Reports from IUPAC bodies

Commission of High Temperature Materials and Solid State Chemistry (II.3)

Summary of the minutes of the meeting in Geneva, 24–26 August 1997

The commission is working primarily on focused international projects concerned with inorganic materials. Current projects reflect the principal function of the Union, i.e. standardization and nomenclature. Other projects are concerned with advancement of teaching solid state chemistry, teaching materials chemistry, and chemistry related to problems of ceramic materials.

The activity of the commission in the area of standardization resulted in the report 'Characterization of SiC powders and influence of powder properties on sintering' by G. Schwier, J. Tensel and M.H. Lewis, published in *Pure and Applied Chemistry*. An important part of the report is the detailed description of the merits and shortcomings of methods for characterizing powder properties, such as particle size, morphology, bulk and surface chemistry.

The objectives of the project 'Characterization of carbonaceous materials and new carbons (CCMC)' are to collect and review the national standards and to point out differences in important parameters (e.g. sample size, particle size, temperature, etc.). The work is performed within the subcommittee project on CCMC. Dr Boehm reported that the various national standards for the characterization of carbon materials, ASTM, ISO, British Standards, DIN (Germany), AFNOR (France), NNI (Netherlands), JIS (Japan) are now compiled. Prof. Heintz (SUNY at Buffalo, NY) is in the process of listing these standards in a format suitable for easy comparison. The format will be similar to that used in an earlier publication in *Pure & Appl. Chem.* (1979). Prof. Heintz hopes to finish this work before the end of the year.

Several projects are devoted to terminology. The project 'Terminology for diffusion in solid state' is in its final stages. A draft manuscript has been prepared and sent to a number of external experts for comment. After revision in light of their comments, and approval by the commission, the revised manuscript will be sent to 15 referees.

The objective of the project 'Terminology of Vapour Deposition Techniques' is to provide definitions for terms used in vapour deposition science and technology. The coordinator proposed a list of terms and is soliciting comments from experts. This input will result in an extended and amended listing which will then be presented to the commission before sending to reviewers.

Provisional recommendations for silicon nitride terminology were accepted for publication in the *Journal of the European Ceramic Society* and announced in the *Bulletin of the American Ceramic Society*. Readers were invited to comment. The coordinator will prepare a revised report for IUPAC review after considering readers comments.

An important commission activity is to promote education in the fields of Solid State Chemistry and High Temperature Materials Chemistry. The purpose of the current project 'Teaching Experiments in Solid State Chemistry' is to widen the collection of instructive, easy-to-perform, tested laboratory experiments illustrating important aspects of solid state chemistry. A list of experiments with comments collected to date by the commission members will be made available to interested readers in the CTC newsletter, with plans to make them available on the World Wide Web.

Two current projects are devoted to ceramic materials 'Chemical research needed to improve High Temperature Processing of Advanced Ceramics' and 'Surface analysis of ceramics'. The purpose of the first project is to interest solid state chemists in devoting their knowledge and techniques to the solution of significant problems of modern technical ceramics, whereas the second project focuses on surface—sensitive experimental techniques directed toward ceramics. It is believed that both projects will be particularly useful to industrial users and processors of advanced ceramic materials. The basic approach in both projects is to engage a number of experts for recommendations and critical evaluation of the field.

The commission continued its highly successful series of conferences on High Temperature Materials Chemistry. HTMC IX was hosted by Prof. Spear at Pennsylvania State University in May 1997 and was attended by more than 130 participants. The plenary lectures were published in *Pure and Applied Chemistry* 1998, **70**, 439–515, and the conference proceedings, issued shortly after the conference, contain papers covering a broad spectrum of material phenomena at high temperatures. These conferences are greatly enhanced by the international composition and unique mix of expertise of the commission. HTMC X will be held at Jülich, Germany, in 2000, organized by Prof. Hilpert.

The commission discussed and verified several new potential projects, related in particular to contemporary inorganic materials. New members with expertise in the proposed projects were identified and proposed for membership in the commission.

Summary of the Minutes of the meeting of the Commission on Molecular Structure and Spectroscopy (I.5) at the IUPAC General Assembly, Geneva, Switzerland 24–27 August 1997

Fifteen members of the Commission on Molecular Structure and Spectroscopy (I.5), including national representatives and observers, met for three days of hard work during the 39th General Assembly in Geneva, Switzerland, with little time for admiring the beautiful setting on the Lac Leman and the famous Geneva fountain. Three new Titular Members, Robin S. McDowell, Noboru Hirota and James E. Boggs, and three Associate Members, Soji Tsuchiya, Qing-Shi Zhu and Paul von Rague Schleyer were elected to the Commission. Four new national Representatives were appointed, Profs P.T. Manoharan (India), J.P. Hawranek (Poland), B.J. Van der Veken (Belgium), and R. Janoschek (Austria).

Several projects were completed and the results published in *Pure & Appl. Chem.*: C.L. Wilkins, Guidelines on Nuclear Magnetic Resonance Computerized Databases *Pure & Appl. Chem.* 1995, **67**, 593; A.M. Bradshaw and N.V. Richardson, Symmetry, Selection Rules and Nomenclature in Surface Spectroscopy, *Pure & Appl. Chem.* 1996, **68**, 457; G. Guelachvili and 23 collaborators, High Resolution Wavenumber Standards for the Infrared, *Pure & Appl. Chem.* 1996, **68**, 193, and this paper was also reprinted in *J. Molec. Spectrosc.* 1996, **177**, 164 and *Spectrochim. Acta* 1996, **52**, 717; C.J.H. Schutte, J.E. Bertie, P.R. Bunker, J.T. Hougen, I.M. Mills, J.K.G. Watson and B.P. Winnewisser, Notations and Conventions in Molecular Spectroscopy part 1. General Spectroscopic Notation, *Pure & Appl. Chem.* 1997, **69**, 1633; C.J.H. Schutte, J.E. Bertie, P.R. Bunker, J.T. Hougen, I.M. Mills, J.K.G. Watson and B.P. Winnewisser, Notations and Conventions in Molecular Spectroscopy part 2. Symmetry Notation, *Pure & Appl. Chem.* 1997, **69**, 1641; P.R. Bunker, C.J.H. Schutte, J.T. Hougen, I.M. Mills, J.K.G. Watson and B.P. Winnewisser, Notations and Conventions in Molecular Spectroscopy part 3. Permutation and Permutation-Inversion Symmetry Notation, *Pure & Appl. Chem.* 1997, **69**, 1651.

