

Minutes of the meeting of the Commission on Molecular Structure and Spectroscopy (I.5) at the IUPAC General Assembly, Berlin, Germany August 8- 10, 1999

The following members of Commission 1.5 were present

Professor John E. Bertie, chairman

Professor Peter Klæboe, secretary

Professor Anton Heyns, titular member

Professor James E. Boggs, titular member

Professor Robin S. McDowell, titular member

Professor N. Hirota, titular member

Dr. Sonia Maria Cabral de Menezes, associate member

Professor Jozef Kowalewski, associate member

Professor A. Oskam, associate member

Professor Robin K. Harris, national representative

Professor Ben van der Veken, national representative

Professor Rudolf Janoschek, national representative

Dr. Brenda P. Winnewisser, observer

Professor Quing-Shi Zhu, associate member

Dr. Karen McNamara observer, attended the session on Sunday

The following members were not present at the meetings of Commission I.5:

Professor Soji Tsuchiya, associate member

Professor Paul von Ragué Schleyer, associate member

Dr. J. J. C. Teixeira-Dias, national representative

Professor Yoon Sup Lee, national representative

Professor Jerzy Hawranek, national representative

Professor Periyakarupan T. Manoharan, national representative

1. Constituting the Commission, Introduction of Titular and Associate Members, National Representatives and Observers. Schedule of Meetings (Document A)

The meeting was conducted by the Chairman, Professor John E. Bertie, who welcomed the members to the commission's meeting. The attendees briefly introduced themselves, mentioning their interests and experience. Some minor changes in the telephone and fax numbers and the E-mail addresses of the attendees were noted.

The agenda had been sent to all members ahead of time and was approved by the commission.

2. Minutes of the Geneva meeting, August 1997 (Document B)

The minutes from the meeting of Commission I.5 at the IUPAC General Assembly in 1997 in Geneva, Switzerland had been sent to all members by the secretary in the fall 1997. The summary of the minutes was published in *Chemistry International* 20, 34 (1998), and the minutes and the summary were approved. There were some comments from A. Heyns regarding the project 150/24/95, "Spectroscopy under Extreme Conditions of Temperature and Pressure," and questions about the proposed project 11.5, "Nomenclature for tensor quantities used in NMR, NQR and ESR Spectroscopies."

3. Matters arising from the Geneva meeting not on the agenda (Document C)

No matters were discussed.

4. Report of the Chairman on the Environment of the Commission within IUPAC

4.1 Basis and purpose of our operation (Documents D1-D2 and E1-E5)

The Chairman discussed the probable future of IUPAC, which has been formulated in various documents from the President and the General secretary. Moreover, the Strategic Development and Implementation Committee (SDIC) established in April 1997 by the IUPAC Executive Committee (EC) has made a recommendation which is published in *Chemistry International* 20, 55 (1998). The implementation of these proposals for the future will be decided by the Bureau during its meetings 11-14 of August at the GA in Berlin 1999.

Among the many changes proposed by SDIC, the abolishment of nearly all the commissions after the General Assembly in 2001 and the introduction of a new project driven system have the largest impact on the future work of the present commissions. The President wants to tighten the connection with industry and governments and expects that more funds from these sources will be available to the Union. Motivation for the changes has particularly come from USA and UK, and the representatives of these countries want a closer tie to the chemical industry. The chairman expressed concern that if these changes were carried out they would lead IUPAC into being a more political than scientific organization.

Sonia Cabral de Menezes forwarded complaints from the Brazilian national organization that the proposed new system would be a disadvantage for Brazil and would have the effect that the national representatives of many developing nations would be weakened, since these representatives apparently would play a minor role in the project driven system.

4.2 Recent Activities of the Physical Chemistry Division (Document F)

It was reported that the Physical Chemistry Division of IUPAC has played a quite active role with a large output of papers, and that eventual complaints about inadequate IUPAC activities must reflect the effectiveness of other divisions.

The Commission agreed that although year 2001 may represent the deadline for the present commissions we should continue with our projects and should also develop new projects which are scientifically relevant and of interest to the chemical community within our mandate.

The President and Vice-president of the Physical Chemistry Division: Professors T. Cvitas and H. G. Wilson visited the Commission at 10.00 o'clock. They greeted the Commission from the Physical Chemistry Division and described some of the proposed new rules. A person proposing an interesting project to the Division will be financed to carry out the project within the framework of an *ad hoc* task force. This work can go on for two years, but might be extended to four years. The average budget for a future project has not been decided and will undoubtedly vary according to the number of persons involved the length of the project and the geographic distribution of the task force members.

