

IUPAC Commission on Physical Organic Chemistry

Newsletter 1994

Introduction

A short history of Commission III.2 was outlined in the 1993 Newsletter, as published in *Chem. Int.*, 1993, 2, 65. Only the developments since that time are considered here.

Recent publications

A major work of the Commission to appear this year is the Glossary,¹ which was prepared for publication by Paul Müller, Chairman of the Commission from 1986–93, with a working party of P. N. I. Ahlberg, M. P. Doyle, W. Drenth, E. A. Halevi, R. A. Y. Jones, J. M. McBride, V. Minkin, M. Ōki, Y. Takeuchi and J. R. Zdysiewicz, and contributions from many others. This work is a major revision of the first Glossary, published in 1983.²

A critical compilation of sigma constants has been prepared for publication as a Technical Report by John Shorter, with the assistance of a working party including Y. Takeuchi (Joint Chairman), M. Charton, O. Exner, C. Hansch, Z. Rappoport, R. D. Topsom and P. Van Brandt.³

Current projects

Glossary of class names for organic compounds and reactive intermediates based on structure

(Joint project with Commission III.1 on Organic Nomenclature)

This compilation recommends terms to denote classes of compounds, substituent groups and reactive intermediates, as contrasted to individual compounds. Such terms are widely in use, but their status of definition varies considerably. The document provides definitions of approved terms, introduces a few new ones, and recommends discontinuation of a selection of terms actually in use.

Commission III.2 originally intended to prepare, as part of the revision of the 'Glossary', a document on class names of reactive intermediates. In parallel, Commission III.1 was working on class names of organic compounds. As the work progressed, we realized that it was impossible to achieve complete and consistent documents and to avoid overlap by working in parallel, and the projects were merged. The final draft is now under external review.

Basic terminology of stereochemistry

(Joint project with Commissions II.2, III.1 and IV.1)

This project, initiated by the late Victor Gold, former Chairman of Commission III.2, provides definitions for a selection of terms in stereochemistry which are in general use (or misuse). The progress of the work was greatly delayed due to the untimely death of its initiator. At that moment, the Divisional Committee decided to transfer the responsibility for the project to Commission III.1, and Professor G. Moss agreed to act as convenor of a working party. There is still much controversy on some basic issues in stereochemistry, but it is hoped that the working party will come to a consensus and publish its final report within a year or two.

Structure–reactivity parameters and relationships

This is a critical compilation of experimental data used in correlation analysis and quantitative structure–activity relationships (QSAR), widely applied in medicinal chemistry. It will provide researchers with a means to obtain with confidence the appropriate substituent constants for the analysis of their data and the appropriate mathematical tool for correct execution and interpretation. The project was initiated in 1989 and involves many specialists who are not members of the commission.

New project proposals presented to the division during the general assembly in Lisbon, August 1993

Compilation and critical evaluation of structure–reactivity relationships. Part 2. Extension of the Hammett σ scale through pK_a measurements of substituted benzoic acids in aqueous organic solvents

This project is an extension of the completed Part 1 and is to be carried out by the same working party.

Glossary of terms used in theoretical organic chemistry

A working party has been formed Chaired by Professor Minkin, and this project is underway. A draft Glossary of 250 terms has already been circulated.

Critical compilation of scales of medium effects

This project is directed by Professor Abboud. A preliminary report will be completed in time for the next meeting of the Commission in Guildford in 1995.

Guidelines for the publication of research results from empirical force field calculations

This project is being Co-chaired by D. J. Raber and W. C. Guida, and has received strong support from the Division and favourable endorsements from referees. A working party has been formed, and will report next year.

Future projects

Education

The topic of chemical education is vital to all the Commissions and Divisions, and the Physical Organic Commission will work with the Division and the IUPAC Committee on Teaching of Chemistry on this subject.

Supramolecular chemistry

Letters have been received from a number of outside experts on the need for an effort in this area. Professor Y. Takeuchi is leading a further survey in this area, with O. S. Tee (Concordia Univ., Montreal).

