

# Report of the IUPAC Organic and Biomolecular Chemistry Division (III)

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## I. Executive Summary and Highlights

The Mission of Division of Organic and Biomolecular Chemistry is to promote the goals of IUPAC in the field of organic and biomolecular chemistry in the broadest sense. To this end the Division consists of a Division Committee and 6 Subcommittees. Together these promote the formulation and execution of Projects on relevant chemical problems, the staging of chemical conferences on important areas of chemistry, the education and professional development of chemists worldwide, the advancement of chemical industry, and the application of chemistry to meet the world's needs. The Division is committed to utilizing the talents of chemists from around the world in these activities, and promoting diversity in our membership.

The Division covers such a broad area of multidisciplinary aspects, and stimulates the fundamental and applied organic synthesis as the top edge science. It includes asymmetric synthesis of Natural products, Process chemistry with Molecular catalysts, and still explosively expanding Organometallic chemistry. Chemical biology or Post genomic chemistry is the key sciences for the biomolecules in this century, and it is also close to Biotechnology. Physical chemistry has been the fundamental mechanistic science, and it is also important in the spectroscopy and/or organic analysis. Photochemistry is of worldwide significance in the standardization for analytical chemistry as well. Green and sustainable chemistry are increasingly recognized as important environmental and limited organic materials from the global scale. The Division coordinates these subjects to be interdivisional activities as well as among the following Subcommittees.

*Subcommittee on Organic Synthesis (Chair: Frank McDonald, USA)*

*Subcommittee on Biomolecular Chemistry (Chair: Vadim Ivanov, Russia)*

*Subcommittee on Green Chemistry (Chair: Pietro Tundo, Italy)*

*Subcommittee on Photochemistry (Chair: Silvia Braslavsky)*

*Subcommittee on Structural and Mechanistic Chemistry (Chair: T. Marek Krygowski)*

*Subcommittee on Biotechnology (Chair: Romas Kazlauskas)*

The Subcommittees have been dealing with the IUPAC sponsored conferences in the various location of the world with quite success. Some of them are recognized as the conference series and planned long time in advance with adjusting the period of time and place for the similar conferences to be held.

The following report style is slightly different from the instruction, since the subcommittees are differently active to fit making this report for the six Goals in the current IUPAC Strategic Plan.

## II. An overall report of Division activities during 2004 and the first part of 2005

- a) *IUPAC will provide leadership as a worldwide scientific organization that objectively address global issues involving the chemical sciences.* Organic Synthesis Subcommittee has long time the tradition as the worldwide leadership in the synthetic chemistry communities; thus, asymmetric synthesis of natural products, new reactions catalyzed by organometallic compounds. In the Biomolecular Subcommittee, it is also recognized as the world leading level for the elucidation of the molecular structures in trace amount and/or complexity and/or biochemical mechanism. These have been indicated in the division-supported series of conferences as Organic Synthesis and Natural Product Chemistry.
- b) *IUPAC will facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion.* Photochemistry is a good example for the standardization since it has been widely applied to various kind of spectroscopy on the basis of physical chemistry such as NMR, Photoluminescence, and Chemical Actinometry. It should be noted that Photochemistry Subcommittee is in good collaboration with major photochemical societies in the world.
- c) *IUPAC will assist chemistry-related industry in its contribution to sustainable development wealth creation, and improvement in the quality of life.* Green Chemistry Subcommittee has contributed to this subject in worldwide starting from South East Asia, India, Arab region, Latin America, Russia, Africa in the strong connection with the economical growth and chemical industry activity.
- d) *IUPAC will foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.* Biomolecular Subcommittee has been achieving the Biodiversity project, which has been completed in the form of IUPAC recommendation (*Pure Appl. Chem.* 74, 697-702, **2002**). It was discussed in Thailand, Brazil, China, and Turkey before the recommendation. Further workshop was held in New Delhi in 2004 during the 4<sup>th</sup> IUPAC Conference on Biodiversity proposed for a Natural Product Center in Bangladesh.
- e) *IUPAC will utilize its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists and the public appreciation of chemistry.* IUPAC prizes have been awarded to young chemists in the ICOS meeting as well as Poster Prize to 3 presentators. Many conferences have similar award system to give presentation awards to young chemists.
- f) *IUPAC will broaden its national membership base and will seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender, and age.* The Division has been committed to these goals for some time, as witnessed by our current 31 members (11 TM, 6 AM, 12 NR, 2 PR), who are from 29 countries (Asia 8), (Europe 15), (North America 3), (South America 3),

and (Africa 2). Only 4 are female but we expect to increase this representation. We are always conscious of the need to recruit younger chemists, but recognize their carriers; In addition our Subcommittee include 73 additional individuals, many of them younger chemists.

