

The Critical Assessment of the IUPAC Divisions Activity

(by V.A. Koptug, September - December 1986)

This brief document is prepared on the basis of my discussions of the activities of the Divisions and of the various Commissions with each Division President at Oxford (September 1986). Some additional information was received later by correspondence.

I. Physical Chemistry Division (President - Dr. D. Lide)

All the Division Commissions worked after Lyon General Assembly productively, 27 from 52 projects have concrete results (projects are completed or will be completed entirely or partly to the end of 1986). Considerable progress has been made on the revised edition of the Green Book (Quantities, Units and Symbols in Physical Chemistry) and on Thermodynamic Tables of the Fluid State. Six projects have been started in the framework of a new Commission on Chemical Kinetics (I.4). The Commission on Colloid and Surface Chemistry has activated its work in the field of catalysis. There is a good basis for cooperation with the Database Committee.

At the same time the Division Committee should consider the situation with "long-living" projects - there are 6 projects started in 1976-77.

In connection with this it is desirable to differentiate in the IUPAC programme listing "on-going" projects (yet not completed) and "permanent" ones (such as - Promotion of the Republications and Translations of the IUPAC Manual).

II. Inorganic Chemistry Division (President - Prof. Kazuo Saito)

This Division is compact and well managed. Among 32 projects mentioned in the 1984 listing 16 are or will be completed to the end of 1986.

Hard work is done for finalizing the manuscript of revised "Red Book" Part 1 (11 chapters) - on nomenclature of inorganic compounds. But there arose the strong controversy in chemical community concerning the Commission II.2. proposal to reformulate the Periodic Table. This is a "hot point" of the Division of Inorganic Chemistry and may be of IUPAC as a whole.

III. Division of Organic Chemistry (President - Prof. J. Bunnett)

Work on three Commissions of this Division is active and efficient. 9 from 34 projects gave concrete results. The total number of projects is reduced to 28 (including 5 new projects).

Some problems are visible in future work of the Commission on Nomenclature of Organic Compounds (III.1). There are some contradictions in requirements to man- and computer-acceptable systems of nomenclature of chemical compounds. Taking into account the high progress in computerization of chemistry and particularly of chemical information it is necessary to define a long-term strategy for development of nomenclature of chemical compounds. The Commission III.1. should organize a broad discussion of this problem. As a starting point I propose to consider the paper prepared for Chemistry International by two Chemists from Novosibirsk (V. Piottuch-Peletskii, V. Scorobogotov).

The Organic Chemistry Division pursues an active policy in organization of international conferences and symposia. Taking into

account the growing interest to computer application in organic chemistry Prof. Jean Mathieu proposed to organize at Novosibirsk in 1988 an IUPAC symposium on the topic "Uses of computers in organic chemistry". It is possible to do this. But there exists the series of International Conferences on Computers in Chemical Research and Education (ICCCRE). The VIII ICCCRE will be at Beijing (China) in June 1987. This series of conferences is stimulated by Prof. Peter Lykos (IIT, Chicago). It seems more desirable to take ICCCRE under sponsorship of IUPAC than to multiply the number of conferences on the same topic.

At the same time it seems very important to organize a series of seminars (or schools) on computer usage training in various fields of organic chemistry (computer aided synthesis, solution of structural problems, prediction of preferable ways of chemical transformations, prediction of properties of chemical compounds and so on).

IV. Macromolecular Division (President - Prof. T. Saegusa)

This Division has two commissions only and uses very efficiently the statute of Working Parties. There were 5 working parties before 1985 and now there are 3 such parties additionally organized for initiation of new important projects:

- Interaction of Polymers with Living Systems (very important for modern medicine)
- Polymeric Liquid Crystals (very important for advanced technologies)
- Computer Modelling of Free-Radical Polymerization

The efficiency of the Division of Macromolecular Chemistry as a whole is very high. Among 29 projects mentioned in the 1984 list-

ing 15 are or will be completed to the end of 1986. It is important to mention that the work on Macromolecular Nomenclature Compendium is finished.

