploration

Abstracts are invited by 9 January 1998, and papers will be published in *Advances in Space Research*.

For more information, please contact: COSPAR Secretariat, 51 bd de Montmorency, 75016 Paris, France. Tel.: +33 1 45 25 06 79. Fax: +33 1 40 50 98 27. E-mail: COSPAR@paris7.jussieu.fr. Information is also available on the WWW at <http://www.mpae.gwdg.de/COSPAR/COSPAR.html>.

IFCC/Roche establish Human Genomics Conferences

The International Federation of Clinical Chemistry (IFCC), an Associated Organization of IUPAC, and Roche Diagnostics have agreed to establish a series of conferences 'Human Genomics: the Basis of the Medicine of Tomorrow'. They aim to highlight progress in molecular genetics and its potential in diagnosis and therapy. The first conference, entitled 'Recent Progress

in Molecular Biology Technology', is to be held in Singapore on 15–18 March 1998. This will focus on improved DNA diagnostics and define the role of the clinical chemistry laboratory of the future.

The organizers wish to bring together scientists specialized in the field of molecular diagnostics for discussion and preparation of recommendations for better clinical use of these new technologies. They also plan to offer interested clinical chemists a high level course in molecular diagnostics after the Conference.

For further information, please contact: Ursula Steeb, IFCC-Roche Conference Secretary, Roche Diagnostics, Bau 223/315, Postfach, CH-4070 Basel, Switzerland. Tel.: +41 61 6872516. Fax: +41 61 687 25 10. E-mail: Ursula.Steeb@Roche.com



'Dictionary of Substances' goes online

The *Dictionary of Substances and their Effects*, produced by the UK's Royal Society of Chemistry (RSC), is now available as an online file (file 307) on Dialog, an online service of Knight-Ridder Information Inc. The online file provides a pay-as-you-go access option, complementing the print and CD-ROM versions already available from the RSC. The dictionary is a specialist reference source of toxicological and environmental data on over 4000 chemicals, updated twice a year.

Names and Addresses

Full details (names, addresses, telephone/telex/Fax numbers and E-mail) of the officers of IUPAC bodies were published in *The IUPAC Handbook 1996–1997*. The IUPAC Secretariat has been notified of the following changes:

Dr David L. Berner (Secretary, Commission on Oils, Fats, and Derivatives), 10 East Pointe, Fairport, New York 14450, USA. Tel. and Fax: +1 (716) 223 9388.

E-mail: amberner@ix.netcom.com

Dr Patrick T. Holland (Secretary, Commission on Agrochemicals and the Environment), HortResearch, Private Bag 3123, Hamilton, New Zealand. Tel.: +64 (7) 838 5045. E-mail: hollandp@hort.cri.nz

Prof. Waldfried Plieth (Chairman, Commission on Electrochemistry), Inst. für Physikalische Chemie und Elektrochemie, Technische Universität Dresden, Mommsenstraße 13, D-01062 Dresden, FRG.

Prof. Rolf D. Schmid (Chairman, Commission on Biotechnology),
E-mail: itbrsc@po.uni-stuttgart.de

IUPAC colleagues deceased

UK: Prof. G. Gee (13 December 1996), Commission on Macromolecules (1953–1961, 1965–1969).

UK: Prof. M.L. McGlashan (18 July 1997), Interdivisional Committee on Nomenclature and Symbols (1969–1975), Physical Chemistry Division Committee (1969–1973), Commission on Physicochemical Symbols, Terminology and Units (1963–1979), Commission on Thermodynamics (1965–1969).

USA: Prof. C.G. Overberger (17 March 1997), Executive Committee/Bureau (1977–1985), CHEMRAWN Committee (1976–1986), President of Macromolecular Division (1977–1979), Macromolecular Division Committee (1967–1977), Commission on Polymer Characterization and Properties (1977–1980), Commission on Macromolecules (1965–1967).

New Publication

Molecular Electronics—a 'Chemistry for the 21st Century' monograph

The study of molecular electronics has an ambitious but realistic goal, the use of synthesis, assembly and miniaturization on the molecular level to achieve a huge diversity of devices: molecular wires, rectifiers, switches, transistors and memories. It foresees applications not only in standard electronics but also some unique to molecular systems, for instance sensors based on molecular recognition, and molecular interfaces with biological systems.

Molecular Electronics recognizes its subject as a multidisciplinary area of research, tracing its origins in both physics (with attempts to replicate on the molecular level devices from solid-state electronics) and biology (where nature has arrived at organic solutions for functions such as memory and photosensitivity). The book, co-edited by IUPAC Vice-President and President-Elect Prof. Joshua Jortner, provides an up-to-date set of authoritative overviews spanning molecular electronics and assessing its future directions.

