

Item 10: Report to Council: Division IV (Macromolecular)

I. Highlights

Projects

Prior to the implementation of the SDIC recommendations, the MMD comprised three Commissions, each of which had a number of Working Parties and projects. The Division has restructured to implement the SDIC recommendations, in a way that ensures continuity for appropriate aspects of the Division activities. The MMD Committee now has Coordinators for three generic areas in polymer science: *Nomenclature and Terminology*, *Characterization* and *Special Projects*. There are currently 40 projects. Since the last report to the Council (1999), there have been 11 publications either appeared or submitted. Three nomenclature reports have also appeared in translation, and two reports published in *Chemistry International*. In Nomenclature and Terminology, 2 projects are ready to be submitted for publication, and 3 are being prepared for IDCNS and public review; in Characterization, 2 projects are ready to be submitted for publication. Since the last report to the Council (1999), 7 projects have been completed and 1 abandoned. About one-third of the active members of current Task Groups are from industry, two-thirds from academia or research institutions. **This high proportion from industry represents a major financial support from industry to IUPAC activities:** although one cannot make any accurate quantification of the monetary value of this, a guesstimate is ~\$10⁵ per year. This is a real contribution, since these individuals' time costs their industry employers money. It is likely that a Division of Chemical Nomenclature will be established in the near future, and Division IV supports this initiative; at the same time, it is noted that macromolecular terminology does not fit properly under this rubric, and the Division will be applying to the Bureau for the creation of a new Commission in this area.

World Polymer Congress

This biennial conference is one of the prime activities of Division IV. The *Macro 2000* conference in this series was held in Warsaw. Delegates from 54 countries attended the meeting, with 1267 active participants, 17 plenary lectures, 84 section invited lectures and a large number of contributed papers, both verbal and poster. Two of the plenaries were by Nobel laureates (Jean-Marie Lehn and Sir Harry Kroto), and another was a masterful overview of future directions in industrial research by Joe Miller, Research Vice-President of DuPont. A special Plenary Lecture was reserved for a young scientist, which was awarded by an international panel to Dr Craig Hawker of the United States. There was also an excellent social program, which enabled delegates to exchange views in an informal atmosphere (including an International Youth Forum which the participating young scientists organized themselves, with some financial assistance from the IUPAC Macromolecular Division).

Improving project impact

In the area of nomenclature and terminology, the Division is making very serious efforts to increase usage of its output. This has started with an **Editors' Round Table** between members of nomenclature and terminology Task Groups and the editors of major polymer journals that was held at the Division Conference in Warsaw, July 2000; a summary of this is given as an Appendix. This led to a number of actions from both groups. (1) It was important for many editors to realize that IUPAC nomenclature does not mean something silly. For example, some editors had the impression that *polystyrene* and *poly(methyl methacrylate)* had to be given complex names, whereas in fact "polystyrene" and "poly(methyl methacrylate)" are acceptable IUPAC names. (2) It was realized by Task Group members that it is important for IUPAC rules to be readily available. We shall soon put highly simplified IUPAC rules onto our website, so that people can easily find and use a simple guide, without having to wade through a large amount of

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complex material. In addition, we are increasing our efforts to insure that the full rules are readily available on the IUPAC website, and can be easily searched. (3) The journal editors have agreed that what they will make explicit reference to this website material (when it becomes available) in their *Instructions To Authors* and *Instructions To Referees*. This will lead to much greater usage of the output from IUPAC Task Groups, to improved international communication, and to a higher profile for the Union. The Division is greatly appreciative of the excellence of the IUPAC website, and the excellence of its maintenance, by IUPAC headquarters. This planned increased profile would be impossible without this excellence, and again Dr Fabienne Meyers is to be congratulated. Another project is to convert the now out-of-print "Purple Book" (the IUPAC Compendium of Macromolecular Nomenclature) into electronic form. This has been achieved by using OCR (optical character recognition) which has enabled the material to be efficiently and accurately converted to a form which (a) can readily be put on the web, and (b) can readily be updated. This Division IV initiative is seen to be a method that can be widely used in other IUPAC endeavours.

Education

The Division has sponsored a number of education initiatives, particularly schools for graduate students from economically-developing countries, held in the Czech Republic and in South Africa.

Impact

Ensuring that the fruits of IUPAC labours are actually used by the international community is recognized as an important matter by the Division. One **critereon for retrospective evaluation** is that publications from certain projects are widely cited in the literature. We also recognize that citations are inadequate as evaluation criteria of nomenclature/ terminology projects, and see that counters on a web page, and visible adoption and/or recommendation by major journals, are also appropriate evaluation criteria. One of many examples of successful Division IV projects is afforded by that on polymerization kinetics (currently IV.2.8). This project has resulted in a series of 8 papers since 1988, which are highly cited in the literature (e.g. 151 citations for a 1995 report), always with the name of IUPAC associated with them. Probably the major reason for this success is that this international collaboration has produced results that are really needed by the international scientific community. Another important reason is that the Task Group is cohesive, and members enjoy working together. Personal contacts are essential, and often a good way of doing this is to create the project, and hold Task Group meetings, at IUPAC-sponsored conferences.

