

IUPAC COMMISSION II.3
High Temperature Materials and Solid State Chemistry
Final Agenda and Outline of Minutes
Aachen, April 15, 2000

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IUPAC COMMISSION II.3
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Minutes
Aachen, April 15, 2000

Attendance

Commission: Chatillon (chairman), Balducci, Boehm, Carlsson, Kizilyalli, Kniep, Leskela, Voronin

Inorganic Division: Rosenblatt

Observers: Hilpert, Spear

1. Introduction and Announcements (Chairman)

Chairman Chatillon welcomed the participants, particularly new members Kniep and Leskela, and introductions were performed. He thanked our host, Klaus Hilpert, for the arrangements. It was agreed to replace the scheduled lunch break and afternoon coffee break by a working lunch of sandwiches to be brought in so that members could catch mid-afternoon trains.

Chatillon and Rosenblatt then told the Commission of the sudden and tragic death of the Commission's respected and beloved secretary, Drago Kolar, due to a heart attack in late February. Commission members expressed their dismay and condolences to Kolar's family and colleagues and co-workers in Ljubljana.

The need for a new Commission secretary was discussed. Chadwick, already a Titular Member, was unanimously selected to become the new secretary and members expressed their hopes that he would accept this appointment. It is only for two meetings, the Commission meeting in Ankara, Turkey in September, 2000, and the IUPAC General Assembly in Brisbane, Australia, in July, 2001, as the Commission will cease to exist after the 2001 General Assembly. In Chadwick's absence, Rosenblatt's offer to prepare minutes for the Aachen meeting was gratefully accepted. [**Added note.** Immediately after the Aachen meeting Chadwick accepted, Division President Corish notified the IUPAC Secretariat, and the IUPAC Executive Committee approved Chadwick's appointment.]

The chairman has been informed of two new National Representatives to the Commission, Milan Drabik (Slovakia) and Pavel Peshev (Bulgaria).

2. Finalization of Agenda (Chairman)

The preliminary agenda had been e-mailed to all Commission members and others on the mailing list by the chairman on 27 March. A major focus of this "informal" meeting (no IUPAC funds used for the meeting) is to organize the submission of project proposals and to discuss the High Temperature Materials Chemistry Conferences that will follow the just completed very successful conference in Jülich, Germany. Minor revisions from the preliminary agenda are reflected in the agenda heading these minutes.

3. Minutes of the Berlin meeting (Chairman)

Drago Kolar, the Commission secretary, had sent out the minutes from the Commission's meeting at the August, 1999 IUPAC General Assembly in Berlin to the Commission mailing list on December 24, 1999 as an e-mail attachment. They are in a Microsoft Word computer file entitled, "Min99_CP.doc." Anyone who did not receive these should contact the chairman or Rosenblatt. Formal acceptance of the Berlin minutes was deferred to the Commission's official meeting in Ankara in September.

4. Reports on items from the Union and Inorganic Division. The future of Commission II.3 within the new structure of IUPAC (Rosenblatt)

Rosenblatt, Division Vice-president, reported on IUPAC decisions and meetings that occurred after the Commission meeting at the August, 1999 Berlin General Assembly. The IUPAC Council meeting at Berlin voted, as had been proposed, to dis-establish all existing Commissions in 2001 after the Brisbane General Assembly. The scientific work heretofore carried out by the Union's Commissions will be carried out on a project basis overseen and coordinated by the Division Committees. There will be opportunity to re-establish a very limited number of Commissions if this is clearly the best way to carry forward the work of the Union.

The newly expanded Inorganic Division met in Berkeley in December, 1999 to consider how best to move forward the present and future activities of the Division under the new IUPAC structure. Chatillon and Rosenblatt participated in this meeting. The Division decided to continue the work of the present, historical atomic weights Commission (Commission II.1 on Atomic Weights and Isotopic Abundances) by requesting a new, broadened Commission to carry on this work combined with that of the current Commission II.4 on Isotope Specific Measurements as Traceable References. The Division will continue specific nomenclature work within the Inorganic Division but supports an IUPAC-wide nomenclature unit. The best organization of nomenclature activities within the Division will depend upon IUPAC-wide plans for nomenclature that are still being formulated. The current work of Commission II.3 in materials chemistry, which is already carried out on a project basis, will continue on a project-by-project basis.