## **SUBCOMMITTEES:**

### ***Subcommittee on Organic Synthesis***

Synthesis covers a central part of the organic chemistry spectrum and ethos. The mission of the Sub-committee on Organic Synthesis is to provide a focus for the dissemination of current knowledge and the development of future directions in all aspects of organic synthesis, including: 1) The development of new molecular transformations; 2) The development of new reagents; 3) The development of environmentally benign synthetic processes; 4) The synthesis of new types of organic structures; 5) The synthesis of target molecules for specific applications; 6) The total synthesis of natural products; 7) Combinatorial and high throughput techniques

IUPAC International Conference on Organic Synthesis (ICOS-15) was held in Nagoya, Japan from Aug. 2004, which was quite successful with nearly 1000 participants. IUPAC Prize was awarded to Prof. Hartwig, and next Prize nomination has just opened since June 20 by co-sponsor with Theme. It will be awarded in ICOS-16, which will be held in Merida, Yucatan, Mexico during June 11-15, 2006 by organizer Eusebio Juaristi. Further ICOS-17 was proposed to be held at Daejeon in Korea during Aug 17-23, 2008; ICOS-18 (2010) in Bergen, Norway; ICOS-19 (2012) in Taiwan.

Heterocyclic Chemistry (FHC-5) was held in Florida, USA in March 2004, and will be held in 2006.

Organometallic Chemistry (ICOMC-21) was held in Vancouver, Canada in July 2004.

There are 2 more conferences planned in 2005; thus, Heterocyclic Chemistry (IHC) in Palermo, Italy in July-Aug, and Organometallic Chemistry (OMCOS-13) in Geneva in July.

### ***Subcommittee on Biomolecular Chemistry***

The Subcommittee will seek to deliver the long-range goals of IUPAC, particularly within the vital interfacial area of molecular science that lies between organic chemistry and biology. It will support the application of the powerful methods of chemistry to current and emerging problems in biology to achieve understanding and, where appropriate, modification of the systems of living organisms at the molecular level. To that end, the Sub-Committee will provide a focus for the dissemination of current knowledge and the development of future directions in the following fields: 1) Structure, function and applications of biomolecules and their analogues; 2) Molecular mechanisms of biological processes and their modulation; 3) Molecular engineering via chemo-enzymatic processes; 4) Analysis, manipulation and application of biomolecular information systems. International Conference on the 4<sup>th</sup> Biodiversity and 24th Natural Products: Chemistry and Medical

Applications was held in New Delhi, India in January 2004 by organizer V. S. Parmar with ca. 1000 participants. A Satellite symposium on Bioresources toward drug discovery and development was held in Mauritius in Feb. 2004 (Org. Am. G. Fakim). The next joint symposia (5<sup>th</sup> and 25<sup>th</sup>) will be held in Kyoto, Japan (D. Uemura) in July 2006; (6<sup>th</sup> and 26<sup>th</sup>) will be held in Australia (Mary Garson).

The 7<sup>th</sup> International Symposium on Biomolecular Chemistry (ISBOC-7) was held at the University of Sheffield, UK in July 2004, which was masterminded by Professor Michael Blackburn in collaboration with the Royal Society of Chemistry. In the Subcommittee meeting in Sheffield, the proposal (# 2004-013-1) submitted by Prof. Mosihuzzaman was recommended to modify the organization of a Symposium in Print. Progress reports of the projects on Post-genomic chemistry (#2001-005-1-300) and Fighting microbial resistance through development of new antimicrobial agent, directed against new specific targets (#2002-030-1-300) was reported by Koomen. Next ISBOC-8 will be held in Florida in March 2007.

### ***Subcommittee on Photochemistry***

Implementation of the overall goals and objectives of IUPAC in the multidisciplinary area of photochemistry and its links to the photosciences (e. g., materials sciences, photobiology, photolithography, photography) can be accomplished only with the inputs of a broad spectrum of experts in the field, including those with ancillary interests in areas covered by all Divisions within IUPAC. 1) Renewable energy sources; 2) Green chemistry; 3) Atmospheric photochemistry; 4) New analytical methods in the biosciences including trace analysis of proteins, nucleic acids, and small bioregulators, both in vivo and in vitro; 5) Industrial photochemistry; 6) Advanced spectroscopic methods in ultra-fast time and ultra-small space resolution; 7) Methods for identifying material fatigue and temporal changes.

