JOURNAL OF PHYSICAL ORGANIC CHEMISTRY, VOL. 6, 193–194 (1993)

NEWSLETTER

IUPAC COMMISSION OF PHYSICAL ORGANIC CHEMISTRY

INTRODUCTION

Physical organic chemistry emerged a few decades ago, when organic chemists started to apply the methods and theory of physical chemistry to the study of organic reactions and their mechanisms. These studies prepared the ground for modern organic chemistry. The way organic chemists think about their science is very much dominated by physical organic concepts, and the teaching of elementary organic chemistry without using a physical organic approach is almost unthinkable.

The IUPAC Commission on Physical Organic Chemistry (Commission III.2) was established within the Organic Chemistry Division in 1973, when classical physical organic chemistry (i.e. mechanisms of reactions in solution) was at its height. Owing to the rapid development of the field, there was much confusion at that time with respect to the language of organic chemistry, and the Commission's first effort consisted in establishing a glossary which defined the terminology to be used in physical organic chemistry.[1] Subsequent work of the Commission dealt with typical problems related to reaction mechanisms,[2,3] but also with topics going beyond the field, such as the development of a nomenclature for organic transformations[4,5] and the nomenclature for hydrogen atoms.[6]

RECENT PUBLICATIONS

During the past few years, the Commission has discussed problems concerning standards of publication. These discussions have resulted in the preparation of two documents, published in the form of technical reports, which recommend guidelines for the publication of research in experimental[7] and computational[8] organic chemistry. These guidelines are intended to assist journal editors in establishing sound editorial standards, and to encourage authors to meet such standards.

A technical report dealing with the physical properties of carbenes and carbene analogues has also appeared recently.

0894–3230/93/030193–02$06.00
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CURRENT PROJECTS

Glossary of terms used in physical organic chemistry, revision 1993 (the 'Glossary')

Most of the effort of the Commission during the last 4 years was spent on this project. The terminology of the previous glossary has been updated, revised and considerably expanded. The document is on the way to outside reviewers, and is planned to be finalized at the 1993 IUPAC General Assembly in Lisbon.

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 with 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, it was 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 owing to the untimely death of its initiator. At that time 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.

FUTURE PROJECTS

There has been much discussion on restructuring IUPAC to make it more efficient and more responsive to the needs of the scientific community and to the needs of society. Conceivably, the activities of the Division of Organic Chemistry might be reoriented, and so will be those of the Commission on Physical Organic Chemistry. For the immediate future, in the selection of projects, the Commission is trying to keep a reasonable balance between the traditional fields of physical organic chemistry and the more recent developments; such projects often will have strong interdisciplinary character and will require participation of experts outside of IUPAC.

Current feasibility studies deal with terminology in theoretical chemistry and with modelling. In addition, the commission is looking for means to make available to a larger audience the projects on terminology which have been going on in the Division of Organic Chemistry; publication of a compilation on IUPAC 'Terminology in Organic Chemistry' is envisaged. Other fields of interest in the future include solvent parameters, steric substituent parameters, language of supramolecular chemistry, physical methods in organic chemistry and physical properties of radicals. Readers of this newsletter are encouraged to offer comments on these projects, and on others that they think the Commission should undertake. Such comments may be addressed to the Chairman or to the Secretary, whose addresses are given below, or to any member of the Commission.

MEMBERSHIP OF THE COMMISSION

Chairman: Professor P. Müller, Department of Organic Chemistry, University of Geneva, 30 quai Ernest Ansermet, CH-1211 Geneva 4, Switzerland. *Secretary:* Professor W. Drenth, Ovidiuslaan 4, 3548 AW Utrecht, The Netherlands. *Titular Members*: Professor J. M. McBride, Yale University, USA; Professor J. Shorter, University of Hull, UK; Professor V. I. Minkin, Rostov University, Russian Republic; Professor Z. Rappoport, Hebrew University, Jerusalem, Israel; Professor Y. Takeuchi, University of Tokyo, Japan. *Associate Members:* Professor P. N. I. Ahlberg, University of Göteborg, Sweden; Professor P. van Brandt, Louvain-la-Neuve, Belgium; Professor E. A. Halevi, Technion, Haifa, Israel; Professor O. M. Nefedov, Zelinski Institute of Organic Chemistry, Moscow, Russian Republic; Professor C. L. Perrin, University of California, San Diego, USA; Dr. D. J. Raber, National Academy of Sciences, Washington, USA; Dr. J. Zdysiewicz, Australian Journal of Chemistry, Melbourne, Australia. *National Representatives:* Professor J. J. Humeres Allende, Campus University Trinidade, Florianopolis, Brazil; Professor T. T. Tidwell, University of Toronto, Canada; Professor X. Jiang, Shanghai Institute of Organic Chemistry, China; Dr. R. Sabbah, CNRS, Marseille, France; Professor E. Baciocchi, University 'La Sapienza,' Rome, Italy; Professor J. A. Silva Cavaleiro, University of Aveiro, Portugal; Professor J. Suh, Seoul National University, Republic of Korea; Professor J.-L. Abboud Mas, CSIC, Madrid, Spain; Professor O. Tarhan, Orta Dogu Technical University, Ankara, Turkey; Professor M. Tisler, University Edvard Kardelj of Ljubljana, Yugoslavia.

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