The first chapter, written by the two co-editors, serves as an introduction, providing a review of some of the goals, concepts, problems, ideas, experiments and theoretical arsenal of molecular electronics. Included is a description of the different categories of devices that have been envisioned—molecular wires, switches, memory elements, electrodes, energy conversion, sensors, optics and optical switches, displays, electrochemical devices, heterostructure and quantum-well devices, information processing, diodes and rectifiers and intrinsically novel molecular devices. The authors relate them to standard solid state systems, and point out their possible uses in actual devices. Then follows a section devoted to the basic chemical physics



Prof. Joshua Jortner

underlying much of molecular electronics, including electron transfer, proton transfer, photo absorption, non-linear optics, descriptions of localization and relaxation, and the coupling of subcomponents. An example analysis based on molecular wires is also presented. The chapter concludes with a consideration of some of the intrinsic limitations and promise of the field of molecular electronics.

Fourteen further chapters, featuring contributors from around the world, deal with topics ranging from molecular control of electron and hole transfer processes to protein-based memories and processors.

Molecular Electronics—a 'Chemistry for the 21st Century' monograph. Edited by J. Jortner, School of Chemistry, Tel Aviv University, Ramat Aviv, Israel, and M. Ratner, Department of Chemistry, Northwestern University, Evanston, Illinois, USA. Published by Blackwell Science, Osney Mead, Oxford OX2 0EL, UK, 1997. 485 pp. + viii. ISBN 0 632 04284 2. Price: USD 125; GBP 75.

Conferences

1st International Conference on Trace Element Speciation in Biomedical, Nutritional and Environmental Sciences, GSF-Forschungszentrum, Neuherberg/München, Germany, 4–7 May 1998

IUPAC
SPONSORED

The conference, organized by the GSF National Re-

search Center for Environment and Health, aims to focus on the broad, new and sometimes diffuse activities relating to speciation and to create a forum for open discussions about very new and perhaps not fully established findings.

The main topics will be:

- Separation and hyphenated techniques
- Quality assurance and reference materials in

speciation analysis

- Speciation in the biomedical field
- Speciation in the environmental field
- Speciation in the nutritional field
- Speciation in occupational health
- Speciation and legislation

The conference programme will comprise three days of oral presentations, posters and extended time for discussion. Oral presentations (invited or submitted) will be 60 or 20 minutes in duration including discussion. Special poster discussions will be organized, where authors will have the possibility of presenting orally the highlights of their poster. Round table discussions will be organized on special topics (for which suggestions are welcomed). On the fourth day, four short courses will be offered: Separation methods using chromatographic techniques; Separation methods using CE techniques; Quality control in speciation analysis; and Sample preparation in speciation for different matrices and elements.

Abstracts of papers must be submitted in English (three copies) to the Chairman of the Organizing Committee by 31 October 1997.

The registration fee is DM 400 before 1 March 1998, DM 500 after 1 March 1998, for participants, and DM 200 for students. A one-day ticket is also available at DM 150. The conference dinner on 5 May is DM 100. The proceedings are DM 75. Each short course is DM 150. A combined ticket for the Speciation Conference and the 5th Conference on Metal Ions in Medicine and Biology (organized from 8 to 10 May at the GSF National Research Center in conjunction with the Hahn-Meitner Institute Berlin) is DM 800 before 1 March 1998, and DM 1000 after 1 March 1998. Members of IUPAC are entitled to a 10% reduction on the registration fee.

For further information on submission of a paper, please contact: First Speciation Conference, c/o Prof. Dr P. Schramel, GSF-Forschungszentrum, Inst. for Ecological Chemistry, Postfach 1129, D-85758 Oberschleissheim, Germany. Tel.: +49 89 31874062.

For further information on registration, please contact: First Speciation Conference, c/o Ulla Schrödel, GSF-Forschungszentrum, Congress Service, Postfach 1129, D-85758 Oberschleissheim, Germany. Tel.: +49 89 31873030/2669; Fax: +49 89 31873362.

Degradation Processes in the Environment, Dubrovnik (Cavtat), Croatia, 24–28 May 1998

IUPAC

SPONSORED

The aim of the conference is to discuss the state-of-the-art in our understanding of environmental degradation processes along the following topics:

- Atmospheric degradation processes
- Degradation processes in water and soil
- Degradation data: sources and quality
- Modelling degradation processes
- Application of research results in environmental management

In particular, attention will be paid to the kinetics and reaction mechanisms, assessment of availability and quality of degradation data, and qualitative and quantitative modelling of degradation processes. It is hoped that the conference will reach recommendations on data quality standards, estimation of degradation rates, and identify the major gaps in knowledge where future research is needed.