V. Analytical Chemistry Division (President - Prof. G.H. Nancollas)

The Analytical Chemistry Division is the largest one in the Union (8 commissions), nevertheless it is managed in whole sufficiently well. 53 projects from 111 presented in the 1984 listing are or will be completed to the end of 1986. At the same time it is desirable to pay attention to the rather large number of "long-living" projects (17). For example, the Commission on Analytical Nomenclature (V.3) has 10 projects started in the period 1976-78 and only 2 of them will be completed to the end of this year (6 to the end of 1987). After the discussion of this problem at the 52nd Meeting of the Bureau, Prof. G.H.Nancollas has organized the work on the critical assessment of Commission's activity by members of the Analytical Division Committee.

High efficiency was again demonstrated by the Commission on Solubility Data (V.8). Four volumes have been published since the Lyon meeting and four other volumes are in press. Fourteen volumes are in advanced stage of preparation.

The Division Committee has completed the work on the project 1/81 - Determination of Trace Metals and Metalloids in Natural Waters. Two volumes of the book "Trace Elements in Water" are ready for press and the third volume is also completed.

The second edition of the Compendium on Analytical Nomenclature ("Orange Book") is also completed.

We should welcome the establishment of a good liaison between the Division of Analytical Chemistry and the Committee on Chemical Databases.

VI. Applied Chemistry Division (President - Dr. P.C. Kearney)

The situation in the Division of Applied Chemistry is on my opinion alarming.

High efficiency has been demonstrated by the Commission on Pesticide Chemistry (VI.5) - 6 from 10 projects will be completed to the end of this year. There is not at this moment sufficient information on the activity of the Commission on Oils, Fats and Derivatives (VI.3).

The Commission on Food Chemistry (VI.1) terminated 6 projects without (?) concrete results, started 10 new projects. Only one project will be completed to the end of this year.

The reconstructed Commission on Atmospheric Chemistry (VI.4) has started only 2 projects. This is not enough for 6 Titular Members, 2 Associate Members and 3 National Representatives.

The new Commission on Water Chemistry initiated only 1 project (6 Titular Members, 2 Associate Members and 2 National Representatives).

The main tasks of the Commission on Biotechnology (VI.2), which is under reconstruction, should be defined more precisely. Judging by the Minutes of Commission VI.2. Meeting in GDR (September 1986), it was decided to initiate a project on terms used in biotechnology and to study as a possible project the compilation of types of biological reactions used in chemical processes. On the whole the revitalization of Commission on Biotechnology goes too slowly.

VII. Clinical Chemistry Division (President - Dr. S.S. Brown)

The work of all Division Commissions is characterized by high activity and efficiency. It is desirable to underline also good cooperation with related bodies of other IUPAC Divisions and IFCC.

The Commission on Automation and Clinical Techniques (VII.1) in cooperation with the Commission on Analytical Nomenclature (V.3) has done a good job on projects related to the bioanalytical nomenclature, classification of analytical systems in clinical chemistry, measurement and presentation of "carry-over effects" in clinical chemistry.

The Commission on Quantities and Units (VII.2) has efficient relations with Commission on Molecular Structure and Spectroscopy (I.5) and with Expert Panel on Quantities and Units of International Federation of Clinical Chemistry. The documents on definitions and units in optical spectroscopy, on nebulizer and flame properties in flame emission and absorption spectrometry, on classification of assays, used in clinical chemistry and on some other subjects are prepared and distributed.

The Commission on Teaching (VII.3) has published a set of interesting documents (mostly in cooperation with IFCC) on problems of regulation and control of clinical chemistry teaching. The activity of this Commission is, on my opinion, helpful for many (especially for developing) countries and we should support them.

The Commission on Toxicology (VII.4) has published or distributed documents on nickel, aluminium and selenium analysis in biological fluids.

Concluding Remarks

On the whole we can be satisfied by the work of the most part of IUPAC Commissions. Some anxiety causes only the level of activity of the Applied Chemistry Division. I believe that we should ask Dr. P.C.Kearney to prepare more detailed report on the current situation in the Division before the next meeting of Bureau.

P.S. (July, 1987)

After discussing the state of things in the Applied Chemistry Division at the 52nd Meeting of the IUPAC Bureau, Prof. Ph.C. Kearney has done comprehensive work on the stimulation of the activity of a number of Commissions. The forming of projects of the Commission on Biotechnology is successfully progressing. Five projects are currently ongoing ("Glossary of Biotechnological Terms", "Symposium on Biotechnology in Chemistry", "Terms, Symbols and Units in Microbial Processes", "Interaction of Biotechnology and Organic Chemistry", "Single Cell Protein-Oil"). Four feasibility studies have been started. The concretization of the areas of the Commission activities is going on. Among new proposals the promotion of the development of new biotechnological methods for the treatment and utilization of industrial and other wastes is of special significance.

