

Meeting reports

ComTox. Commission on Toxicology (VII.4)

Unconfirmed Minutes of the Commission Meeting. Geneva, IUPAC General Assembly. 23–26 August 1997.

Minutes prepared by: Birger Heinzow and Rita Cornelis.
Dr John Duffus reported about the International Semi-

nar on Assessment of Carcinogenic Risk from Occupational Exposure to Inorganic Substances, Luxembourg, 17–20 October 1995. The publication of the proceedings is now being organized by the Royal Society of Chemistry and will be published later this year.

Recommendations for the biological monitoring of VOCs

Coordinators: Drs Jakubowski, Regine Heinrich-Ramm

and Heinzow.

A revised and shortened draft, prepared by Dr Heinrich-Ramm and Dr Heinzow, was presented and discussed within the working party. As the outcome of the fruitful discussion, specific tasks were assigned and will be sent to Dr Heinrich-Ramm by the end of September.

A further meeting was regarded as necessary for the final discussion. It was proposed that the meeting of the members of the working party be on 21–23 November 1997. Funding was requested from the Division. (Participants: Drs Aitio, Jakubowski, Molin Christensen, Heinzow, Olsen and Heinrich-Ramm).

Calculation and application of coverage intervals for biological reference values

The manuscript prepared by O.E. Poulsen, E. Holst, J.M. Christensen has been published in PAC as a technical report (*Pure Appl. Chem.* 1997, **69**, 1601-1611). A computer program will be made available by Dr Christensen upon request.

Decision rules in compliance testing for implementation of exposure limits

Coordinator: Dr J.M. Christensen and E. Olsen

A revised version focusing on human health was circulated by Dr Christensen. Additional input was obtained from the ISO. The project will be completed by 1999.

Risk assessment group

Working group: Drs Duffus, J.M. Christensen, E. Olsen and R. Herber

A first meeting of the exploratory working party was held in Amsterdam in 1996 and in 1997 in Stockholm. The problems of terminology were discussed.

Dr Duffus has prepared a first draft for teaching risk assessment. The project will mainly focus on the occupational environment and will be prepared as educational material.

Dr Duffus proposed as an additional project: risk assessment for inhalation of particulate matter (especially for metal). International input for the working party (e.g.) Fraunhofer Inst. Hannover (D) will be established.

The Commission recommended these proposals to become projects for the next two year. Cooperation with ICPS will be sought and was welcomed by Dr Mercier, director of IPCS.

Recommendations for exposure assessment using a logbook method.

Coordinator: E. Olsen

Erik Olsen reported that the logbook project will be based on papers circulated previously. He gave a report on the basic methodology. Dr Rappaport is a co-worker. The paper will be revised soon.

Combined effects of drugs and toxic agents. Recommendations for study design, methods, evaluation and nomenclature.

Coordinators: Drs G. Poech and B. Heinzow

Dr Heinzow outlined the status of the project. A first draft has been presented by Dr Poech. The approach to use dose–response curves as the basis for a description of combined effects was supported. Examples should be given, a software package is available by Dr Poech. The project will be completed within the next two years.

A new project presented by O. Hertel (DK): Modelling of human exposure to outdoor air pollution, was accepted by the commission. It was recommended to include practical examples. A computer program will possibly be made available for use of exposure assessment. This activity was received with great interest also by Dr Mecier (IPCS). Co-operation with Division VI (Chemistry and the Environment), Commission on Atmospheric Chemistry, was established.

Cooperation within IUPAC

Analytical Chemistry Division, Commission on Microchemical Techniques and Trace Analysis, Division VI, Chemistry and the Environment, Commission on Fundamental Environmental Chemistry, and Division VII Chemistry and Human health, Commission on Toxicology.

Dr Cornelis and Dr Templeton represented ComTox. Working definitions on speciation were agreed upon and distributed. A manuscript: 'Terms related to speciation of trace elements' following the results of the discussion in Guildford and Ispra is under preparation.

A document co-ordinated by Dr Cornelis should be ready by November

Future co-operation on the project: 'Speciation analysis of biomolecules by hyphenated techniques' is planned with V.C2. Co-ordinator is Dr Ryszard Lobinski.