To coordinate and provide project management for its diverse activities the Division Committee will organize three Coordinating Groups, one for Elements, one for Molecular Compounds, and one for Materials. The membership of these Coordinating Groups will consist of Division Committee members in that area plus one or two leaders of significant projects. The initial membership of the Inorganic Division's Coordinating Group for Materials is anticipated to be Chatillon, Corish, Interrante, Rosenblatt, and West.

5. Need to submit project proposals (Chairman/Rosenblatt)

Chatillon and Rosenblatt emphasized how the organizational changes just described make it important that current Commission members submit project requests to cover those ongoing and anticipated Commission projects that will not be completed before the 2001 Brisbane General Assembly. So far, only Voronin has submitted a formal project submission to the Division and Secretariat. A major purpose of the

Aachen meeting is to identify current and clearly defined new projects that should be submitted. The chairman distributed sample Project Submission Forms. They are available on the World Wide Web at www.iupac.org. The form is not onerous. Chatillon asked that Commission members submit current projects within the next 4-6 weeks. This will enable the Commission to concentrate on considering new project areas at its Ankara meeting in September.

6. Chemical Research Needed to Improve High Temperature Processing of Advanced Ceramics (230/24/93) (Rosenblatt/Spear)

A very close-to-final draft of this report was distributed by Kolar three weeks before the August 1999 GA at Berlin. The Commission approved the report for publication at Berlin but Kolar anticipated that some minor editing changes would still be made before the report was put into the publication process by the Commission Chairman. Following Kolar's untimely death Rosenblatt obtained the computer file of the report from Kolar's secretary so that the Commission could see Kolar's work through to completion. Metselaar and Spear looked over the manuscript one last time and suggested minor corrections that Rosenblatt will incorporate into the document. Rosenblatt will then send the report to Chatillon for formal review and publication. Corish and Metselaar will ascertain the number of referees needed. Since this is a technical report and 14 experts contributed to it, an extensive number of reviewers may not be necessary. Spear and Metselaar will suggest referees to Chatillon. After the referee comments are received Spear and/or Metselaar will make any necessary changes and transmit them to Rosenblatt who will keep the master document. Kolar will be kept as author and the report will be published in his honor. [Added note. After the Aachen meeting Metselaar notified Rosenblatt that no additional referees are needed for this technical report. Rosenblatt submitted the corrected manuscript to the IUPAC Secretariat for review by the IDCNS officers and publication in *Pure and Applied Chemistry*.]

7. Terminology of Vapor Deposition (230/27/95) (Carlsson/Spear)

Carlsson took over the lead on this project at Berlin after Spear's extensive other commitments, regrettably but understandably, led him to resign from the Commission. Spear recently gave additional information to Carlsson and Leskela. This is a large, ambitious undertaking so the project will focus on finalizing terminology for *chemical* vapor deposition. Leskela and Chatillon can help with the project. Carlsson will go through the literature and interact with the editor of the *Handbook on Deposition*. Carlsson will prepare a formal project proposal for IUPAC and send it to Chairman Chatillon within six weeks, by May 15.

8. Subcommittee on Characterization of Carbonaceous Materials and New Carbons (SC-2) (232/1/91) (Boehm)

Boehm summarized some of the history leading up to this subcommittee project. Fitzer's subcommittee project (SC-1) on carbon terminology was completed with the end of Fitzer's tenure. Fitzer proposed a second subcommittee project dealing with carbon, specifically with international standardization of characterization methods and procedures for carbon materials, in 1991. Boehm was asked to chair this with the understanding that

Fitzer would provide much of the effort but Fitzer, unfortunately, suffered a stroke. Heintz at Buffalo has been working on collating input into the project but there has been no progress in quite a while and Boehm is worried.

Boehm will contact Heintz and ascertain status. He will then, within the next six weeks, complete the formal IUPAC project proposal that he started including an action plan for completion of the project. Rosenblatt will look at the initial draft proposal Boehm prepared and send comments to Boehm.

9. Project on Calculation of Equilibrium Thermodynamic Properties of High Temperature Superconductors (Voronin)

This project was advanced from a preliminary survey team (PST-18) to a project in 1999 at Berlin. A manuscript describing the first part of the final results, “Thermodynamic characterization of high-temperature superconductors in the yttrium-barium-copper-oxygen system. I. The Y123 solid solution,” was approved by the Commission at Berlin for publication in PAC. Voronin has sent the final manuscript to *Pure And Applied Chemistry* at the IUPAC Secretariat and the paper is scheduled to appear in the March, 2000 issue. Preprints are available as an Adobe “pdf” file.