It is believed that ecological problems in general could be presented in the activities of the Applied Chemistry Division more significantly than it is today. These problems are touched upon in the projects of the Commission on Food Chemistry and the Commission on Pesticide Chemistry especially. They could be made the central point also on Atmospheric Chemistry and the Commission on Water Chemistry. At present there is great demand for the information on the lists of ecotoxicants discharged into the atmosphere and water by various industries (non-ferrous metallurgy works, paper and pulp and textile industries, microelectronic plants and so on); on the economic methods of waste water purification and the purification of the discharges into the atmosphere, the utilization of wastes; on the permissible standards of wastes and discharges of chemical substances per one unit of output; on the time of the half-decay of different types of organic substances in water and atmosphere and so on.

Generally speaking the IUPAC position concerning the ecological problems is of great importance. It is desirable that one of the CHEMRAWN conferences is devoted to discussing these problems.

Divisions and Commissions	Number of Projects				
	in the listing of 1984 (among them permanent)	completed or will be completed entirely or partly to the end of 1986	abandoned or suspended	started in the period of 1985-86	in the listing of 1986 (among them permanent)
1	2	3	4	5	6
<u>I. Physical Chemistry Division</u>					
Subcommittee on Physicochemical Measurements and Standards	2(0)	1	1	0	1(0)
Subcommittee on Plasma Chemistry	2(0)	1	0	1	2(0)
I.1. Commission on Physicochemical Symbols, Terminology and Units	4(2)	0	0	0	4(2)
I.2. Commission on Thermodynamics	3(0)	0	2*	1	3(0)
- Subcommittee on Thermodynamic Tables	5(0)	3	0	3	6(0)
- Subcommittee on Transport Properties	1(0)	0	0	2	3(1)

* Projects 5/83 and 6/83 replaced by 9/85

1	2	3	4	5	6
I.3. Commission on Electrochemistry	13(2)	5	2	2	11(2)
I.4. Commission on Chemical Kinetics (established in 1983)					
- Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry				1	1
- Subcommittee on Symbolism and Terminology in Chemical Kinetics	-	-	-	5	5(0)
I.5. Commission on Molecular Structure and Spectroscopy	6(0)	4	0	3	8(0)
- Subcommittee on Infrared and Raman Spectroscopy	6(0)	4	1	2	5(0)
- Subcommittee on Mass Spectroscopy	2(0)	1	0	0	2(0)
- Subcommittee on Chiroptical Phenomena (disbanded in 1983)	1(0)	1	0	0	1(0)
- Subcommittee on Notations and Conventions for Molecular Spectroscopy	1(0)	2	0	2	3(0)
I.6. Commission on Colloid and Surface Chemistry including Catalysis	6(0)	5	0	2	5(0)

1	2	3	4	5	6
- Subcommittee on Catalyst Characterization	-	-	-	1	1
- Subcommittee on Reference Material	-	-	-	-	-
- Subcommittee on Characterization of Porous Solids	-	-	-	1	1
- Working Party on Thin Films	-	-	-	1	1

41 EM + 51 AM	52	27	6	27	63
<u>II. Inorganic Chemistry Division</u>					
II.1. Commission on Atomic Weights and Isotopic Abundances	5(3)	2	0	0	3(3)
- Subcommittee on Isotopic Abundances Measurements	-	-	-	1	1(1)
- Working Party on Measurements, Sensors and Measuring Instruments	-	-	-	1	1(1)
- Working Party on Natural Isotopic Fractionation	-	-	-	1	1(1)
II.2. Commission on Nomenclature of Inorganic Chemistry	15(0)	10	0	4	19(0)

1	2	3	4	5	6
II.3. Commission on High Temperature and Solid State Chemistry	12(1)	4	1	6	16(1)
22 TM + 30 AM	32	16	1	13	41
<u>III. Organic Chemistry Division</u>					
III.1. Commission on Nomenclature of Organic Compounds	17(0)	3	2+1*	0	13(0)
III.2. Commission on Physical Organic Chemistry	11(0)	3	6**	0	5(0)
- Working Party on Quantum Chemical and Computational Data	-	-	-	-	1
- Working Party on Standards for Presentation of Data	-	-	-	-	1
III.3. Commission on Photochemistry	6(0)	3	1***	5	8(0)
20 TM + 25 AM	34	9	10	5	28