Managing the transition to a project-based system

Generally this transition has been smooth, and most (but not all) of current Task Group Leaders are now happy with the procedure and the way it is administered. There have been minor difficulties but these are seen as teething problems. For the majority of new projects, it was found that the new system involves very little extra work, and that this extra work is worthwhile. Part of the DP's and Coordinators' job is to help people submitting projects state outputs, milestones, outcomes and retrospective evaluation criteria. This requirement has meant that Task Group members are now very seriously thinking about means of increasing the impact of IUPAC projects on the international scientific community and about completing projects in a reasonable timeframe.

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II. Report of Division/Committee activities in 2000–2001.

These are listed under the IUPAC Goals (given in *italics*).

1. *IUPAC will serve as a scientific, international, non-governmental body in objectively addressing global issues involving the chemical sciences. Where appropriate, IUPAC will represent the interests of chemistry in governmental and non-governmental forums.*
 - Nomenclature and terminology activities
 - Report on polymer recycling
2. *IUPAC will provide tools and forums to assist international advances of research in the chemical sciences.*
 - World Polymer Congress
 - Many other conferences which are sponsored by IUPAC in which the Division is actively consulted and represented.
 - Activities in polymer characterization, including high level of citation.
3. *IUPAC will assist chemistry related industry in its contributions to sustainable development, wealth creation and improvement in the quality of life.*
 - The high proportion of Task-Group members from industry attests to the importance of Division activities to international industry.
4. *IUPAC will facilitate the development of effective channels of communication in the international chemistry community.*
 - Nomenclature and terminology activities
 - World Polymer Congress
5. *IUPAC will promote the service of chemistry to society in both developed and developing countries.*
 - Graduate Schools for postgraduate students from economically-developing countries
6. *IUPAC will utilize its global perspective to contribute toward the enhancement of education in chemistry and to advance the public understanding of chemistry and the scientific method.*
 - Graduate Schools for postgraduate students from economically-developing countries
7. *IUPAC will make special efforts to encourage the career development of young chemists.*
 - Special activities for young scientists at World Polymer Congresses (including prizes and forums).
8. *IUPAC will broaden the geographical base of the Union and ensure that its human capital is drawn from all segments of the world chemistry community.*
 - Graduate Schools for postgraduate students from economically-developing countries
 - Active promotion of the Union through opening addresses by Division IV representatives at international conferences.
9. *IUPAC will encourage worldwide dissemination of information about the activities of the Union.*
 - Publications in both printed and web form
 - Putting current and old (including out-of-print) material on the IUPAC website.

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- Production of highly-cited papers which bear the IUPAC imprimatur.
10. *IUPAC will assure sound management of its resources to provide maximum value for the funds invested in the Union.*
- All new projects have carefully planned and managed budgets.

III. Other substantive information

All this has been dealt with in the Highlights section.

IV. Tabular material.

Publications

- “Blends Containing Core Shell Impact Modifiers. Part 1: Structure and Tensile Deformation Mechanisms”, by C. B. Bucknall, submitted to PAC (2000)
- “Blends Containing Core Shell Impact Modifiers. Part 2: Melt Rheology of Rubber Toughened Plastics”, by M. Kozłowski and C. B. Bucknall, submitted to PAC (2000)
- “The Influence of Reprocessing on the Structure-Property Characterisation of a Plasticised PVC Compound”, by C. Dehennau and D. R. Moore, submitted to PAC (1999)
- “Manifestation of phase separation processes in oscillatory shear: droplet-matrix systems versus co-continuous morphologies”, by I. Vinckier and H. M. Laun, *Rheol. Acta* 38 (1999) 274-286
- “Manifestation of spinodal decomposition in oscillatory shear measurements” by I. Vinckier and H. M. Laun, *Macromol. Symp.* 149 (2000) 151-156. *Macromol. Chem. Phys.* 201, 1355-1364 (2000)
- "Rheology and morphology of phase-separating polymer blends", Z.I. Zhang, H.D. Zhang, Y.L. Yang, I. Vinckier and H.M. Laun, *Macromolecules* 34 (2001) 1416-1429.
- "Studies of biodegradable poly(hexano-6-lactone) fibres. II. Environmental degradation.", M. Mochizuki, K. Nakayama, R. Quian, B.-Z. Jiang, M. Hirami, T. Masuda, and A. Nakajima, *Pure Appl. Chem.* 71 (1999) 2177-2188.
- "Characterization of the flow behaviour, structure, and properties of thermotropic and polymer liquid crystals and aromatic polycondensates", J. L. White, L. Dong and P. Han, submitted to *Pure & Appl. Chem.* (2001).
- "Compatibility of poly(a-methylstyrene-co-acrylonitrile) with PMMA. A neutron and cloud point study", D. Schubert, *Mat. Res. Innovat.* 4 (2001) 353-359.
- "Critically evaluated rate coefficients for free-radical polymerization 3, Propagation rate coefficients for Alkyl Methacrylates", Beuermann, S.; Buback, M.; Davis, T. P.; Gilbert, R. G.; Hutchinson, R. A.; Kajiwara, A.; Klumperman, B.; Russell, G. T. *Macromol. Chem. Phys.* 2000, 201, 1355.
- Recommendations on “Recycling of Polymers” (Chairman: Dr. Norbert Bikales): *Macromol. Symp.* 135, 287-94 (1998)
- P. Kratochvil: UNESCO/IUPAC Postgraduate Course in Polymer Science. *Chem. Int.* 23, No. 1, p. 16 (2001)
- P. Kratochvil: 40th Microsymposium on Polymers in Medicine. *Chem. Int.* 23, No. 2, pp 48-49 (2001)