The registration fee is USD 200 before 1 February 1998 and USD 300 after 1 February 1998. The fee will include a book of abstracts, a get-together party, morning and afternoon tea or coffee and an excursion to the historic sites of Dubrovnik. Students will have a 50% discount on the fee.

For further information, please contact: Dr Aleksandar Sabljic, Ruder Boskovic Institute, PO Box 1016, HR-10001 Zagreb, Croatia. Tel.: +385 14561089. Fax: +385 1425497. E-mail: dpe@indigo.irb.hr.

Conference Calendar

1997

Electron transfer processes

3–7 September

International Symposium on Electron Transfer Processes and Reactive Intermediates in Macromolecular and Organic

Chemistry. Zabre, Poland.

Prof. Z.J. Jedlinski, Institute of Polymer Chemistry, Polish Academy of Sciences, ul. Marii Curie Skłodowskiej 34, 41-800 Zabrze, Poland. Tel.: +48 (32) 1716077; Fax: +48 (32) 1712969; E-mail: polymer@usctoux1.cto.us.edu.pl

Colloquium spectroscopicum internationale

21–26 September

30th Colloquium Spectroscopicum Internationale 1997. Melbourne, Australia.

The Meeting Planners, 108 Church Street, Hawthorn Victoria 3122,

Australia. Tel.: +61 (3) 98193700;
Fax: +61 (3) 98195978.

Emulsions

23–26 September

2nd World Congress on Emulsions: Industrial Applications of Emulsions. Bordeaux, France.

Mr A. Le Coroller, Directeur-Général, CME, 50 place Marcel Pagnol, 92100 Boulogne-Billancourt, France. Tel.: +33 (1) 47617689; Fax: +33 (1) 47617465.

Green chemistry

28–30 September

International Conference on Green Chemistry: Challenging Perspectives. Venice, Italy.

Conference Secretariat, Green Chemistry: Challenging Perspectives, Consorzio Interuniversitario Nazionale 'La Chimica per l'Ambiente', Facoltà di Scienze Matematiche, Fisiche e Naturali, Calle Larga S Marta 21.37, 30123 Venezia, Italy.

Visas

It is a condition of sponsorship that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all *bona fide* chemists from throughout the world to attend irrespective of race, religion, or political philosophy. IUPAC sponsorship implies that entry visas will be granted to all *bona fide* chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting the IUPAC Secretariat should be notified without delay by the applicant.

Macromolecule–metal complexes

6–10 October

7th International Symposium on Macromolecule-Metal Complexes (MMC-7). Noorwijkerhout, Netherlands.

Prof. J. Reedijk, Leiden Institute of Chemistry, PO Box 9502, 2300 RA Leiden, Netherlands. Tel.: +31 (71) 5274459. Fax: +31 (71) 5274451; E-mail: reedijk@rulgca.leidenuniv.nl

Biodiversity and bioresources

23–27 November

International Conference on Biodiversity and Bioresources—Conservation and Utilization. Phuket, Thailand.

IUPAC Biodiversity Conference, National Center for Genetic Engineering and Biotechnology, National Science and Technology Development Agency Building, 73/1 Rama VI Road, Bangkok 10400, Thailand. Tel.: +66 (2) 6448150-4, ext. 505, 532, 534; Fax: +66 (2) 6448107-8; E-mail: iupacconf@biotec.or.th

1998

Polymer sciences and technology

5–10 January

International Symposium on Advances of Polymer Sciences and Technology. Madras, India.

Dr K.S.V. Srinivasan, Deputy Director & Head, Polymer Division, Central Leather Institute, Council of Scientific & Industrial Research, Adyar, Madras - 600 020, India.

Calorimetry and chemical thermodynamics

5–9 April

International Conference on Calorimetry and Chemical Thermodynamics. Campinas, Brazil.

Prof. C. Airoidi, Instituto de

Química, UNICAMP - CP 6154, Universidade Estradal de Campinas, 13081-970 Campinas sp, Brazil.

<http://www.iqm.unicamp.br/wloh/conf/>

Trace element speciation

4–7 May

1st International Conference on Trace Element Speciation in Biomedical, Nutritional and Environmental Sciences. Neuherberg, Munich, Germany.

First Speciation Conference, c/o Ulla Schrödel, GSF-Forschungszentrum, Congress Service, Postfach 1129, D-85758 Oberschleissheim, FRG. Tel.: +49 (89) 31873030 (2669); Fax: +49 (89) 31873362.

Degradation processes in the environment

24–28 May

International Conference on Degradation Processes in the Environment. Dubrovnik, Croatia.

Dr A. Sabljic, Institute Boskovic, POB 1016, HR-10011 Zagreb, Croatia

Organic synthesis

28 June–2 July

12th International Conference on Organic Synthesis. Venice, Italy.