In principle, it is planned to get more involvement from countries, which are not represented, in the present IUPAC structure. However, it is difficult to see how this can be done in a project driven system in which the persons asked to carry out the projects on an *ad hoc* basis will be selected from leading authorities in the field. There seems to be no role for the national representatives in the new system. The cost of maintaining these representatives is presently carried out by the national organizations. Thus, the project driven system suggested, may be more and not less expensive to the IUPAC budget.

After the President and Vice-president of the Physical Chemistry Division had left, the Commission proceeded with the agenda, and the chairman referred to the Physical Chemistry Divisions meeting in Frankfurt a/M February 25-26, 1999. He elaborated the draft minutes of March 4, 1999 (F in the agenda), which mostly concerned the impact of the proposed changes to IUPAC on the Physical Chemistry Division.

4.3 The Current IUPAC Environment (Documents G)

4.3A Statements by the President and Secretary-General (Document H) in Chemistry International 20, 163 (1998) (document H)

The President and Secretary-General's statements concerning the reorganization of IUPAC were briefly discussed. The future publication of the IUPAC journals: Pure and Applied Chemistry (PAC) and Chemistry International and of books were reported. Blackwell has for a long time had a contract for these publications. However, this company does not do a satisfactory job publishing these books since they are not easily available, particularly in North America. In the future, PAC will be published by IUPAC, and other publishers are being considered for the books.

4.3B Project Submission and Approval Processes; Chemistry International 21, 8 (1999). (Document I)

The Bureau approved at its meeting in Frankfurt a/M a new system for the submission and approval of projects funded by IUPAC. During the period 1999-2001 funding will be made both by the current method of funding commissions and by the new system of funding projects. The funding procedures were briefly discussed by the Commission.

4.4 Report on the Physical Chemistry Division Meeting of Saturday August 7, 1999

The chairman briefly reported from the meeting, which mostly had dealt with the role of the physical chemistry in the new organization of IUPAC

5 Brief Report of the Chairman on the Activities of the Commission

5.1. General (Document J)

The chairman outlined the activities of Commission I.5 between the General Assemblies in Geneva and in Berlin as formulated in Document J on the Agenda.

5.2. Reports of the Chairman to the President of the Physical Chemistry Division (Documents K and L)

First, the chairman registered an official protest against the statements of the President and General Secretary concerning the work of the commissions within IUPAC. These statements were made in connection with the drastic changes proposed for IUPAC in which the commissions will be abolished after year 2001, and the scientific work of IUPAC is carried out on an *ad hoc* basis. The probable adverse consequences for the future work were outlined, leading to an orientation of IUPAC from scientific towards political goals. No comments from members of Commission I.5 were made contradicting this protest, which therefore in general terms express the opinion of its members.

A brief summary of the status of the current projects of Commission I.5 and from the Subcommittees on Notations and Conventions for Molecular Spectroscopies and on Theoretical Chemistry were listed in the report.

5.3. Commission (IUPAC) Web Site:

It should be known to the members of Commission I.5 that the names of the titular members, associate members, national representatives and of the subcommittees are listed on the home page of IUPAC. In the future the minutes from the General Assemblies and the various projects will probably be written on the web.

6. Joint meeting of Commission I.5 and Commission on Spectrochemical and other Optical Procedures for Analysis (V.4)

The members of Commissions I.5 and V.4 presented their names and the current projects of each commission were described by the chairmen John E. Bertie and T. Vo-Dinh.

From Commission I.5 the following projects were reported:

1. 150/18/93 "Provisional Recommendations for NMR Nomenclature, Nuclear Spin Properties and Conventions for Chemical Shifts" (authors) R. K. Harris, E. Becker, W. Bremser, S. Cabral de Menezes, R. Goodfellow and P. Granger.

2. 150/19/93 "Specification of Components, Methods and Parameters in Fourier Transform Spectroscopy by Michelson and Related Interferometers," (author John E. Bertie) Pure and Appl. Chem. 70, 2039-2045 (1998).

3. 150/20/93 "Nonlinear Spectroscopy for Molecular Structure Determination" (edited by R. W. Field, E. Hirota, J. P. Maier and S. Tsuchiya) appeared as a book published by Blackwell 1998 containing 276 pages and 10 chapters written by different authors, describing the various non-linear techniques as an introduction for non-specialists.