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Japanese translations:

"Source-based Nomenclature for Non-Linear Macromolecules and Macromolecular Assemblies"
Kobunshi 49 (2) 85 (2000)

"IUPAC Recommendations on Macromolecular Nomenclature" Kobunshi 49 (2) 92 (2000)

A Russian Translation of "Source-based Nomenclature for Non-Linear Macromolecules and Macromolecular Assemblies" has been submitted to Vysokomolec. Soed. and will be published in October 2000.

IUPAC- Round Table Discussion with Editors of Leading Journals in the Field of Polymers to Improve the Impact of IUPAC Recommendations.

Warsaw, July 10th 2000

It was generally agreed that there is a need for a commonly used nomenclature and terminology in science, and that the use of a common language in this sense should be encouraged. IUPAC Nomenclature Commissions are providing the corresponding information in their recommendations, published in *Pure & Applied Chemistry* and on the IUPAC web-site (<http://www.iupac.org/divisions/IV/IV.1/index.html>). This web-site contains many of the documents in full text, the most recent ones are already down-loadable.

Although there are journals (e. g.: *Helvetica Chimica Acta*) which demand the use of an accepted nomenclature, most of the editors argued that resources were not available to help this. Furthermore, some authors appear to understand IUPAC Recommendations as kind of a law which leads to a psychological barrier. The feeling appears to be rather strong that many authors do not like to "obey laws" set by any organization and that the authors should not be bothered more than necessary (they might switch to another journal). IUPAC members pointed out that the recommendations are to be understood as recommendations in the truest sense of the word, recommendations which have been published after long and intense discussions, reviewed by well-known (external) experts, and opened to public review. They are necessary for all scientists to speak in one unequivocal common scientific language. It is imperative that authors understand the importance of their use in publications and especially in textbooks so that the students become familiar with them as early as possible. The editors were invited to participate in meetings of the Nomenclature Commission of Division IV to experience its work and to give feedback.

It was agreed that the editors would recommend the use of IUPAC recommendations in their Instructions for Authors and that, especially those journals with electronic versions, promised to provide links to IUPAC web-sites. IUPAC will improve its web-site and accelerate the publication of the full documents in electronic version and give any support possible. Commission IV.1 has an ongoing discussion on how to make its recommendations more accessible and to provide more tools to develop a common scientific language (such as: a polymer dictionary, computer "searchable" documents, a comprehensive list of terms, abbreviations, commonly used names, assistance in solving of problems).

Short-term Action Items arising from the Warsaw Meeting

Web document which gives abbreviated instructions for macromolecular nomenclature. The URL address of this will be used by Editors in their *Instructions to Authors* and *Instructions to Referees*. An English-language, web-based version of the IUPAC recommendations (which are the same as CAS principles) for correct identification, orientation, and naming of CRUs/SRUs and other important aspects of macromolecular nomenclature. This will be a "do-it-yourself" mini-manual that gives readers step-by-step instructions for most polymers. Information will be included on where to go for help for difficult examples. This item has high priority.

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Participants

Editors

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* indicates that this member of Division IV is also an editor of an important journal.