Voronin in January submitted a 3-year project proposal containing the following project description to the Inorganic Division and IUPAC Secretariat: “The work is to be done: (1) critical assessment and accommodation of existing thermodynamic data for solid phases Y123, Y247, Y124 and liquid solutions of components, (2) analytical representation of the Gibbs energy functions for these phases, and (3) computer-assisted optimization analysis to obtain a set of functions parameters with the best fitting to the experimental results and fulfillment of thermodynamic relations. The first stage of this project concerning the Y123 solid solution is completed.” The proposal is currently being evaluated.

10. Project on Teaching of High Temperature Materials Chemistry at University (Balducci)

This project was advanced from a preliminary survey team (PST-16) to a project in 1999 at Berlin. Balducci distributed a summary and rationale for the project. The objective is to propose a list of topics that should be included in chemistry courses to help in understanding the properties and behavior of high temperature materials. The list will be accompanied by a bibliography of helpful references. After the list of topics is at hand, a short introduction or explanation of each topic will be written, possibly indicating areas of application. Balducci will draft a proposal before the September Commission meeting in Ankara. In parallel, he will contact potential contributors to the project.

11. High Temperature Mass Spectrometry Ionization Cross Sections (230/9/83) (Chatillon)

This long-standing, monumental effort is nearing completion so a post-Brisbane proposal is not required. It is planned to send the manuscript send out for review this year. Jean Drowart will become secretary and editor of the final revisions and will prepare an appendix during the summer. Hilpert mentioned additional sources of cross-

section measurements and evaluations and computational capabilities at NIST and Merck; he will e-mail Drowart directly.

12. Surface Analysis of Ceramics (230/25/93) (Mintmire)

No report was received. The Chairman will contact Mintmire to ascertain the status and encourage a formal proposal.

13. Teaching Experiments in Solid State Chemistry (230/29/95) (Kizilyalli)

As noted in the Berlin minutes, Kizilyalli had presented a list of 25 experiments developed and edited by various authors at the Ljubljana meeting in 1998. The plan was to make the experiments available to interested persons on the IUPAC web site with a link to CTC. Corish informed Jost, who is ready to arrange this, but it has to be in correct format; contact Fabienne Meyers in the IUPAC Secretariat. When the experiments are posted on the web, this should be announced in *Chemistry International* and the CTC newsletter and possibly in *J. Chem. Education*.

As noted at Ljubljana and Berlin, the completed experiments, although they have been checked in the laboratory, still need editing for English clarity and to include at the beginning of each write-up: (1) equipment needed, (2) chemicals needed, (3) time required, and (4) safety aspects. Kizilyalli sent the report to Spear for editing some time ago but he will not have time to do this. Carlsson, with possible help from Leskela, will see if he can do the required editing or find someone at Uppsala to help. Spear provided Carlsson with a disk containing all of the experimental write-ups in an electronic format (MS Word).

Kizilyalli will prepare a formal IUPAC project proposal for work in this area – collection and dissemination of experiments in solid state and materials chemistry – before the Ankara meeting.

14. Glossary of Terms for Polymer Gels, Networks, Pre-Ceramic Materials, and Sol-Gel Processing (with Div. IV) (TF-20, 27/95) (Chadwick)

Jones, Macromolecular Division, and Chadwick sent the Chairman a report dated 31 March, 2000 on the status and plans for the project. The nomenclature system for basic sol-gel processing has been incorporated into the project and the title of the project has changed accordingly, as reflected above. Seven collaborators from Division IV have been identified. The group has identified an extensive list of terms, summarized on a 7-page spreadsheet, along with references to potential sources of definitions.

According to the 31 March report the project has been submitted for formal approval under the new IUPAC scheme. Chatillon will ask Chadwick where the proposal stands and whether anything is needed to complete its submission.

15. Thermochemical and Thermophysical Properties of Refractory Metal Carbides (PST-19) (Balducci)

Balducci envisions a project, analogous to those led by Kolar and Voronin, that will summarize current knowledge and point out what is needed, focusing on the

thermodynamic properties of certain refractory metal carbides important, or potentially so, in applications. Balducci will draft an IUPAC proposal during the next six weeks and send the draft to Commission members for comment with a 2-3 week deadline. He will then submit a revised proposal to the Inorganic Division before Ankara.