Future co-operation with CTC may focus on educational programs on toxicology for chemistry students and for school teachers

It was recommended that an abbreviated version of the textbook on Toxicology be prepared and a curriculum for a training course for chemists and chemistry school teachers on Toxicology be developed. It was recommended that questions and answers put forward most often to school teachers by students and the public be included.

Project: Abbreviated textbook: 'Introduction to toxicology'

Coordinator: Dr Duffus and Dr Worth; B. Heinzow, R. Herber, J. M. Christensen, D. Templeton. Co-operation will be sought with WHO.

Committee on Quantities and Units

The manuscript: 'Properties and Units in the clinical laboratory sciences, XI. Properties and Units in Trace Elements', by Rita Cornelis, X. Fuentes, I. Brunshuis and D. Templeton was finalised and will be published in *PAC, Clin. Chim. Acta* and *Eur. J. Clin. Chem. Clin. Biochem.*

A new project: 'Metrological nomenclature in toxicology' will be co-ordinated by Drs X. Fuentes, R. Cornelis and J. M. Christensen.

Co-operation and exchange of expertise will continue

Contacts were established to the Chemistry and the Environment Division, Commission on Food Chemistry. Possible projects and future topics were presented by Dr Elke Anklam, M. Miraglia and C. Brera.

As a possible joint project: 'Review of endocrine disruptors in foodstuff and its health implications' was agreed. This project might also become part of the planned White Book on Endocrine Disruptors. This matter will be discussed within the Divisions, whether to include the project as a chapter in the white book or to initiate a separate project.

A discussion on metals in food was initiated and Dr Templeton will contact Dr Szeke (PL).

Cooperation with other scientific bodies

Cooperation with WHO and IPCS on risk assessment will continue and be intensified. It was recommended that Dr Cornelis be nominated as liaison to IPCS. Dr Mercier attended the Commission meeting and gave an overview of IPCS activities. The input by ComTox was very much welcomed and the discussion for a training course on toxicology will be further explored.

Next meeting of the commission

The next venue will be in Edinburgh in September 1998. Dr Duffus will be the local organizer.

Summary of the minutes of the meeting of the Commission on Molecular Structure and Spectroscopy (I.5) at the IUPAC General Assembly, Geneva, Switzerland 24–27 August 1997

Fifteen members of the Commission on Molecular Structure and Spectroscopy (I.5), including national

representatives and observers, met for three days of hard work during the 39th General Assembly in Geneva, Switzerland, with little time for admiring the beautiful setting on the Lac Lemman and the famous Geneva fountain. Three new Titular Members, Robin S. McDowell, Noboru Hirota and James E. Boggs, and three Associate Members, Soji Tsuchiya, Qing-Shi Zhu and Paul von Rague Schleyer were elected to the Commission. Four new national Representatives were appointed, Profs P.T. Manoharan (India), J.P. Hawranek (Poland), B.J. Van der Veken (Belgium), and R. Janoschek (Austria).

Several projects were completed and the results published in *Pure Appl. Chem.* (PAC): C.L. Wilkins, *Guidelines on Nuclear Magnetic Resonance Computerized Databases*, PAC 1995, **67**, 593; A.M. Bradshaw and N.V. Richardson, *Symmetry, Selection Rules and Nomenclature in Surface Spectroscopy*, PAC 1996, **68**, 457; G. Guelachvili and 23 collaborators., *High Resolution Wavenumber Standards for the Infrared*, PAC 1996, **68**, 193, and this paper was also reprinted in *J. Molec. Spectrosc.* 1996, **177**, 164 and *Spectrochim. Acta* 1996, **52**, 717; C.J.H. Schutte, J.E. Bertie, P.R. Bunker, J.T. Hougen, I.M. Mills, J.K.G. Watson and B.P. Winnewisser, *Notations and Conventions in Molecular Spectroscopy part 1. General Spectroscopic Notation*, PAC 1997, **69**, 1633; C.J.H. Schutte, J.E. Bertie, P.R. Bunker, J.T. Hougen, I.M. Mills, J.K.G. Watson and B.P. Winnewisser, *Notations and Conventions in Molecular Spectroscopy part 2. Symmetry Notation*, PAC 1997, **69**, 164; P.R. Bunker, C.J.H. Schutte, J.T. Hougen, I.M. Mills, J.K.G. Watson and B.P. Winnewisser, *Notations and Conventions in Molecular Spectroscopy part 3. Permutation and Permutation-Inversion Symmetry Notation*, PAC 1997, **69**, 1651.