* Project 15/83 is included in 2/81 and 6/81

** Projects 5/81-10/81 are amalgamated with 2/81

*** Project 7/83 is combined with 3/81

1	2	3	4	5	6
<u>IV. Macromolecular Division</u>					
IV.1. Commission on Macromolecular Nomenclature	10(0)	7	0	5	14(0)
IV.2. Commission on Polymer Characterization and Properties					
- Working Party on Structure and Properties of Commercial Polymers	9(0)	4	1	2	5(0)
- Working Party on Molecular Characterization of Commercial Polymers	5(0)	4	1	3	6(0)
- Working Party on Supported Polymer Films	3(0)	0	0	0	3(0)
- Working Party on Thermal Properties of Polymers	1(0)	0	0	1	2(0)
- Working Party on Kinetic Parameters for Free Radical Polymerization	1(0)	0	0	0	1(0)
15 TM + 16 AN	29	15	2	11	31

1	2	3	4	5	6
<u>V. Analytical Chemistry Division</u>					
Analytical Chemistry Division Committee	5(0)	2	1	1	4(0)
V.1. Commission on Analytical Reactions and Reagents	9(0)	8	0	3	10(0)
V.2. Commission on Microchemical Techniques and Trace Analysis	20(0)	13	0	3	17(0)
- Working Party on Organic Trace Analysis	-	-	-	4	4(0)
- Working Group on Surface Analysis	-	-	-	2	2(0)
V.3. Commission on Analytical Nomenclature	18(0)	2	1	3	20(0)
V.4. Commission on Spectrochemical and other Optical Procedures for Analysis	12(0)	4	1	1	12(0)
V.5. Commission on Electroanalytical Chemistry	18(0)	8	2	2	12(0)
- Subcommittee on Electroanalytical Methods of Environmental Trace Analysis	7(0)	1	1	6	11(0)
V.6. Commission on Equilibrium Data	9(0)	2	2	5	12(0)
V.7. Commission on Radiochemistry	-	-	-	5	5(0)
V.8. Commission on Solubility Data	2(1)	1 (partly)	0	0	2(1)
- Subcommittee on Gas Solubilities	3(0)	5	0	2	5(0)
- Subcommittee on Liquid Solubilities	3(0)	3	0	2	5(0)
- Subcommittee on Solid Solubilities	5(0)	4	0	3	7(0)
51 2M + 89 AM					
	111	53	8	42	128

1	2	3	4	5	6
<u>VI. Applied Chemistry Division</u>					
Applied Chemistry Division Committee	1(0)		0	0	1(0)
VI.1. Commission on Food Chemistry	9(0)	1	6	10	12(0)
VI.2. Commission on Biotechnology (under review)	3(0)	-	-	-	-
VI.3. Commission on Oils, Fats and Derivatives	17(0)	3	0	0	15(0)
VI.4. Commission on Atmospheric Chemistry (previously - on Atmospheric Environment)	-	-	-	2	2(0)
VI.5. Commission on Pesticide Chemistry	10(0)	6	1	0	6(0)
VI.6. Commission on Water Chemistry	-	-	-	1	1(0)
33 TM + 34 AM	40	10	7	13	37

1	2	3	4	5	6
<u>VII. Clinical Chemistry Division</u>					
Clinical Chemistry Division Committee	1	1	0	1	1
VII.1. Commission on Automation and Clinical Chemistry Techniques	3	1	0	0	3
VII.2. Commission on Quantities and Units	8	4	0	2	7
VII.3. Commission on Teaching	6	4	0	5	10
VII.4. Commission on Toxicology	-	-	0	1	1
- Subcommittee on Environmental and Occupational Toxicology of Nickel	5	1	3*	0	2
- Subcommittee on Environmental and Occupational Toxicology of Cadmium	3	1	1	0	1
- Subcommittee on Toxicology of Selenium	2	1	0	0	2
- Subcommittee on Analytical Methods	-	-	-	2	2
- Subcommittee on Harmonization	-	-	-	2	2
- Subcommittee on Risk Assessment	-	-	-	1	1

22 EM + 23 AM	28	13	4	14	32

* are transferred to other Subcommittees