The Subcommittee works in close contact with the three major Photochemical Societies of the world, i. e., the Inter-American Photochemical Society, IAPS, The European Photochemical Association, EPA, and the Japanese Photochemical Association.

Miguel Miranda organized a meeting of the Sub-Committee on Photochemistry, plus colleagues participating in or chairing projects, during the XX-IUPAC Sponsored symposium of Photochemistry in Granada, Spain in July 2004. The 21 Symposium is planned to be held in Kyoto, Japan in April 2006 (Masahiro Irie).

Project on Chemical Actinometry (#2002-008-1-300) has been published in *Pure Appl. Chem.* 76, 2105-2146 (2004) by H. J. Kuhn etc. Reference methods, standards and applications of photoluminescence Project (#2004-021-1-300) was carried out (by interdivision ally with III, I and V) by Task group (Chair E. S. roman and F. Brouwer). This is an updating of the previous 2 relevant documents *PAC*, 60(7), 1107-1114 (1988), and *PAC*, 62(8), 1631-1648 (1990). The scope of this work is not only limited to the theoretical field in single molecule fluorescence, but also applicable to the material sciences and biology through fluorescence microscopy, etc.

### ***Subcommittee on Structural and Mechanistic Chemistry***

The Subcommittee should handle problems concerning the many aspects of structural and mechanistic organic chemistry. Specific examples include: 1) Environmentally friendly chemical processes and degradative pathways of organic contaminants; 2) Reactions in solution, gas phase, and solid state; 3) Solvents for organic reactions; 4) Acidity and basicity of organic compounds; 5) Supramolecular chemistry.

The 17<sup>th</sup> IUPAC Conference on Physical Organic Chemistry (ICPOC-17) was held in Shanghai, China in August 2004 (Guo Zhen Ji). The next ICPOC-18 is planned in Warsaw in Aug 2006; and ICPOC-19 will be in Santiago, Spain (Galicia) in 2008. Next group conference will be held in Essen, Germany in 2007 (Roland Boese). CAIC-10 was held in Bussan, Korea in August 2004 (Dae Dong Sung).

Subcommittee meeting in Shanghai approved the name of “Correlation Chemistry” to change to “Correlation and Modeling in Chemistry). This change aims at fostering research in all aspects of the modeling of the structure-property quantitative relationship (SPQR); thus, between structural variations and measurable properties as equilibrium constants, (enzyme catalyzed) reaction rates, etc.

### ***Subcommittee on Green Chemistry***

The aim of this Subcommittee is to develop actions devoted to the cause of green chemistry for its wider benefit to the future of chemistry and society as whole.

Activities are introduced in *Chemistry International*, Vo. 26, No. 2, March-April, 2004 by Pietro Tundo and Mohamed Tawfic Ahmed as follows. “Green Chemistry is an emerging field concerned with the safe practice of chemistry—a goal that people all over the world are interested in attaining. Green chemistry addresses some of our most precious values; human well-being, environmental sustainability, integrity, and safety, and the worldwide need for green chemistry practices should allow human development and property, along with environmental ethics. The IUPAC working party on Synthetic Pathways and Processes in Green Chemistry defined Green Chemistry (2000) as *The invention, design, and application of chemical products and processes to reduce or to eliminate the use and generation of hazardous substances.*

Projects of the Green (Sustainable) Chemistry are of south East Asian (#2002-028-1-300), IUPAC coordinated web page (#2002-029-1-300), in the Arab region (#2003-043-1-300), are still in progressing; and Green Chemistry in Russia (#2003-026-1-300) and in Latin America (#2002-064-1-300) have been completed. There has been a proposal for the translation and dissemination of a monograph for secondary schools on ‘Global Climate Change” by Tundo (#2005-015-1).

### ***Subcommittee on Biotechnology***

The International Biotechnology Symposium and Exhibition (IBS-12) was held in Oct. 2004 in Santiago, Chile

(J. A. Asenjo). The program included 10 sections with newer areas of Molecular tools, Cellular tools, Genomic tools, applied genome research, Cultivation technology, downstream processing, Biocatalysis, Health care, Plant and food biotechnology, and Environmental Biotechnology.

