

## Commission on Molecular Structure and Spectroscopy-I.5

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### **Summary of Minutes of Commission Meeting at the IUPAC General Assembly, Brisbane, Australia, 30 June-2 July 2001**

*For greater utility, this report has been updated to include activities completed by December 17, 2001.*

Twelve members of the Commission on Molecular Structure and Spectroscopy (I.5) with two subcommittees and including two observers, met for two days during the 41st General Assembly at the Queensland University of Technology in Brisbane. The participants enjoyed the pleasant winter weather in Queensland and the beautiful setting of the “river city” Brisbane. The reorganization of IUPAC is final and Commission I.5 like many other bodies will cease to exist at the end of 2001. The activity must therefore be concentrated on getting the pending projects finished.

Three projects which were completed earlier have been published in additional journals: 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), Magnetic Resonance in Chemistry **36**, 145-149 (1998), Solid State NMR **10**, 111-116 (1998), Quimica Nova **22**, 622-629 (1999) in Portuguese; J. E. Bertie, *Specification of Components, Methods and Parameters in Fourier Transform Spectroscopy by Michelson and Related Interferometers*; Pure Appl. Chem. **70**, 2039-2045 (1998), Austr. J. Chem. **52**, 721-725 (1999), Appl. Spectrosc. **55**, 510-513 (2001); 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), Some journals have reprinted the paper, others have sent it to referees and authors.

One project was completed since Berlin: J. J. P. Stewart, *Guidelines for the Presentation of Methodological Choices in the Publication of Computational Results, part B. Semiempirical Electronic Structure Calculations*, Pure Appl. Chem. **72**, 1449-1452 (2000).

The following project was already approved by the Commission: R. K. Harris, E. D. Becker, S. Cabral de Menezes, R. Goodfellow and P. Granger; *Nuclear Spin Properties and Conventions for Chemical Shifts*, providing guidelines for nomenclature and containing accepted spin properties of all the nuclei commonly used in NMR spectroscopy. As part of the long IUPAC review process for IUPAC recommendations, the paper has been sent to 16 experts and received very favorable comments and has been presented on the IUPAC web site for 6 months seeking comments from the general public before it is finally accepted by IUPAC and sent to PAC, and subsequently to other specialized journals, for publication. The document as modified by the comments received has very recently been returned to IDCNS, the Interdivisional Committee on Nomenclature and Symbols, for final review and publication

The final report of another project: R. Janoschek, *Quantum Chemical B3LYP/cc-pvqc Computation of Ground State Structures and Properties of Small Experimentally Known Molecules for H-Ar*, had been approved by the Commission in February 2001. This report had been considerably revised since Berlin and, it had been sent to the Commission and to 10 experts inside and outside of IUPAC early in 2001. Certain minor details in this paper containing comprehensive tables of calculated and observed molecular parameters of small molecules were discussed in Brisbane. The report has been accepted by the Physical Chemistry Division and is published in *Pure Appl. Chem.* Vol. 73, No. 9, pp. 1521-1553 (2001)

Three projects were presented to the Commission in nearly completed forms, and all of these were comprehensive papers with many pages of text.

A. M. Heyns, *Infrared and Raman Spectroscopy under Extreme Conditions of Pressure and Temperature*. This paper (60 pages containing many figures) was first presented to the commission members in Brisbane although certain drafts had been discussed at earlier meetings. It deals with many experimental techniques in high pressure spectroscopy employing the diamond anvil cell. The paper is particularly concerned with Raman spectra recorded at very high pressures (and in some cases under high or low temperatures) and many very recent applications are included. Many details were discussed and certain improvements were suggested by the Commission. A slightly revised version was approved by the Commission in October 2001 and has been sent to the President of the Physical Chemistry Division for approval and to IDCNS for preliminary approval and classification as a Technical Report rather than a IUPAC Recommendation.

M. Terazima, N. Hirota, S.E. Braslavsky, A. Mandelis, S. E. Bialkowski, G. J. Diebold, R. J. D. Miller, D. Fournier and A. Tam, *Quantities, Terminology and Symbols in Photothermal and Related Spectroscopies*. Two of the authors were present at the meeting and they reported the changes made after the earlier discussions in Berlin. The report covers very many branches of spectroscopy, several of these have different terminologies, and a uniform nomenclature is therefore suggested. Some minor changes were suggested by the Commission and the report was later approved by the Commission in October. It has been approved by the President of the Physical Chemistry Division, and is currently undergoing minor revision of terminology and symbols suggested by IDCNS during their initial review. It will then be sent to 15 experts and continue with the long IUPAC review process for IUPAC recommendations.

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*. This paper gives a description of the symbols and notations used in rotational-vibrational spectroscopy, based upon the work of R. S. Mulliken and G. Herzberg. The experimental spectra can be studied of samples present in the vapor phase in

infrared and Raman spectra. The report was nearly completed in 1999 and further improvements of a revised version were discussed in Brisbane. Unfortunately, no further progress appears to have been made to date and the future of the project is uncertain.

It was decided to terminate the following two projects: Project 154/6/97, *Notations and Conventions in Molecular Spectroscopy: Part 5. Electronic-Vibration-Rotation Spectroscopy* and Project 155/1/95 part C, *Guidelines for the Presentation of Methodological Choices in the Publication of Computational Results, C. Molecular Mechanics Calculations*. These projects which are both very important for physical chemistry, would have required a large amount of work to be completed. Due to the termination of Commission I.5 at the end of 2001 it was not possible to continue this work.

A joint session was held with Commission on Physicochemical Symbols, Terminology and Units (I.1) and the new, revised version of the green book was presented to the Commission. Members of Commission I.5 had objections to the new chapters 2.6 Spectroscopy and 2.7 Electromagnetic Radiation, and certain modifications of the footnotes to some tables were discussed. A planned joint session with Commission on Spectrochemical and Other Procedures for Analysis (V.4) was cancelled since this commission was not found by members of Commission I.5 in Brisbane.

A new project between members of Commission, I.5 (J. E. Boggs and R. Janoschek) and Commission on Chemical Kinetics, I.4 (T. Bérczes) had been approved and funded by IUPAC under the new rules. It would involve six theoreticians and seven experimentalists who plan to study thermodynamic functions which cannot be easily measured for species important to atmospheric chemistry.

At this very last meeting of the Commission, the chairman, Professor John E. Bertie, thanked the members for their time and efforts devoted to IUPAC, and he was complimented for his hard work and excellent leadership of Commission I.5 since 1993.

**Peter Klæboe**  
**Secretary, IUPAC Commission I.5**