The following book has been published: J.E. Bertie, C.D. Keefe and R.N. Jones, Tables of Intensities for the Calibration of Infrared Spectroscopic Measurements in the Liquid Phase, 263 pp., Blackwell Science Ltd, 1995. A joint article from Commissions I.5 and V.4 describing the work in the two commissions has been published in *Applied Spectroscopy* 1996, **50**, 12A: J.E. Bertie and T. Vo-Dinh, Spectroscopy Commissions of the International Union of Pure and Applied Chemistry.

Other articles which were in press or the projects were very close to completion were: R.K. Harris, J. Kowalewski and S. Cabral de Menezes, Parameters and Symbols for Use in Nuclear Magnetic Resonance, *Pure & Appl. Chem.* 1997, **69**, 2489–2505; E.D. Becker, W. Bremser, S. Cabral de Menezes, R. Goodfellow, P. Granger and R.K. Harris**,** Recommendations for NMR Nomenclature A. Nuclear Spin Properties and Conventions for Chemical Shifts; and J.E. Bertie, Specification of Components, Methods and Parameters in Fourier Transform Spectroscopy by Michelson and Related Interferometers. The latter paper has been divided into one part for modest resolution spectroscopy (0.1 cm^{-1} or less) and one for high resolution spectroscopy (10^{-3} cm^{-1} or better). In addition, a part pertaining to FT-Raman spectroscopy is included. The following manuscript of a book was approved in Geneva: E. Hirota, R.W. Field, J.P. Maier and S. Tsuchiya, Editors, Nonlinear Spectroscopy for Molecular Structure Determination. It constitutes a monograph of 268 pages and 10 chapters, probably suitable both for teaching and as a reference book to nonlinear spectroscopy. The book will be published by Blackwell early in 1998.

Projects from the Sub-Committee on Theoretical Chemistry are in progress: Guidelines for Presentation of Methodological Choices in the Publication of Computational Results, A. *Ab Initio* Electronic Structure Calculations (Project leader J.E. Boggs) *Pure & Appl. Chem.* 1998, **70**, 1015–1018. The paper was approved by the Commission for immediate publication. A draft for semi-empirical calculations is in progress (part B) and should be completed in two years. A third paper (part C) is planned to deal with computation of large molecules by molecular mechanics. An extensive report comprising 194 compounds was presented to the Commission for discussion and suggestion: R. Janoschek, The Quantum Chemical Computation of Structures and Properties of Small Experimentally Known Molecules I. Diatomic Molecules for H-Ar. It was agreed that the project would be completed following consultations with an international group of specialists.

Various new projects were initiated: Notations and Conventions in Molecular Spectroscopy. Part 4. Vibrational-Rotational Spectroscopy (Project leaders R.S. McDowell and J.K.G. Watson); Notations and Conventions in Molecular Spectroscopy. Part 5. Electronic-Vibrational-Rotational Spectroscopy (Project leaders J.K.G. Watson and R.S. McDowell). The Commission approved both these projects. Another proposed project was also approved: Quantities, Terminology and Symbols in Photothermal and Related Spectroscopies (Project leaders N. Hirota and M. Terazima); these methods are very sensitive and of increasing importance in applied science. R.K. Harris successfully sought approval-in-principle for a project to recommend Nomenclature for tensor quantities used in NMR, NQR and ESR Spectroscopies (Project leader R.K. Harris);

formal IUPAC approval for this project will be sought when the working party members have been recruited and the goals have been more precisely formulated.

Joint meetings were held between Commission I.5 and three other commissions: Commission V.4 (Commission on Spectrochemical and Other Optical Procedures for Analysis) of the Analytical Division; Commission I.3 (Commission on Electrochemistry) and Commission I.1 (Physicochemical Symbols, Terminology and Units). With each of these commissions various projects of common interests were discussed. These joint meetings are very important to avoid overlap between projects of different commissions and to provide stimulation for joint projects of greater breadth than is usually achieved by a single commission. In particular, the meetings in Geneva gave good ideas to both parties about new proposals and cooperation on existing projects. With Commission I.1 it was agreed on additions and alterations which should be included in the next edition of The Green Book (Quantities, Units and Symbols in Physical Chemistry).

Theoretical chemistry plays an ever increasing role in chemistry and the Subcommittee on Theoretical Chemistry, which was established at the General Assembly in Guildford, continues with its chairman Prof. James E. Boggs. The subcommittee is strengthened with five new members. The Subcommittee on Notations and Conventions for Molecular Spectroscopy has a new chairman Dr J.K.G. Watson, and Dr Robin S. McDowell and Prof. Jean-Marie Flaud will join the subcommittee.

The commission discussed the use of the World Wide Web and it was suggested that a Home Page be established. However, no decision was made concerning the content and who should be responsible for the Web Site.

The chairman, John E. Bertie, expressed his thanks to the outgoing members for their contributions to the work of Commission I.5 and looked forward seeing the members at the next IUPAC General Assembly to be held in Berlin in August 1999.

Peter Klaeboe
(Secretary of Commission I.5)