4. 150/2/95 "The Computation of Experimental Structure and Properties of Small Molecules by *Ab Initio* Calculations," (author Rudolf Janoschek). The report computes the bond distance, vibrational anharmonicity, dipole moments and spectral parameters of

ca. 200 diatomic molecules by density functional methods. Results for some larger molecules (up to 6 atomic) are included.

5. 150/24/95 "Spectroscopy under Extreme Conditions of Pressure and Temperature," (author A. M. Heyns, contributors D. M. Adams, W. B. Holzapfel, M. N. Nicol, Ph. Pruzan). A preliminary report of 220 pages has been written and a summary of 6 pages was presented in Berlin. The report will be mostly concerned with high pressure rather than high temperature, and will focus predominantly on the Diamond Anvil Cell (DAC) applied to infrared and Raman spectroscopy. Dr. Heynes reported that the paper is not focussed particularly on applications and is not a review article. It should be completed before the next General Assembly.

6. 150/25/98 "Quantities, Terminology and Symbols in Photothermal and Related Spectroscopies," (authors M. Terazima and N. Hirota). A report of 29 pages has been presented, describing the various photothermal effects. For analytical applications it would be advantageous for the authors to cooperate with Commission V.4.

7. 154/5/97 "Notations and Conventions in Molecular Spectroscopy Part 4. Vibrational-Rotational Spectroscopy" (authors R. S. McDowell, J. E. Bertie, P. R. Bunker, J.-M. H. Flaud, J. T. Haugen, P. Rosmus, J. K. G. Watson, B. P. Winnewisser). A 40-page report has been written, soon ready to be submitted to Pure Appl. Chem. for publication. Earlier reports: parts 1, 2 and 3 have been published in Pure Appl. Chem. in 1997.

8. 154/6/97 "Notations and Conventions in Molecular Spectroscopy Part 5. Electronic-Vibrational-Rotational Spectroscopy" is planned, but the progress will depend upon the workload of J. K. G. Watson.

9. 155/1/95 "Guidelines for the Presentation of Methodological Choices in the Publication of Computational Results," A. *Ab Initio* Electronic Structure Calculations (author J. E. Boggs) published in Pure and Appl. Chem. 70, 1015-1018 (1998)

10. "Guidelines for the Presentation of Methodological Choices in the Publication of Computational Results, B. Semiempirical Electronic Structure Calculations," (author J. J. P. Stewart). A report of four pages was presented to be published shortly in PAC.

From Commission V.4 the following projects were reported

1. 540/15/95 "Waveguides," The manuscript will be sent by the authors to the Commission (V.4) in February.

2. 540/16/95 "Supersonic Jet," A new draft has been prepared. No direct information from Commission I.5 was intended. After reorganization the manuscript will be forwarded to IDCNS and later to the experts. This paper should be ready for publication soon. It has been discussed whether a 10-page database should also be included. The decision was to extract some essential data and put the whole database to the WebSite of the Commission. The paper will then be distributed to Commission I.5 for review.