Depha Congress SRL, Viale Majno 21, 20122 Milano, Italy. Tel.: +39 (2) 76008190; Fax: +39 (2) 782400; E-mail: dephadue@mbox.vol.it

Chemistry in Africa

6–10 July

7th International Chemistry Conference in Africa (7th ICCA). Durban, South Africa.

The Secretary, 7th ICC & 34th SACI Convention, Department of Chemistry & Applied Chemistry, University of Natal, Durban 4041, South Africa. Tel.: +27 (31) 3603090. Fax: +27 (31) 2603091; E-mail: 7icca@che.und.ac.za

Macromolecules

13–17 July

37th International Conference on Macromolecules, Gold Coast, Australia.

Prof. R.G. Gilbert, School of Chemistry, F11, Sydney University Polymer Center, University of Sydney, New South Wales 20006, Australia. Tel.: +61 (2) 351 3366; Fax: +61 (2) 351 3329; E-mail: gilbert@chem.usyd.edu.au

20–23 July

18th Discussion Conference of Macromolecules: Mechanical Behaviour of Polymeric Materials. Prague, Czech Republic.

P.M.M. Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, CZ-162 06 Prague 6, Czech Republic. Tel.: +420 (2) 360341; Fax: +420 (2) 367981; E-mail: sympo@imc.cas.cz

Chemical thermodynamics

26 July–1 August

15th International Conference on Chemical Thermodynamics. Porto, Portugal.

Prof. M.A.V. Ribeiro da Silva, Department of Chemistry, Faculty of Science, Rua do Campo Alegre 687, P-4150 Porto, Portugal.

Pesticide chemistry

2–7 August

9th International Congress on Pesticide Chemistry. London, UK.

Dr John F. Gibson, Secretary (Scientific), Royal Society of Chemistry, Burlington House, London W1V 0BN. Tel.: +44 (171) 4378656; Fax: +44 (171) 7341227.

Novel aromatic compounds

2–7 August

9th International Symposium on Novel Aromatic Compounds, Hong Kong.

Prof. H.N.C. Wong, Chairman, Local Organizing Committee, 9th International Symposium on Novel Aromatic Compounds, Department of Chemistry, Chinese University of Hong Kong, Shatin, New Territories, Hong Kong.

Solubility phenomena

5–8 August

8th International Symposium on Solubility Phenomena. Niigata, Japan.

Prof. H. Akaiwa, Faculty of Engineering, Gunma University, Kiryu 376, Japan.

Chemical education

9–14 August

15th International Conference on Chemical Education: Chemistry and Global Environmental Change. Cairo, Egypt.

Prof. Saad S.M. Hassan, Department of Chemistry, Faculty of Science, Ain Shams University, Cairo, Egypt.

Physical organic chemistry

16–21 August

14th International Conference on Physical Organic Chemistry, Santa Catarina, Brazil.

Prof. E. Humeres, Universidade Federal de Santa Catarina, Departamento de Química, 88040-900 Florianópolis S.C. Brazil.

Coordination chemistry

30 August–4 September

33rd International Conference on Coordination Chemistry. Florence, Italy.

33rd ICC Secretariat, Department of Chemistry, University of Florence, Via Gino Capponi 7, 50121

Firenze, Italy. Tel.: +39 (55) 2757549. Fax: +39 (55) 2757555.

Medicinal chemistry

6–10 September

25th International Symposium on Medicinal Chemistry. Edinburgh, Scotland.

Dr John F. Gibson, Secretary (Scientific), Royal Society of Chemistry, Burlington House, London W1V 0BN. Tel.: +44 (0)171 437 8656; Fax: +44 (0)171 734 1227.

Natural products

11–16 October

21st IUPAC Symposium on the Chemistry of Natural Products. Beijing, China.

Prof. Xibai Qiu, Secretariat of ISCNP-21, c/o Chinese Chemical Society, PO Box 2709, Beijing 100080, China. Tel.: +86 (10) 62568157 or 62564020; Fax: +86 (10) 62568157; E-mail: qiuxb@infoc.3.icas.ac.cn

2000

Macromolecules

9–14 July

MACRO 2000: International Symposium on Macromolecules. Warsaw, Poland.

Prof. S. Penczek, Centrum Badan Molekularnych i Makromolekularnych, Polskiej Akademii Nauk, ul. Sienkiewicza 112, PL-90-363 Lodz, Poland. Tel.: +48 (42) 819815; Fax: +48 (42) 847126.

Biotechnology

3–8 September

11th International Biotechnology Symposium. Berlin, Germany.

Prof. G. Kreysa, DECHEMA e.V., PO Box 15 01 04, D-60061 Frankfurt am Main, Germany.