### **III. Any other substantive information**

Budget of Division III for 2004-2005 is allocated to the 6 Subcommittees in part, and the rest are available for projects. Further funding is available for good proposals. The generation of new projects remains the most urgent business of the Division.

Many potential proposals have been discussed among the subcommittee meetings to generate most important and timely projects.

### **IV. Tabular material**

List of publications

#### **Current Projects**

2000-012-1-300 - Single molecule spectroscopy\*

2001-005-1-300 - Post-genomic chemistry\*

2001-018-1-300 - Space- and time-resolved fluorescence spectroscopy and photochemistry

2001-020-1-300 - Glossary of terms and basic protocols used in photodynamic therapy

2001-036-1-300 - Glossary of terms in photocatalysis and radiation catalysis\*

2002-024-1-300 - Glossary of terms used in photochemistry (3rd version)\*

2002-028-1-300 - South East Asian, and neighbouring countries, Green Chemistry Network

2002-029-1-300 - A IUPAC coordinated web page on Green/Sustainable Chemistry

2002-030-1-300 - Fighting microbial resistance through development of new antimicrobial agents, directed against new specific targets

2003-043-1-300 - Green chemistry in the Arab region

2003-046-1-300 - Workshop for formulation of plans for the establishment of a "Center of Natural Products Research (CNPR)"

2004-021-1-300 - Reference methods, standards and applications of photoluminescence\*

\* Interdivisional project

#### **OTHER INTERDIVISIONAL PROJECTS**

2001-014-1-800- Fullerene nomenclature - part II

2001-031-1-800 - Alignment of nomenclature in areas of overlap between the preferred names for

organic nomenclature and the revision of the nomenclature of inorganic chemistry

2001-043-1-800 - Preferred names in the nomenclature of organic compounds

2002-010-1-050 - Toward a core organic chemistry curriculum for Latin American universities

2003-006-1-100 - NMR chemical shifts: updated conventions

#### PROJECTS NEAR COMPLETION / IN PRESS

301/1/93 - Development of guidelines for the transmission of information on organic synthesis  
(Abbreviation guidelines and glossary of terms for protecting groups in synthesis)

#### Recently Completed

2003-026-1-300 - Green chemistry in Russia

2002-064-1-300 - Green Chemistry in Latin America

2002-008-1-300 - Chemical actinometry

#### Representation on other IUPAC Bodies

*Committee on Chemical Education (CCE)* M. Fatima d. G. F. da Silva.

*Interdivisional Committee on Nomenclature, Terms, and Symbols (ITCNS)* Gerrit Koomen.

*Subcommittee on Materials Chemistry* Shunichi Fukuzumi and Istvan Horvath.

*Division VIII Nomenclature* Warren Powell.

#### Recent Reports from ORGANIC AND BIOMOLECULAR CHEMISTRY DIVISION (III)

Chemical actinometry (IUPAC Technical Report)

*Pure Appl. Chem.* **76**(12), 2105-2146 (2004)

Phane nomenclature. Part II. Modification of the degree of hydrogenation and substitution derivatives of phane parent hydrides (IUPAC Recommendations 2002) (III)

*Pure Appl. Chem.* **74**(5), 809-834 (2002)

Molecular basis of biodiversity, conservation, and sustained innovative utilization

*Pure Appl. Chem.* **74**(4), 697-702 (2002)

Nomenclature for the C<sub>60</sub>-I<sub>h</sub> and C<sub>70</sub>-D<sub>5h</sub>(6) fullerenes (IUPAC Recommendations 2002) (III.1)

*Pure Appl. Chem.* **74**(4), 629-695 (2002)

Critical evaluation of proven chemical weapon destruction technologies

*Pure Appl. Chem.* **74**(2), 187-316 (2002)

Organic photochromism (IUPAC Technical Report) (III.3)

*Pure Appl. Chem.* **73**(4), 639-665 (2001)

Figures-of-merit for the technical development and application of advanced oxidation technologies for both electric- and solar-driven systems (IUPAC Technical Report) (III.3)

*Pure Appl. Chem.* **73**(4), 627-637 (2001)

Synthetic Pathways and Processes in Green Chemistry. Introductory Overview (III.2)

*Pure Appl. Chem.* **72**(7), 1207-1228 (2000)

That is the *Introductory Overview* to the PAC special topic issue on Green Chemistry.

Revised Section F: Natural products and related compounds (III.1)

*Pure Appl. Chem.* **71**(4), 587-643 (1999)

+ Errata, *Pure Appl. Chem.* **76**(6), 1283-1292 (2004)