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Background. The restructuring program approved by the Bureau in 1998 and by Council in 1999 envisions the discontinuation of all current Commissions at the end of 2001. Division Committees have available a variety of mechanisms for planning activities, ensuring continuity of ongoing activities, and managing their portfolio of projects, in the absence of Commissions. Nevertheless, the restructuring program recognized the possibility that new Commissions might occasionally be required, and the Bylaws provide a framework for forming new Commissions.

Proposed Commissions. In general, the Divisions have found that most of their programs can be handled without Commissions. However, the Bureau has received requests from the Physical and Biophysical Chemistry Division and from the Inorganic Chemistry Division to each form one Commission:

- *Commission on Physicochemical Symbols, Terminology and Units*. This represents a reestablishment of the present Commission I.1, but with changes in emphasis and responsibility, as noted later.
- *Commission on Isotopic Abundances and Atomic Weights*. This represents a reestablishment of the present Commission II.1, which is devoted to Atomic Weights and Isotopic Abundances, with the inclusion of the International Measurement Evaluation Program, now under the purview of Commission II.4. The proposed Commission would be divided into two subcommittees to carry out these related but rather different activities, as discussed later.

Review Procedure. Bylaw 4.301 provides very specific directions for the process of forming a commission, saying in part:

> If a Division or Section Committee wishes to create a Commission, it must apply to the Bureau for the appointment of an ad hoc committee of three persons which shall study the question and then report back to the Bureau. The report, if favorable to the creation of a new body, shall contain an indication as to the probable duration of the life of the new body and an estimate of its annual cost.

As noted in more detail later, two ad hoc committees were appointed by the President and have considered the proposals from Divisions I and II. The issue is not whether the work proposed for the Commissions should be carried out by IUPAC but whether a Commission, rather than some other managerial arrangement, is desirable. The Bylaws provide no specific guidance, but the program to convert the Union's scientific activities largely to a project-driven system anticipates the formation of Commissions under only special circumstances. The report of the Strategy Development and Implementation Committee [1998], as well as subsequent discussions in the Bureau and Executive Committee, suggest that a number of factors might be important, such as broad impact throughout IUPAC, need for interactions with other Unions, "visibility" of IUPAC in an emerging or interdisciplinary field, assurance of long-term need, and perhaps to some extent "tradition." The ad hoc committees were aware of their role in helping to develop criteria for these cases that might serve as precedent for guiding the formation of future Commissions.

Reports by the *ad hoc* Committees

- The ad hoc committee considering the formation of a new *Commission on Physicochemical Symbols, Terminology and Units* initially had serious concerns about the need for this body as a Commission, but discussions with the Division President resulted in a clarification of

several points and a revision in the proposal. As a result, *the report of the ad hoc committee to the Bureau endorses this new Commission.*

- The ad hoc committee considering the formation of a new *Commission on Isotopic Abundances and Atomic Weights* concluded that the core work, as carried on by the current Commission I.1, merited formation of a new Commission. However, the inclusion of the IMEP as a subcommittee within this Commission raised serious concerns, as indicated in the detailed report on later pages. The committee suggested that the proposal be modified to restrict the Commission to the core work, but the Division President felt that there are sufficient mutual interests to warrant pursuing the proposal as presented initially. Under these circumstances, *the committee regrets that it cannot support the proposal and will recommend that the atomic weight work and the IMEP continue without the formation of a Commission.*

The reports of the ad hoc committees, provided in subsequent pages, will be presented to the Bureau for discussion and action. The Bureau is not required to accept the reports in framing its recommendations to Council.

Item 14.3: Proposed New Commissions

Proposal for a New Commission on Physicochemical Symbols, Terminology and Units

April 2001

Aims: To oversee the development of a system of units, symbols, and terminology in Physical Chemistry, and to advise all parts of IUPAC and the broad chemistry community on their use.

IUPAC Core Activity: Physicochemical terminology, with its accompanying symbols and units is an IUPAC core activity requiring a continuing authoritative body to achieve and stand for wide consensus obtained by consultation with the full range of experts in the international community in weights and measures, physics, biology, and other disciplines.

Details of composition and practice: The Commission, with three permanent members, would act as a coordinating group with the aims of:

(a) Disseminating best practices in the use of units and symbols via the Green Book
(b) Highlighting and addressing new physicochemical terminology problems that may have an impact in Physical Chemistry and in other chemical disciplines
(c) Publicity for the resulting works (i.e. the Green Book and the Web)
(d) Initiate new projects within the Physical Chemistry Division where terminology issues are important, and where more specific work and consensus on definitions is required.
(e) Maintain a network of experts who will be consulted (usually not required to attend meetings)
(f) Serve as a link between the chemical sciences community and other international organizations concerned with quantities and symbols in physical chemistry in its broadest sense.

