The Project Place

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Update of IUPAC Glossary of Physical Organic Chemistry

A task group has been formed to update the IUPAC *Glossary of Terms Used in Physical Organic Chemistry*. The original glossary had been compiled under the auspices of the IUPAC Subcommittee on Physical Organic Chemistry and published in *Pure and Applied Chemistry*, 1994, 66, 1077–1184. In 1997, a Web version was created: www.chem.qmul.ac.uk/iupac/gtpoc/. The glossary will be updated to include new terminology that has developed, to revise ambiguities, to respond to inquiries, to make it consistent with other IUPAC glossaries, and to establish procedures for continual revision and expansion.

For more information and comments, contact Task Group Chair Charles L. Perrin <cperrin@ucsd.edu>

www.iupac.org/web/ins/2009-002-1-300

Reference Methods, Standards, and Applications of Photoluminescence

More than 20 years ago, David Eaton undertook the task of collecting information on fluorescence methods and materials as a task of the IUPAC Commission on Photochemistry. Two relevant documents evolved from this work: "Reference Materials for Fluorescence Measurement," [*Pure and Applied Chemistry*, 1988, 60(7), 1107–1114]; and "Recommended Methods for Fluorescence Decay Analysis," [*Pure and Applied Chemistry*, 1990, 62(8), 1631–1648]. Since Eaton's documents were written, new reference materials have been published and the subject has evolved rapidly with the incorporation of new areas and methods of fluorescence that were not understood or poorly developed at that time. A few examples are single molecule fluorescence, ultrafast fluorescence detection, and fluorescence microscopy. Many of these subcategories are of utmost relevance in materials science and in biology. In general, interest has shifted to organized, (micro) heterogeneous systems.

A nearly completed IUPAC project, begun almost six years ago, has been systematically updating all IUPAC documents on fluorescence, including advances registered during the last 20 years. Nearly 15 documents will be issued and published as an outcome of this project, which gives particular attention to newly developed reference materials and methods.

The scope of the work has been broadened for this project to include luminescence from molecular emitters in their triplet state or states with mixed spin multiplicity, quantum dots, and more. Thus, the term "fluorescence" appearing in the earlier documents has been replaced by the far more comprehensive term "photoluminescence." "Reference methods will include recommendations for the calibration of luminescence measuring systems; the correction of emission, excitation, action, and polarization spectra; the determination of quantum yields in different spectral ranges; and the determination of lifetimes or decay kinetics in the various achievable time scales. Whenever possible, extension to nondilute, unclear, or complex systems of applied interest will be performed.

At present, 13 documents have been drafted, all of which will be issued under the signature of one or more authors. They carry the primary responsibility for the written material. However, all documents have profited from the criticism and the contribution from all Task Group members, whether they participated or not in active writing. Style uniformity and fulfillment of IUPAC rules will be pursued in a final step, in which internal and external consistences will be checked. Final documents will be submitted successively.

The first titles in the series are as follows:

1. Fluorescence Standards: Classification, Terminology and Recommendations on their Selection, Use and Production, by U. Resch-Genger, P.C. DeRose
2. Characterization of Photoluminescence Measuring Systems, by U. Resch-Genger, P. C. DeRose
3. Determination of the Photoluminescence Quantum Yield of Dilute Dye Solutions, by K. Rurack, U. Resch-Genger
4. Standards for Photoluminescence Quantum Yield Measurements in Solution, by A.M. Brouwer
5. Fluorescence Anisotropy Measurements in Solution: Methods and Reference Materials, by M. Ameloot, M. vandeVen, A. U. Acuña , B. Valeur
6. Time-Resolved Fluorescence Methods, by H. Lemmetyinen, N. Tkachenko, B. Valeur, N. Boens, M. Ameloot, N. Ernsting, T. Gustavsson, J.-I. Hotta

Preview drafts are available on request as opinions, criticisms and comments from the photochemical community are kindly requested.

The project is divided into different sections:

I. Steady-state Luminescence Measurements
II. Time-resolved Spectroscopy and Decay Analysis
III. Single Molecules and Microfluorimetry
IV. Luminescence Measurement in

Microheterogeneous, Heterogeneous, Highly Absorbing and Complex Systems

Documents 1 to 4 belong to Section I, as they deal mainly with steady-state measurements, document 6 to Section II, and document 5 pertains to both sections, as it involves both steady-state and time-resolved measurements. The remaining documents to be issued correspond to Sections III and IIV.

For more information and comments, contact Task Group Chairs Albert M. Brouwer <fred@science.uva.nl> or Enrique San Román <esr@qi.fcen.uba.ar>.

www.iupac.org/web/ins/2004-021-1-300

Experimental Requirements for Single-Laboratory Validation

The objective of this recently initiated project is to provide expert guidance on the scope and scale of experiments required for single-laboratory method validation, enabling regulatory agencies to harmonize validation requirements.

This new project will develop guidance on experimental designs suitable for determining method performance characteristics during single laboratory validation experiments. Where possible, the resulting report will include guidance on numerical values for such performance characteristics.

The output is intended to support implementation of the existing IUPAC Harmonized Protocol on Single-Laboratory Validation (*PAC* 2002, Vol. 74, No. 5, pp. 835–855), which specifies the performance characteristics to be assessed, but currently includes no quantitative guidance on the scale of experimentation required.

It is currently envisaged that the guidance will be informed by statistical power considerations; that is, experimental requirements will be set so as to achieve a particular probability of correctly identifying significant adverse effects (such as a specified upper limit for bias). The guidance will indicate the power appropriate for different situations. For example, verification of performance of an established method, validation of a new method, or validation of a new method intended for critical uses would attract increasingly stringent requirements. It is envisaged that the report will include example simple-experiment designs and associated tables of replicate numbers for each such situation so that regulators can easily specify the level of stringency required and analysts can easily identify the scale of experimentation necessary to meet the requirement.

The requirements will be chosen so that they broadly reflect and harmonize current best practice. The advantage of specifying requirements in terms of test power as well as listing specific experiments and experiment sizes is that it then becomes possible to permit any experiment design that is designed to achieve the necessary confidence. This provides for flexibility in specifying single-laboratory validation requirements, and allows analysts to design improved experiments which have greater efficiency while being able to demonstrate that the stringency is sufficient.

For more information and comments, contact Task Group Chair Steven L.R. Ellison <s.ellison@lgc.co.uk>.

www.iupac.org/web/ins/2009-006-1-500

Provisional Recommendations

Name and Symbol of the Element with Atomic Number 112

A joint IUPAC/IUPAP Working Party (JWP) has confirmed the discovery of the element with atomic number 112 by the collaboration of Hofmann et al. from the Gesellschaft für Schwerionenforschung mbH in Darmstadt, Germany. In accordance with IUPAC procedures, the discoverers proposed a name, copernicium, and symbol, Cn, for the element. The Inorganic Chemistry Division now recommends these proposals for acceptance.

This proposal lies within the long tradition of naming elements to honor famous scientists. Nicolaus Copernicus was born on 19 February 1473 in Torún, Poland, and died on 24 May 1543 in Frombork/Frauenburg. His work has been of exceptional influence on the philosophical and political thinking of humankind and on the rise of modern science based on experimental results.

Comments by 31 January 2010
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www.iupac.org/reports/provisional/abstract09/corish_310110.html