3. 540/17/95 “LIDAR,” This project was presented at the meeting, but has later been cancelled since Dr. D. Moore has moved to the Analytical Chemistry Division Committee and he ran out of time to complete the project.
4. 540/18/95.” Hyphenated Techniques,” The general concept was presented at the joint meeting with Commission on Separation Method in Analytical Chemistry (V.3).
Hyphenation: Combination of different (e.g., separation and spectroscopic) methods (not simply detection). Hyphenated techniques involve the on-line coupling of a separation and an optical detection method, and the system has to provide more than a pure signal, but rather a spectrum. Hyphenated techniques combine two different types of analytical techniques: separation and spectroscopy, each technique has to supply multi-dimensional information. Thermal desorption/MS has to be included. The influence of the interface and the environment also have to be considered.
5. 540/19/95. “ Optical biosensors and bioprobes,” The project deals with biosensors and spectroscopic techniques. What is a biosensor? The performance criteria of biosensors are discussed, and the various spectroscopic techniques employed, e.g.: absorption, fluorescence, polarization are described in the report. A mini-meeting is scheduled along with Europt(r)ode 2000, approx. April 18, 2000 for completing the project.
6. 540/20/95: “Identification, coordination, and extension of bioanalytical sensors projects,” This project is closely related to the former 540/19/95 and represents a project oriented activity since biosensors do not belong to any of the earlier commissions.
7. 540/21/97: “Surface/Interface, Elemental Analysis,”
deals with optical methods for studying surfaces, definitions, operating principles (figures and equations), instrumentation and performance criteria (LOD, selectivity, etc.)
The recently published project from Commission I.5: A. M. Bradshaw and . V. Richardson, Symmetry, Selection Rules and Nomenclature in Surface Spectroscopy, Pure Appl. Chem. 68, 457 (1996) will be considered. The title will be modified to Part I: Elemental Analysis by Glow Discharge, Atomic Emission Spectrometry and Laser-Induced Break-down Spectrometry.
8. 540/24/98: “Femtosecond Techniques.”
This field is very actual in view of the Nobel Prize in Chemistry in 1999 to A. Zewail for femtosecond chemistry (added Oct 16). A subtitle is proposed as Part I: Multiphoton Ionization Mass Spectrometry. The content will be restricted to analytical applications and the project has to have global applications. The present outline is restricted to a small area. For this reason Commission V.4 considered the following points: emphasis on the advantages of femtosecond lasers in modern spectrochemical analysis, why does one need such type of lasers, advantages and limitations and compare femtosecond techniques with nanosecond techniques.

7. Reports on the Status of Projects of Commission I.5

7.1. Project 150/18/93: (Document M) R. K. Harris, E. Becker, W. Bremser, S. Cabral de Menezes, R. Goodfellow and P. Granger, **Provisional Recommendations for NMR Nomenclature, Nuclear Spin Properties and Conventions for Chemical Shifts**.

The project is nearly finished and written in a report of 21 pages, it has 74 references and contains 4 tables giving spin properties of Spin 1/2 nuclei, of quadrupolar nuclei, lanthanide and actinide nuclei and alternative secondary references.

7.2. Project 150/19/93: (Document N) John E. Bertie, **Specification of Components, Methods and Parameters in Fourier Transform Spectroscopy by Michelson and Related Interferometers**, Pure Appl. Chem. **70**, 2039-2045 (1998).

The parameters are listed with one table for Fourier transform spectrometers of modest resolution ($0.25\text{-}8\text{ cm}^{-1}$), one table for instruments of high resolution (better than 0.01 cm^{-1}) and one table dealing with Fourier transform Raman spectroscopy. The paper has been distributed to ca. 55 journals of molecular spectroscopy, analytical chemistry, physical chemistry, polymer chemistry and organic chemistry, asking the editors to adopt these standards and distribute them to authors and referees, for example through the web. The paper is presently being reprinted in Australian J. Chem.

7.3. Project 150/20/93: editors R. W. Field, E. Hirota, J. P. Maier and S. Tsuchiya, **Nonlinear Spectroscopy for Molecular Structure Determination**, Blackwell, Oxford 1998.

The book contains 276 pages and 10 chapters written by well known international specialists. The first chapter (by M. Takami) gives an introduction to the basic principles of laser spectroscopy while the 9 remaining chapters describe the various non-linear techniques with their common acronyms in terms of theory, instrumentation and a few applications. These methods have proved to be powerful tools for the study of molecular structure and dynamics, sometimes giving orders of magnitude more precise results than with conventional light sources. Written as an introductory monography for non-specialists with many references and a comprehensive index, the book should be useful as a hand book for molecular spectroscopists and a text for graduate courses in molecular spectroscopy.

7.4. Project 150/2/95: (Document O) R. Janoschek, **The Computation of Experimental Structure and Properties of Small Molecules by *Ab Initio* Calculations**.

This project was also discussed in detail by the commission at the General Assembly in Geneva in 1997 as reported in the minutes. The present report was revised according to this discussion and presents comprehensive calculations using density functional theory.

The report computes the relative electronic energy T_e , bond distance r_e , harmonic vibrational wavenumber ω_e , absolute absorption intensity A , electric dipole moments μ , ionization potential IP and dissociation energy D_0 of ca. 200 diatomic molecules at the level B3LYP/cc-pVQZ by density functional theory. Special tables are presented for 50 selected polyatomic molecules (up to 6 atomic) where the calculated structures are compared with experimental values from ED and MW experiments and 50 molecules where the computed NMR shifts are compared with the experimental values. Another table presents 20 polyatomic radicals in which the hyperfine splitting is compared with results from ESR spectroscopy. In 30 diatomic molecules the anharmonicity $\omega_e x_e$ are compared with results from IR spectroscopy. The report might fill ca. 70 pages and in

addition 30 pages of references. The Commission expressed compliments to R. Janoschek for the large amount of work he has done single handed on this project.