Visibility for these and other activities will be achieved by:

(a) Raising the profile of the Commission at international conferences
(b) Targeting of graduate students in chemistry by providing them with a clear guide to symbols, units and terminology
(c) Promoting the advantages of an internationally-approved system to enhance clarity in the communication of scientific information.
(d) Improving links with journal editors and text book writers
(e) Creation of a mail list of interested groups (mailbase systems)

Current and Proposed Projects

The proposed Commission would, in part, follow from the current Commission I.1. As such, there are a number of current and proposed projects already under way. In order to carry out the aims stated above, the Commission would coordinate projects on:

(a) Production of the Green Book, Third Edition
(b) Production of an undergraduate student version of the Green Book
(c) Production of a flat web version as an initial Web presence
(d) Production of a fully interactive, hyperlink version of the Green Book

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Proposed Terms of Reference: To promote uniform practice by the chemical community in the usage of symbols, terminology, and units, and to assure proper coordination with other IUPAC bodies and international organizations in all matters related to symbols and units.

Additional clarifying comments by the Division President: When I joined IUPAC some 14 years ago, Commission I.1 was a largely autonomous unit within the Division. Decisions about what to include in the Green Book were not generally made in consultation with the "users" of the terminology. Thus the frequent complaint was, "Why create symbols and terminology that no one will use?" The Third Edition, shortly to be released, is the product of significant consultation and discussion with the various constituencies within the Physical Chemistry Division. I believe that generally a good balance of usage vs. rigor and consistency has been achieved. Certainly this remains a work in progress. The Green Book is "thin" physically because every effort is made to include only those terms and symbols that are generally applicable in the chemical sciences and leave specialized terminology up to specialized groups. For this reason, I believe it can be said that the Green Book provides an essential base for physicochemical terminology and symbols, not just for Physical Chemistry, but for IUPAC as a whole. Our model for the future operation of the proposed commission is based on the very successful experience of detailed consultation with users over the last few years.

The activities of the proposed commission will be supported with Division funds. The core of three individuals is considered crucial to maintaining the necessary continuity and experience required for making consistent decisions concerning terminology and symbols. This group will, as in the past, provide an essential training ground for future members of IDCNS in this area. This model provides, in our opinion, a good balance between flexibility derived from a "lean" unit, and a pool of experience needed to implement such an activity.

As the proposal itself indicates, dissemination of the Green Book via the Web and in various forms is currently under active discussion. This will require a proactive stance, and will require emphasis on the importance of consistent scientific language as the exchange of ideas occurs on a world-wide scale. Because the commissions will no longer exist, this core group will establish a network of experts to provide input on improvement and enhancements. This will be implemented through the database that the Physical Chemistry Division is setting up at the Secretariat, and through organization of mini-workshops at international meetings, where a representative of the proposed commission could meet with specialists in a particular area. Projects will be created as needed and we anticipate involvement of other divisions as the flexibility of our new structure will easily accommodate. As in the past, activities will be coordinated with IUPAP, BIPM and other scientific unions. Thus the new format of the Commission (smaller and more flexible) is entirely compatible with our recent positive experience and with the future goals of IUPAC.

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Report of the *ad hoc* Committee:
Proposed Commission on Physicochemical Symbols, Terminology and Units

The current Commission I.1 has carried out excellent work over many years in systematizing a broad range of physicochemical symbols and related terminology. The results of its work have been presented largely in three editions of the manual commonly known as the "Green Book," a book in which the Division justifiably takes pride. It has been an IUPAC "best seller," which provides an indication of its widespread use by chemists throughout the world. The proposal highlights the past accomplishments and cites future plans for updating and promoting the Green Book.