Michael Hess, Chairman Commission IV.1; R G Gilbert, Division President

Current projects

COMMISSION ON MACROMOLECULAR NOMENCLATURE (IV.1)

410/18/87 - Basic Definitions of Terms Relating to Liquid Crystals

410/19/89 - Nomenclature of Regular Single-Strand Organic Polymers (Revised Edition)

410/21/93 - Source-Based Generic Nomenclature for Polymers

410/22/93 - Guide to Polymer Terminology and Nomenclature

410/24/93 - Terminology Related to Multi-Phase Polymer Composites and Blends

410/25/95 - Asymmetric Polymerization

410/26/95 - Kinetics and Thermodynamics of Polymerization

410/28/97 - Terminology and Structure-Based Nomenclature of Dendritic and Hyperbranched Macromolecules

410/29/97 - Terminology and Nomenclature of Macromolecules with Cyclic Structures

410/30/97 - Glossary of Polymer Chemical and Topological Class Names (revised title)

410/31/97 - Polymerization Processes and Polymers in Dispersed Systems

2000-006-1-400 - Terminology of Polymers with Ionizable Groups and Polymers Containing Ions

1999-051-1-400 - Source-Based Nomenclature for Modified Polymers

1999-048-1-400 - Definitions of Terms Relating to Reactions of Polymers and Functional Polymers

2000-007-1-400 - Glossary of terms relating to polymeric gels and networks, hybrid inorganic polymeric materials and the processing thereof (previous 410/27/95)

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COMMISSION ON POLYMER CHARACTERIZATION AND PROPERTIES (IV.2)

WORKING PARTY ON STRUCTURE AND PROPERTIES OF COMMERCIAL POLYMERS

421/15/86 - Melt Rheology and Concomitant Morphology in Polyblends and Polyalloys

421/28/89 - Structure-Property Relationship of Discontinuous Fibre Reinforced Plastics

421/29/91 - Rubber Toughening of Plastics

421/31/93 - Structure and Properties of Hydrogenated NBR

421/32/95 - Future Requirements in the Characterization of Continuous Fibre Reinforced Polymeric Composites

421/33/95 - Rheological and Mechanical Properties of PaMSAN/PMMA Blends in Miscible and Phase Separated Regimes of Various Morphologies

421/34/95 - Property Improvement via Interfacial Chemical Reaction - Reactive Extrusion of EVOH/SMA and Polyamide/MAH-EPR

421/35/97 - Effects of Side-Chain Branching on Processability of Commercial Polycarbonates

421/36/97 - Studies on Biodegradable Poly(epsilon-caprolactone)

1999-020-1-400 - Quantifying scratch resistance of commercial polymers

WORKING PARTY ON MOLECULAR CHARACTERIZATION OF COMMERCIAL POLYMERS

422/1/98 - Nomenclature of chromatography of polymers and related substances

422/2/98 - Characterization of polyelectrolytes in aqueous solution by GPC, light scattering, viscometry, ultracentrifuge or similar methods

422/3/98 - Size exclusion chromatography dispersion correction

422/4/98 - Precise determination of molecular weight distributions of polyolefins by high temperature size exclusion chromatography and hyphenated techniques

422/5/98 - SEC/GPC of polystyrenes

422/6/98 - Molecular characterization of polyamides 6, 11 and 12

COMMISSION ON FUNCTIONAL POLYMERS (IV.3)

1999-029-1-400 - Postgraduate course in polymer science

1999-024-1-400 - Polyaniline: Recommendations for Preparation of Conducting Polymer and its Colloidal Form

2000-001-1-400 - Critically Evaluated Propagation Rate Coefficients for Free-Radical Polymerizations of Methacrylic Acid Esters with Functional, Cyclic and Branched Ester Groups

1999-039-1-400 - Structure and Properties of Cyclic Olefin Copolymers

2000-005-1-400 - University Education in Polymer Science

2000-006-1-400 - Terminology of Polymers with Ionizable Groups and Polymers Containing Ions

1999-021-1-400 - Round Robin Test on the Molecular Characterization of Epoxy Resins by Liquid Chromatography

1999-051-1-400 - Source-Based Nomenclature for Modified Polymers

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2000-028-1-400 - Critically evaluated termination rate coefficients for free-radical polymerization. 1. Current status, evaluation of experimental methods, data for styrene and methyl methacrylate

Completed projects:

421/30/93 - The Influence of Reprocessing on the Structure-Property Characteristics of a Plasticized PVC Compound

401/1/93 - Recycling of Polymers

410/9/83 - Source-Based Nomenclature for Non-Linear Macromolecules and Macromolecular Assemblies (revised title)

410/23/93 - Definition of Terms Relating to the Non-Ultimate Mechanical Properties of Polymers

428/5/93 - Critically Evaluated Database of Kinetic Parameters for Free-Radical Polymerization

428/6/97 - Critically Evaluated Database of Kinetic Parameters for Free-Radical Polymerization -
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430/1/91 - Polymer Liquid Crystals (abandoned)

Robert G Gilbert (President, Division IV)