Theoretical and computational chemistry

It is certain that this multidisciplinary area will become increasingly important, and future activities on this topic are planned. There is an effort in this area underway in the Physical Chemistry Division, and our efforts are being co-ordinated with

theirs. They are producing a list of acronyms and a booklet on common methods of theoretical and computational chemistry.

Keeping records

Efforts in this area will be co-ordinated with other Divisions.

Acidity of strong acids

This is an area of major industrial and academic interest. Several expressions of support for such a project have been received, and further information is being solicited.

IUPAC Conferences on physical organic chemistry

The very successful 12th Conference was held in Padova, Italy, August 28–September 2, 1994 and the lectures will be published in *Pure and Applied Chemistry*. The 13th Conference is scheduled in Seoul (Inchon), Korea, August 25–29, 1996, and information regarding this Conference may be received from Professor Junghun Suh, Department of Chemistry, Seoul National University, Seoul 151-742, Korea, Fax +82 2 889 1568. The Commission has recommended Brasil as the site of the conference in 1998. Sites for the 2000 Conference are under consideration, and suggestions for possible locations may be sent to the Chair of the Commission.

Recent developments

An important recent development in the Organic Division is the formation of a fledgling Commission on Organic Chemical Synthesis, which had its first meeting in Padova at the time of the Conference on Physical Organic Chemistry.

The Commission is making an effort to ensure that its reports are widely circulated so that the chemical community can fully evaluate their usefulness. In particular the 1989 report on a 'System for Symbolic Representation of Reaction Mechanisms' and the latest Glossary¹ are being circulated to textbook authors and publishers to gain greater exposure for the documents.

References

1 Glossary of Terms Used in Physical Organic Chemistry, ed. P. Müller, *Pure Appl. Chem.*, 1994, **66**, 1077.

2 Glossary of Terms Used in Physical Organic Chemistry, ed. V. Gold, Provisional: *Pure Appl. Chem.*, 1979, **51**, 1725; Final: *Pure Appl. Chem.*, 1983, **55**, 1281.

3 Compilation and Critical Evaluation of Structure–Reactivity Parameters and Equations. Part I. Values of σ_m and σ_p Based on the Ionization of Substituted Benzoic Acids in Water at 25 °C, *Pure Appl. Chem.*, 1994, **66**, 2451.

Membership of the Commission

Chairman: Professor T. T. Tidwell, Department of Chemistry, University of Toronto, Toronto, Ontario, Canada M5S 1A1.

Secretary: Professor Emeritus W. Drenth, Utrecht University, Ovidiuslaan 4, 3584 AW Utrecht, The Netherlands.

Titular Members: Professor C. L. Perrin, University of California, San Diego, USA; Professor Emeritus J. Shorter, University of Hull, England; Professor V. I. Minkin, Rostov University, Russian Republic; Professor Z. Rappoport, Hebrew University, Jerusalem, Israel; Professor Y. Takeuchi, Kanagawa University, Japan.

Associate Members: Dr M.-F. Ruasse, CNRS, Paris, France; Dr A. J. Kirby, University of Cambridge, UK; Dr D. J. Raber, National Academy of Sciences, Washington, USA; Dr J. R. Zdysiewicz, Australian Journal of Chemistry, Melbourne, Australia; Professor H.-U. Siehl, University of Tübingen, Germany; Professor Per N. I. Ahlberg, University of Göteborg, Sweden; Professor E. Baciocchi, University 'La Sapienza', Rome, Italy.

National Representatives: Professor J. J. Humeres Allende, University Trinitade, Florianopolis, Brazil; Professor Guo Zhen Ji, Shanghai Institute of Organic Chemistry, China; Dr R. Sabbah, CNRS, Marseille, France; Professor J. A. Silva Cavaleiro, University of Aveiro, Portugal; Professor S. S. Kim, Inha University, Inchon, Republic of Korea; Professor J.-L. Abboud Mas, CSIC, Madrid, Spain; Professor O. Tarhan, Middle East Technical University, Ankara, Turkey; Professor Miha Tisler, University of Ljubjana, Slovenia; Professor J. Chandrasekhar, Indian Institute of Science, Bangalore.