The following book has been published: J.E. Bertie, C.D. Keefe and R.N. Jones, *Tables of Intensities for the Calibration of Infrared Spectroscopic Measurements in the Liquid Phase*, 263 pp., Blackwell, 1995. A joint article from Commissions I.5 and V.4 describing the work in the two commissions has been published in *Applied Spectroscopy* 1996, **50**, 12A: J.E. Bertie and T. Vo-Dinh, *Spectroscopy Commissions of the International Union of Pure and Applied Chemistry*.

Other articles were, in press or the projects were very close to completion: R.K. Harris, J. Kowalewski and S. Cabral de Menezes, *Parameters and Symbols for Use in Nuclear Magnetic Resonance*, PAC, in press; E.D. Becker, W. Bremser, S. Cabral de Menezes, R. Goodfellow, P. Granger and R.K. Harris, *Recommendations for NMR Nomenclature A. Nuclear Spin Properties and Conventions for Chemical Shifts*; and J.E. Bertie, *Specification of Components, Methods and Parameters in Fourier Transform Spectroscopy by Michelson and Related Interferometers*. The latter paper has been divided into one part for modest resolution spectroscopy

(0.1 cm^{-1} or less) and one for high resolution spectroscopy (10^{-3} cm^{-1} or better). In addition, a part pertaining to FT-Raman spectroscopy is included. The following manuscript of a book was approved in Geneva: E. Hirota, R.W. Field, J.P. Maier and S. Tsuchiya, editors, *Non-linear Spectroscopy for Molecular Structure Determination*. It constitutes a monograph of 268 pages and 10 chapters, probably suitable both for teaching and as a reference book to nonlinear spectroscopy. The book will be published by Blackwell early in 1998.

Projects from the Sub-Committee on Theoretical Chemistry are in progress: *Guidelines for Presentation of Methodological Choices in the Publication of Computational Results, A. ab initio Electronic Structure Calculations* (Project leader J.E. Boggs). The paper was approved by the Commission for immediate publication. A draft for semiempirical calculations is in progress (part B) and should be completed in two years. A third paper (part C) is planned to deal with computation of large molecules by molecular mechanics. An extensive report comprising 194 compounds was presented to the Commission for discussion and suggestion: R. Janoschek, *The Quantum Chemical Computation of Structures and Properties of Small Experimentally Known Molecules I. Diatomic Molecules for H-Ar*. It was agreed that the project would be completed following consultations with an international group of specialists.

Various new projects were initiated: *Notations and Conventions in Molecular Spectroscopy. Part 4. Vibrational-Rotational Spectroscopy* (Project leaders R.S. McDowell and J.K.G. Watson); *Notations and Conventions in Molecular Spectroscopy. Part 5. Electronic-Vibrational-Rotational Spectroscopy* (Project leaders J.K.G. Watson and R.S. McDowell). The Commission approved both these projects. Another proposed project was also approved: *Quantities, Terminology and Symbols in Photothermal and Related Spectroscopies* (Project leaders N. Hirota and M. Terazima); these methods are very sensitive and of increasing importance in applied science. R.K. Harris successfully sought approval-in-principle for a project to recommend *Nomenclature for tensor quantities used in NMR, NQR and ESR Spectroscopies* (Project leader R.K. Harris); formal IUPAC approval for this project will be sought when the working party members have been recruited and the goals have been more precisely formulated.