Our committee recognizes the importance of the Green Book but believes that the updating and management of any IUPAC book on nomenclature, symbols or terminology is an inadequate justification for the formation of a Commission. A book can be updated as a project, a continuing oversight of needs in the field can be provided by the Division Committee or a subcommittee, and the use of the web can facilitate these processes. However, the committee recognized broader implications in the area of physicochemical symbols and terminology. Discussions with the Division President served to clarify several aspects and resulted in the revised proposal now presented to the Bureau and Council. Several points made in the proposal and supporting comments are particularly important:

1. The value of the Commission as a body to promote a system of symbols, units and physicochemical terminology throughout IUPAC and the chemistry community. Although every specialty has its own terminology, the symbols, units and terminology dealt with by the Commission are not restricted to physical chemistry, but rather are widely used throughout chemistry. Thus, this Commission is expected to be an IUPAC-wide resource.
2. The need for a *consistent set* of symbols and units, which parallels in some ways the need for systematic nomenclature of chemicals. Both are of much broader value than in the Division responsible for their development, and both require considerable experience and continuity. For nomenclature of chemicals, the Executive Committee has endorsed a proposal to Council to establish a new Division of Systematic Nomenclature and Structural Representation. In the present case, a new Division is not needed, but a Commission with ties to other Divisions and responsibility for IUPAC-wide efforts seems appropriate.
3. The importance of having a small continuing body in this area with a large number of experts "on call" as a training ground and a backup to IDCNS. All Recommendations and Technical Reports are reviewed by IDCNS for consistency in chemical nomenclature, symbols and units. The proposed new Division will provide backup in nomenclature, and the proposed Commission can serve a similar role in the specialized expertise and interest in symbols, units, and the whole SI.
4. The value of having a Commission to interact with similar bodies in IUPAP, BIPM and other international bodies. The "prestige" of the title Commission provides an ancillary benefit but is not in itself justification for the formation of the Commission.

In conclusion, the committee believes that the Division has provided convincing arguments for the formation of the new Commission. As pointed out in the Division President's comments, the cost is expected to be minimal and will be met from the Division's operating budget. If formed, the Commission will be subject to annual renewal under the provisions of Bylaw 4.302. Although there is no apparent limit to the need for the work to be carried out by the Commission,

in keeping with the requirement of Bylaw 4.301 for "an indication of the probable duration of the life of the new body," the committee recommends that the need for continuing the Commission be examined in detail by the Bureau, not only the Division, in eight years.

Mostafa A. El-Sayed (former member of the Physical Chemistry Division Committee)

Folke Ingman (President, Analytical Chemistry Division)

Edwin D. Becker (Secretary General)

Item 14.3: Proposed New Commissions

Recommendation to the Bureau of the International Union of Pure and Applied Chemistry for the Creation in 2001 of a Commission entitled "Commission on Isotopic Abundances and Atomic Weights"

Justification for a Commission on Isotopic Abundances and Atomic Weights

Isotopic abundances and atomic weights are of fundamental importance in science, technology, trade, and commerce. Atomic weights relate mass to molar quantities, both base quantities in the International System of Units (SI). The Table of Atomic Weights produced by IUPAC is one of the most fundamental sets of scientific data. Atomic weights are essential to all of the physical sciences, for quantitative chemistry and analysis, and for the understanding of chemical reactions, energies, formulae, and stoichiometry. It is therefore not surprising that the measurement of isotopic abundances and atomic weights has played a central role in the development of chemistry and that knowledge of their accuracies continues to be a key component in the progress of chemistry and allied sciences. Recently, new applications have come into prominence, among them the ability to use subtle differences in isotopic compositions for identifying sources of materials, studying manufacturing processes, and investigating biological, environmental, geological, hydrological, and nuclear processes.

Background

In 1892 the American Chemical Society formed a Committee on Atomic Weights. By 1900 the International Committee on Atomic Weights was formed, and it became affiliated with IUPAC when the Union was formed in 1920. In 1969 there was a move within IUPAC to eliminate the Atomic Weights Commission because atomic weights were then thought to be so accurate that any further improvement was at most an "academic" exercise and of no interest or relevance to professional chemists or chemical technology, and certainly not to commerce. But in the 1980's it became clear that the isotope measurement techniques that gave more accurate atomic weights could be employed to perform chemical analyses and other physical measurements to equal accuracy. Currently, application of highly precise isotope ratio techniques to a wide range of significant physical and biological problems is undergoing a rapid increase.

The emphasis over many years on increasing the accuracy of atomic weights has significantly contributed to the development of many high accuracy techniques and instrumentation that are applied to all manner of novel, practical and important problems. These open new windows of scientific opportunity that in turn stretch the demands on procedures and instruments.

The further significant improvement in mass spectrometric equipment strongly suggests that a differentiation between sources of elements is likely to be found for those elements that so far have appeared invariant in atomic weight. More generally, this increased precision in relative isotopic abundancies and atomic weight measurements clearly signals a need for suitable reference materials with certified atomic weights to be developed, measured, evaluated for reliability, and distributed to users under the auspices of the proposed Commission.