Various details concerning the paper were discussed in the commission: should the total energy be omitted to save space? There are reasons to include quadrupole moments, and the signs of the dipole moments should be explained in a footnote. In Table 4 ClO_2Cl and C_5O give poor agreement with the experiments, also in a very important molecule like CO_2 there are large discrepancies between calculated and observed values. The paper should if possible be published in *J. Mol. Struct. (Theochem)*. The importance of good references was stressed, if too extensive for an article they could be put on the web.

7.5. Project 150/22/95: (Document P) R. K. Harris, J. Kowalewski and S. Cabral de Menezes, **Parameters and Symbols for Use in Nuclear Magnetic Resonance**, *Pure Appl. Chem.* **69**, 2489-2495 (1997). This paper has also been published in two journals devoted to NMR spectroscopy.

7.6. Project 150/23/95: J. E. Bertie, **Spectroscopic Intensities; Related Quantities, Nomenclature and Symbols**.

This project has contributed to the Green book and to project 154/5/97 and has been terminated.

7.7. Project 150/24/95: (Document Q) A. M. Heyns and collaborators D. M. Adams, W. B. Holzapfel, M. N. Nicol and Ph. Pruzan, **Spectroscopy under Extreme Conditions of Pressure and Temperature**.

Anton Heyns reported that a very extensive report will result from this project, and that a preliminary report of 220 pages has been completed whereof a summary of 6 pages was presented in Berlin. Dr. Heyns gave a comprehensive description of the report. The paper will mostly be concerned with high pressure rather than high temperature, and will focus predominantly on the Diamond Anvil Cell (DAC) first developed by Weir, Lippincott, Valkenburg and Buntling in 1959, and applied to UV, visible, infrared and Raman spectroscopy. There will be no reference to Mössbauer and other spectroscopic techniques. Conventional piston-cylinder cells, anvil cells, belt systems and Drickamer cells, employed by specialists are described, but emphasis is put on high pressure measurements with the DAC, which is very widely used. The sample is confined between two diamond anvils within a hole in a metal spacer of typically 0.4 mm inner diameter and the cell can be easily interfaced with optical UV, visible, IR and Raman spectrometers. The cell was interfaced to old dispersive instruments with a beam condenser, but the vastly improved signal/noise ratio with modern FT instruments makes the recording much easier. Sapphire cells can be employed for lower pressures. Sophisticated ways of drilling the holes by lasers and interfacing to spectrometers with fibre technique have been described by Pruzan et al.

Emphasis has been put on pressure determination which is not straightforward with the DAC. The ruby chip method, based upon the pressure induced shift of the fluorescence band has been widely used and can be employed up to 500 kbar (Pa will be used as the pressure unit) although there is a pressure broadening at high pressure. The report will not review all the papers which have appeared in the literature, but ca. 50 pages will describe various applications.

Several aspects of this work were discussed by the commission, Anton Heyns was praised for the large amount of work invested in the project, it was suggested to include optical spectroscopy in the title, and that the author should look for possible overlap with earlier review articles. The report should hopefully enable many spectroscopists to carry out high-pressure experiments. The publication of the report was discussed, it should if possible be written as a book rather than publishing in PAC, and the work will hopefully be completed in the near future.

7.8. Project 150/25/98: (Document R) M. Terazima and N. Hirota, **Quantities, Terminology and Symbols in Photothermal and Related Spectroscopies.**

A preliminary report of 30 pages was presented, defining the field, systemizing the nomenclature and describing the various spectroscopic and calorimetric techniques involved. Photoacoustic detection, and the methods of thermal lens, thermal grating and interferometry, in which changes in the refractive index of the sample are measured, represent applications of these means of light detection. The methods are very sensitive and of increasing importance in applied science.

N. Hirota described the progress and had contacted various possible collaborators. A meeting in this field will be held in Kyoto in July 2000. The chairman thought IUPAC could support possible collaborators to attend this meeting in order to facilitate the work. Hopefully, the work should be completed before the year 2001. A long list of physical parameters was included in the report (pages 27-28) and John Bertie emphasized that all the units should be employed according to the green book. Brenda Winnewisser believed that the applications of these techniques should not be included in the paper, but if applications are included they should be made in cooperation with Commission V.4. The commission felt that the photothermal and related spectroscopies would be very important in analytical chemistry in the future.