Joint meetings were held between Commission I.5 and three other commissions: Commission V.4 (Commission on Spectrochemical and Other Optical Procedures for Analysis) of the Analytical Division; Commission I.3 (Commission on Electrochemistry) and Commission I.1 (Physicochemical Symbols, Terminology and Units). With each of these commissions various projects of common interests were discussed. These

joint meetings are very important to avoid overlap between projects of different commissions and to provide stimulation for joint projects of greater breadth than is usually achieved by a single commission. In particular, the meetings in Geneva gave good ideas to both parties about new proposals and cooperation on existing projects. With Commission I.1 it was agreed on additions and alterations which should be included in the next edition of The Green Book (Quantities, Units and Symbols in Physical Chemistry).

Theoretical chemistry plays an ever increasing role in chemistry and the Subcommittee on Theoretical Chemistry; which was established at the General Assembly in Guildford, continues with its chairman Professor James E. Boggs. The subcommittee is strengthened with five new members. The Subcommittee on Notations and Conventions for Molecular Spectroscopy has a new chairman Dr J.K.G. Watson, and Dr Robin S. McDowell and Professor Jean-Marie Flaud will join the subcommittee.

The commission discussed the use of the World-wide Web and it was suggested that a Home Page be established. However, no decision was made concerning the content and who should be responsible for the Web site.

The chairman, John E. Bertie, expressed his thanks to the outgoing members for their contributions to the work of Commission I.5 and looked forward seeing the members at the next IUPAC General Assembly to be held in Berlin in August 1999.

Peter Klæboe
(Secretary of Commission I.5)

Latin American Workshop on Mycotoxins—methods of analysis

Food Chemistry Commission WPAC project: 650/88/96 (Working Group: Mycotoxins)

Coordinator(s): M. Sabino (local), J. Gilbert, E. Sydenham and H. van Egmond

This workshop was held in São Paulo (Brazil) at the Instituto Adolfo Lutz, from 18 to 22 November 1996. Dr Myma Sabino was responsible for the local organization. The workshop was sponsored by ILSI Brazil, FAPESP, Instituto Adolfo Lutz and IUPAC. Additional funding was provided by industry. Eighty participants from four South American countries attended the workshop.

The workshop was aimed at providing training through a series of lectures from invited experts and through open discussion sessions covering methods of analysis for aflatoxins, ochratoxin A, zearalenone, patulin, trichothecenes and fissionisins. There were also a number of presentations on activities in the field of mycotoxins by participants from South America.

The workshop was evaluated by participants and

judged to have been successful and contributing strongly to spreading the IUPAC mission in the region. The success of this Workshop encouraged the organizers to bid to host the Xth IUPAC Symposium on Mycotoxins and Phycotoxins. The bid was successful, the conference will be held in São Paulo, Brazil, 22–25 May 2000.

IUPAC CNOC—1997 Meeting—Summary

As part of the IUPAC 1997 General Assembly, the IUPAC Commission on Nomenclature of Organic Chemistry (Commission III.1—CNOC) met in Geneva, Switzerland for three full days, 24–26 August. Twenty-four people participated in some or all of the sessions. Most of the working time was spent on the P-names document, which was completed, except for editing, and adopted by the Commission. Other documents requiring only minor editing, at most, before submission to IDCNS or public review include:

- Phane Nomenclature. Part 1: Parent Hydride Names, Recommendations 1997. (Prepared for publication by W. H. Powell; O. Weissbach, coordinator.)
- Extension and Revision of the von Baeyer System for Naming Polycyclic Compounds (Including Bicyclic Compounds). (Prepared for publication by G. P. Moss.)
- Extension and Revision of the Nomenclature for Spiro Compounds. (Prepared for publication by G.P. Moss.)

Recommendations on fusion nomenclature [Nomenclature of Fused Ring and Bridged Fused Ring Sys-

tems, (Prepared for publication by G. P. Moss)] are scheduled for publication in *Pure and Applied Chemistry* in January 1998.