In 1989 a Commission on "Isotopic Specific Measurements as Traceable References" was created as a Limited Lifetime Commission within IUPAC's Inorganic Chemistry Division

because of the mass spectrometry expertise residing in the Division's Commission on Atomic Weights. The combination of metrological and isotopic experience combined with the early cooperation of several national measurement laboratories assured the scientific success of the International Measurement Evaluation Programme (IMEP) operated by the Commission. By the mid 1990s, the IMEP programmes had become well established and more recently they have been adopted by a number of regional laboratory accreditation schemes. The Limited Lifetime Commission became a full Commission in 1995 with very solid support from the Committee on Chemistry and Industry (COCI). The list of IMEP programmes now numbers about 16, or about one new one per year. There have been a number of publications presenting results from these programmes. The number of participating laboratories for some IMEPs has grown to more than 200 distributed around the world.

The New Commission

Recognizing the continuing and increasing importance of isotopic abundance studies, the Inorganic Division recommends that a Commission be created after 2001 entitled "Commission on Isotopic Abundances and Atomic Weights."

This commission would regularly:

- evaluate published data in the scientific literature on isotopic abundances of the chemical elements;
- examine the literature on measurements of variations in isotopic abundances in a wide range of natural (including non-terrestrial) materials;
- critically assess this literature, prepare an authoritative Table of Standard Atomic Weights and a Table of Isotopic Compositions of the Chemical Elements;
- assist the wider scientific community with recommendations for isotopic standards and reference materials and evaluations and calibrations thereof;
- meet to review progress on new and old IMEP programmes and to develop requirements for future programmes;
- examine and evaluate potential new reference materials from national measurement laboratories for use in new IMEPs and propose new methods of preparing and distributing the IMEP rounds.

These goals require continuity and dedication that cannot be accomplished within short-term projects.

Organization of the Commission

The Commission will consist of a small group of experts in isotope mass spectrometry, statistics, and measurement science who are concerned with:

- measurement of isotopic abundances, and variation of those abundances in a wide range of naturally occurring materials;
- maintaining a link to the International Organization for Standardization (ISO) recommendations on principles of measurement science which are supported by IUPAC and most relevant international associations;
- preparing, certifying and distributing suitable reference quality materials for the IMEP programmes.

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The professional diversity and institutional memory of this group that are provided by a commission are critical to maintain effective working continuity and a rapid response for isotope information to the needs of the scientific community.

To carry out its tasks, it is envisioned that the Commission will contain two subcommittees:
(1) a subcommittee for the assessment of isotopic abundance measurements and atomic weights, the assessment of the natural variation of isotopic abundances, and for the compilation of isotopic variations in non-terrestrial materials;
(2) a subcommittee for the operation of the IMEP programmes

Products

Due to the increasing importance of isotopic abundances in numerous fields of chemistry, earth sciences, physics, forensics, and biology, the primary work of the Commission will be to evaluate continually the literature on isotopic abundances and so provide accurate information to the scientific community on a regular basis. Such data provide the basis of IUPAC's Tables of Isotopic Compositions of the Elements and of investigations on variations of isotopic abundances. The Commission will also invest substantial effort in abstracting and summarizing literature information on the isotopic compositions of materials of non-terrestrial origin. These IUPAC Tables serve as the authoritative source for atomic weights and isotopic compositions and are used for many purposes, including the refinement of fundamental chemical and physical constants.

IMEP rounds utilizing a variety of natural-matrix "real world" samples of direct interest to chemical and other industries yield numerous, directly comparable, analytical data from participating laboratories around the world. These data are classified and evaluated, for example, according to the analytical technique used. Since the IMEP programme provides for each element (compound) a certified range obtained by several independent national laboratories, each participating laboratory can determine how far its results are biased from the certified range. IMEP results classified according to analytical methods, experience, accreditation, etc. and evaluated against the certified range are of great value for education and training in academy and industry. IMEP materials can be used as test samples to demonstrate the degree of equivalence between results from national metrological institutes through key comparison studies conducted by the Consultative Committee on Amount of Substance (CCQM) of the International Bureau of Weights and Measures (BIPM). The results of the IMEP rounds will be published and will also be made available on the IUPAC website.

Benefits

A Commission on Isotopic Abundances and Atomic Weights will maintain IUPAC's leadership role in atomic weights and isotopic abundances, and provide authoritative data sets to the worldwide scientific community on a regular basis.