8. Reports on the Status of Projects of the Subcommittee on Notations and Conventions for Molecular Spectroscopies.

8.1. Project 154/5/97: (Document S) R. S. McDowell, J. E. Bertie, P. R. Bunker, J. -M. H. Flaud, J. T. Hougen, P. Rosmus, J. K. G. Watson and B. P. Winnewisser, **Notations and Conventions in Molecular Spectroscopy: Part 4. Rotation-Vibration Spectroscopy.**

A nearly completed draft of 36 pages text and an appendix of 8 pages consisting of an index of symbols and a subject index was presented to the Commission by R. S. McDowell. I. M. Mills has also contributed to the paper. The earlier reports in the series: Notations and Conventions in Molecular Spectroscopy, part 1, General Spectroscopic Notation; part 2, Symmetry Notation and part 3, Permutation and Permutation-Inversion Symmetry Notation, have been published in Pure Appl. Chem. 69, 1633 (1997); 69, 1641 (1997) and 69, 1651 (1997), respectively. The present paper gives a complete description of the symbols and notations used in rotational-vibrational spectroscopy as can be observed in the vapor phase by infrared and Raman spectroscopy, and is based upon the work of R. S. Mulliken and G. Herzberg. The Mulliken-Herzberg nomenclature will be documented for future spectroscopists. New techniques have made it possible to measure spectral transitions, which have not been measured earlier, and the recommendations should be exact. Hopefully, the paper will be completed in the fall and it will be sent to various specialists for comments.

The Commission discussed various details of the paper. Brenda Winnewisser asked about Cartesian coordinates in the *ab initio* calculations and the need for the A-matrix and if internal coordinates can be introduced initially. Inexactness in the point group symbols of the green book was pointed out which should be corrected in cooperation with Commission I.1.

8.2. Project 154/6/97, **Notations and Conventions in Molecular Spectroscopy Part 5. Electronic-Vibrational-Rotational Spectroscopy**, is planned, but the progress will depend upon the workload of J. K. G. Watson. If he cannot carry it through, the project will have to be cancelled.

9. Reports on the Status of Projects of the Subcommittee on Theoretical Chemistry

9.1. Project 155/1/95, (Document T) J. E. Boggs, **Guidelines for the Presentation of Methodological Choices in the Publication of Computational Results, part A. *Ab Initio* Electronic Structure Calculations**, Pure Appl. Chem. **70**, 1015-1018 (1998). This paper has been sent to various journals of which some have reprinted the paper and others will send it to referees and authors.

9.2. Project 155/2/95, (Document T) J. J. P. Stewart, **Guidelines for the Presentation of Methodological Choices in the Publication of Computational Results, B. Semiempirical Electronic Structure Calculations**.

This paper was approved by the commission and a few changes were recommended. A few minor changes have been made by the author and the paper has later been submitted to PAC (according to information from J. E. Boggs on October 13, 1999).

9.3. Project 155/3/95, (presented by James E. Boggs) **Guidelines for the Presentation of Methodological Choices in the Publication of Computational Results, C. Molecular Mechanics Calculations**.

At the General Assembly in Geneva and shortly afterwards it was agreed that this project should be a joint undertaking of Commissions I.5 and I.7 and that it should be led by Dr. Terry Stouch of Commission I.7. No progress appears to have been made since then. Further, Terry Stouch was not present in Berlin, and the Chairman of Commission I.7 has indicated his intention to terminate the project. In 1998 the Organic Division published a related paper [PAC, vol. 70, pp 2047-2049 (1998)] which is insufficiently detailed to satisfy the needs of theoreticians. The members of Commission I.5 agreed that this is a very important project because many scientists are interested in very large molecules for which molecular mechanics calculations are essential. Also because many such calculations are being done by people who are not expert theoreticians and who need the guidance of experts in deciding how much computational detail should be published in order for the significance of the study to be judged meaningfully by other scientists. Accordingly, it was agreed that it should be left in the hands of Professor Boggs to seek experts to pursue the project. N. L. Allinger has shown interest in the past, but may prove to be too busy to work on this project.