The Commission has now completed full review of points left pending in the *Guide*: namely, phane nomenclature (part 1), hydro/dehydro prefixes, and priority among classes of compounds. New substantive decisions on principles for the P-names document include:

- (a) Seniority order for rings and ring systems.
- (b) Seniority order for chains. This order includes <a> replacement names and a major change pertaining to compounds containing multiple carbon–carbon bonds. The longest continuous chain, with or without the multiple-bond linkage, is the parent chain.
- (c) Alkyl vs. alkanyl style names. *Alkyl* will be used when the free valence (or point of attachment) is at a terminal position of the longest chain; *alkanyl* (with locant) will be used when the free valence (or point of attachment) is at a non-terminal position on the longest chain.
- (d) Deletion of several previously retained (non-systematic) names, including isobutyl, sec-butyl, and phosgene.

No substantive decisions remain to be made by the Commission on any of its current projects, only editing of the documents before submission to IDCNS. For the next biennium, the Commission expects to work on four new projects:

- 1 Fullerene nomenclature
- 2 Stereochemistry: concepts, terms, notation.
- 3 Phane nomenclature, part II
- 4 Seniority based on CIP priorities

Prepared by James G. Traynarn, Secretary, CNOC



Meeting of the Commission on Physical Organic Chemistry in Geneva. From left to right: *Standing*—Prof. J.-L. Abboud, Prof. E. Humeres, Prof. E. Baciocchi, Dr J. R. Zdysiewicz, Prof. M. Tisler, Prof. S. Fukuwmi, Dr D. J. Raber, Prof. T. T. Tidwell, Prof. U. Sieffi, Prof. J. Shorter, Prof. S. S. Kim, Prof. R. Louw, Prof. V. I. Minkin, Prof. C. L. Perrin, Prof. P. Muller, Prof. Z. Rappoport; *Sitting*—Prof. P. Tundo, Prof. N. Nudelman, Prof. D. Lenoir, Prof. U. G. Edlund, Prof. M.-K. Ruasse, Prof. M. Oki, Prof. Y. Takeuchi.

Summary minutes of the meeting of the Commission on Physical Organic Chemistry (III.2), Geneva (Switzerland), 24–26 August 1997

The largest part of the meeting was devoted to the review of the status of the current projects as well as to the discussion of new projects. The Commission was pleased to find that the project *Critical Compilation of Scales of Medium Effects* can be considered finished and the project *Guidelines for Publication of Research Results from Empirical Force Field* is very close to the conclusion. The projects *Glossary of Terms Used in Theoretical Organic Chemistry* and *Glossary of Terms Used in Supramolecular Chemistry* are also well under way and their completion is expected within the next year.

Two new projects related to the environment were also discussed and approved. The first project *Reaction Pathways and Processes in Green Chemistry* was presented by Professor Tundo, the second, *Evaluation of Methods for Obtaining Physicochemical Properties of Environmentally Important Organic Compounds* by Professor Lenoir. Both projects are expected to be complete in two years. A feasibility study for a project concerning Gas-phase and Solution Data of Carbocations will be carried out by Professor Abboud. Continuing interest was shown for projects related to

materials and education. A project on biomolecular mechanisms is also under consideration.

A joint meeting with the Commission of Photochemistry (III.3) was held on 25 August. In this meeting information was exchanged on the ongoing and future projects of the two Commissions. The possibility of a joint project was also considered.

Profound changes in the Commission Membership were recorded. Professor Tidwell will leave the Commission, having been nominated Secretary of the Organic Chemistry Division Committee. From January 1st, 1998, Professor C. Perrin will be the new Chairperson of the Commission. Professors Abboud and Ruasse were proposed as Titular Members of the Commission to replace Professors Shorter and Takeuchi (completed term of service). Professors Tundo and Lenoir were proposed as Associate Members.

Before concluding its work, the Commission wished to express the most grateful thanks to Professor Tidwell for his very efficient chairmanship and to Professors Shorter and Takeuchi for their numerous effective contribution to the Commission activity.

The next series of meetings of the Commission will be held in Florianópolis (Brazil) in the occasion of the 14th IUPAC Conference on Physical Organic Chemistry (16–21 August 1998).

Prof. T. T. Tidwell (Chair) and Prof E. Baciocchi (Secretary)