The results obtained by participating in the IMEP rounds have great economic importance in terms of assistance to the individual laboratories as they evaluate their need to change or modify their laboratory methodology.

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The recommended Commission will play a premier role in addressing the IUPAC objective to study topics of international importance to pure and applied chemistry, which need standardization and codification.

Item 14.3: Proposed New Commissions

Report of the *ad hoc* Committee:
Proposed Commission on Isotopic Abundances and Atomic Weights

The International Committee on Atomic Weights was formed in 1900, thus antedating IUPAC, and joined the Union in 1920. IUPAC has long been the recognized international authority on atomic weights, and updated tables of atomic weights are always of widespread interest. As the proposal points out, in recent years the availability of highly accurate mass spectrometric methods of measuring atomic mass have led to new applications in analytical chemistry, geochemistry and other areas.

Our committee recognizes the importance of this work and its potential future value. It would be almost inconceivable for IUPAC to relinquish its leadership position in this field. The question is the need for the work to be carried out by a Commission, rather than in a set of projects managed by the Division Committee or another body, such as a Division subcommittee. In fact, it seems likely that much of the work can and should be carried out under the project system. The need for planning and coordinating activities could indeed be handled by a subcommittee of the Division Committee. However, our committee believes that the prominence of this subject as an IUPAC activity, together with the 100-year tradition of the Atomic Weights Commission, provide a strong argument for the retention of the title. The proposed inversion of the name to emphasize the rapidly developing area of Isotopic Abundances is regarded by the committee as appropriate.

The proposal, as presented to the Bureau, envisions the incorporation into the new Commission of the International Measurement Evaluation Program [IMEP], which is currently handled by a separate Commission within the Inorganic Chemistry Division. The IMEP depends on the use of isotope dilution mass spectrometry to carry out highly precise quantitative analyses in a manner that provides metrological traceability. The proposal points out that this program developed within IUPAC, and specifically within the Inorganic Chemistry Division, in 1989 as a result of mass spectrometric expertise that resided within Commission II.1. Our committee recognizes this historical connection but believes that the IMEP as presently operated does not fit into a Commission that is justified on the basis of the discussion in the preceding paragraph.

The committee suggested to the Inorganic Division that the proposal would be strengthened by focusing it on the core atomic weight and isotopic abundance work. However, the Division President declined to modify the proposal, noting that "a check over the documentation used to prepare the original request and my renewed consultation with the principals involved revealed no reason to change the decision reached by the Division Committee. I do want to stress again that this decision was made only after careful consideration of the science involved, of our understanding of the need for renewal within IUPAC and of the even greater need to continue to have the Union to be clearly seen to be doing meaningful and internationally useful work."

As a result, the committee regrets that it cannot provide a favorable report to the Bureau on the formation of the new Commission. The committee is sensitive to its role in helping to establish criteria and procedures for formation of future Commissions, and this factor plays a role in our conclusions. Our reasoning can be summarized as follows:

- The justification for the reestablishment of the Commission on Isotopic Abundances and Atomic Weights rests largely on the historically important role that it has played as a Commission and on the anticipated continuation of its important core activities.

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- By all accounts, IMEP is an excellent program, and IUPAC may well wish to continue and expand its role in the program. However, the work can be carried out largely under the project system, with support by the Inorganic Chemistry Division and possibly other IUPAC bodies. Most work within the Divisions will be carried out in this way, and the incorporation of this program into a Commission justified on other grounds would set a poor precedent for the formation of future Commissions.
- It appears that there are conflicting views, both within and outside IUPAC, on the role that the Union plays in IMEP and might play in the future. Although it is outside the purview of this committee to go into the details here, we believe that the Division Committee needs to address these questions directly. Relegating IMEP to a subcommittee of a new Atomic Weights Commission might preclude the attention that the matter deserves.

In conclusion, the committee believes that the future of the core work on atomic weights and isotopic abundances will be better served by having a body that focuses on that program alone. At the same time, IMEP should be better able to develop on an international scale if it is managed separately. Although we would be glad to recommend a Commission focused on the core atomic weight work, it is our opinion that the proposal as submitted should not be approved. Both the core atomic weight / isotopic abundance work and IMEP should certainly continue as important IUPAC endeavors but at present without Commission status.

Norman Greenwood (Former President, Inorganic Chemistry Division)

Hitoshi Ohtaki (Elected Member of the IUPAC Bureau)

Edwin D. Becker (Secretary General)