10. Joint meeting of Commission on Electrochemistry (I.3) and Commission I.5.

The scheduled meeting between Commission on Electrochemistry, I.3 and I.5 was cancelled.

11. Joint meeting of Commission on Physicochemical Symbols, Terminology and Units, I.1 and Commission I.5.

The members of Commissions I.1 and I.5 presented their name and affiliation, and the projects of Commission I.5 which would give rise to additions and/or alterations in the next edition of the Green Book (Quantities, Units and Symbols in Physical Chemistry) were discussed.

A slightly revised version of the green book has been written by Commission I.1 and Chapter 2.6 Spectroscopy and 2.7 Electromagnetic Radiation were sent to Commission I.5 ahead of time. However, neither the copy sent to John Bertie nor to Peter Klaeboe arrived in time before leaving for Berlin. During the joint session various details in these chapters were corrected by Commission I.5. Particularly in the field of NMR spectroscopy, R. Harris, J. Kowalewski and S. Cabral de Menezes suggested various corrections to the new version of the green book. These parts of the corrected manuscript will be sent to M. Quack from Commission I.5.

12. Plans for the Future

12.1 Recommendations for Future Activity: How to proceed if commissions close.

It was felt necessary to discuss the future work of the commission on the background of the completely new organization of IUPAC, and various aspects of the new routines were discussed.

- A. New proposals can be still be forwarded. As many strong projects as possible should be suggested. Projects will be approved differently in the future. Meetings once a year would speed up the projects.
- B. The members of commissions will in the future be appointed and supported on an *ad hoc* basis and a distinction between titular and associate members will not be meaningful.
- C. What about National representatives? When working groups (new commissions) are assembled to work on a special project, there may be no place for NRs. This may have an adverse effect on many developing nations who will have less chance to participate in the new commissions. These countries will loose contact with IUPAC. National representatives have different meaning in unlike countries.
- D. There may be less reason to go to General Assemblies in the future, meetings of the commissions can be held anywhere, such as in connection with international conferences.
- E. The Physical Chemistry Division Committee will presumably be selected from a "charmed circle" of insiders in the future since there will be no commissions to elect its members as is now the case.

New projects, various possible future projects were suggested:

Nomenclature for tensor quantities used in NMR, NQR and ESR Spectroscopies, this project was also suggested in 1997 in Geneva.

Project 150/25/98, "Quantities, Terminology and Symbols in Photothermal and Related Spectroscopies," may be completed before 2001 or may be extended beyond that date.

Mössbauer spectroscopy.

X-ray crystallography. This field is handled by International Union of Crystallography.

Infrared and Raman spectroscopy of biological molecules

Intensities, liquids-vapors

Chemometrics applied to near-infrared (NIR), mid infrared (MIR) and Raman spectroscopy. NIR spectroscopy with typical broad overlapping bands is depending upon chemometric techniques for analytical applications.

12.2 Subcommittee on Notations and Conventions for Molecular Spectroscopy

The only remaining project of this subcommittee is

Project 154/6/97, Notations and Conventions in Molecular Spectroscopy Part 5. Electronic-Vibrational-Rotational Spectroscopy. If this project will not be carried out the subcommittee will be discontinued.

12.3 Subcommittee on Theoretical Chemistry

Theoretical chemistry is a field in very rapid development due to the vast progress in computers and programs, making calculations available for non-specialists. The award of the Nobel prize in Chemistry for 1998 to Walter Kohn and to John A. Pople supports this conclusion. The Subcommittee on Theoretical Chemistry established in 1995 within Commission I.5 is the only body within IUPAC working systematically in this field and this work should continue in the future. The present Project 155/3/95, Guidelines for the Presentation of Methodological Choices in the Publication of Computational Results, C. Molecular Mechanics Calculations should be continued and new projects proposed.

12.4 People who might we willing to work for IUPAC in the future

This part of the agenda was not discussed

13. Other Business

Commission members raised the following points which were briefly discussed without reaching unique conclusions. What is the best way to get IUPAC documents, that are now typically published in the little-read Pure and Applied Chemistry, widely known in the chemical community? It was generally agreed that it would help to refer to them in journals, present them at conferences, to make them available at the web and to advertise their existence on the web to the chemical community in citations and by word of mouth.

The meeting of Commission I.5 was terminated, the chairman thanked the members and looked forward to see them at the General Assembly in Brisbane, Australia in 2001.