16. Project on Classification and Nomenclature of Borophosphate Compounds (PST-20)
(Kizilyalli)

This potential project has developed from an earlier, more general, discussion of a new project in the area of “Classification and nomenclature of phosphorus compounds.” The Berlin minutes on that potential project state: “The project is still justified. Kizilyalli illustrated the need by quoting several inconsistencies and ambiguities in the phosphate literature.... Corish contacted the Chairman of nomenclature commission and was advised to produce a list of chemical formulae as examples which may need proper identification. Kizilyalli should prepare the list of examples, possibly of B/Si/P complex compounds, and send it to Chatillon who will contact the nomenclature commission.” After Berlin Kizilyalli started to prepare such a list of formulas to be named and found ‘thousands’ of them making it difficult to prepare the requested list.

The length of the potential list of examples led Kizilyalli to suggest that the new project concentrate on borophosphates, changing the title of the potential project from that discussed earlier to the one listed here. Borophosphates are new compounds which have been prepared in the last 10 years. Nomenclature for these solids is not covered currently in the Red Book. Kniep’s and Kizilyalli’s research groups are active in the preparation of these compounds. Kizilyalli has drafted an outline for a project that Kniep would coordinate with Kizilyalli’s help. Kizilyalli and Kniep will submit a formal proposal after Kniep reviews and corrects the initial draft. The proposal should be sent to Commission II.2 (Kaes) before or when it is submitted to the Inorganic Division.

17. Project proposals, potential new projects (Chairman/members)
Particles/clusters (Carlsson)

Carlsson envisions a project concerned with how one characterizes particles and clusters with respect to size and shape but the idea is not yet sufficiently formulated to define a project. It will be discussed further at Ankara.

Acting secretary Rosenblatt presented the list of potential future projects that had been discussed at earlier meetings and that should be considered again at Ankara. Those not appearing elsewhere in these minutes are:

- Characterization of porous solids
- Terminology for inorganic composites
- Round robin measurements of grain boundary composition
- Use of synchrotron radiation for materials characterization

18. Red Book revision (Metselaar/Rosenblatt)

The IUPAC Red Book on Nomenclature of Inorganic Compounds is under revision by Commission II.2. The chapter on solids was drafted by Metselaar about a decade ago for the last edition of the Red Book and needs to be gone over and updated.

Knief volunteered to help Metselaar with this. Rosenblatt will notify Metselaar and Corish.

19. HTMC-X in 2000 (Hilpert)

The just completed IUPAC High Temperature Materials Chemistry Conference was very successful and sets a new standard for future conferences in this series. The success of the conference was greatly facilitated by the German science foundation providing 20,000 DM to bring scientists from the former “east” and another 25,000 DM for general conference support. There was also excellent help and support from the conference organization group at Jülich.

There were excellent science lectures in both the invited and contributed categories. Engagement of industry was outstanding and particularly successful. A number of the industrial participants expressed to Hilpert how gratified they were by their interactions with fundamental and academic researchers at the conference and how valuable those interactions were.

The proceedings will be published by the Jülich Research Center: half of the papers have already been received. There were 240 registrations and 250 contributions. The conference is now as large as it become if it is to remain an interactive meeting with no overlapping sessions. Posters must be an increasingly prominent part of the conference agenda.

20. HTMC-XI in 2003 (Rosenblatt)

The IUPAC conference committee (Rosenblatt-chairman, Balducci, Corish, Hastie, and Spear) has received five strong applications to host HTMC-XI in 2003. The applications are from:

- Atlanta, USA (J. Gole);
- Kalpakkam, India (V. Rao);
- Tokyo, Japan (M. Yamawaki);
- Tsukuba, Japan (H. Yokokawa);
- Xian, China (Bingbo Wei).

The committee is close to a final decision and will announce the venue of the next conference before August so that Hilpert can include this with the mailing of the HTMC-X proceedings. [**Added note.** After the Aachen meeting and extensive deliberation the committee decided to accept the proposal from M. Yamawaki at the University of Tokyo to host HTMC-XI in 2003. The sites were essentially tied and it was difficult to choose among these fine proposals.]

21. HTMC-XII in 2006 (Rosenblatt)

Rosenblatt pointed out that it is time to refresh the conference committee. The new committee which will select the site of HTMC-XII and will oversee interactions with the host of HTMC-XI after 2000 will consist of Spear-chairman, Balducci, Hilpert, Rosenblatt, plus one member to be selected at Ankara after the site of HTMC-XI is known.

A very preliminary discussion of potential sites for HTMC-XII generated the following possibilities assuming that HTMC-XI is held in Asia:

- Ankara, Turkey (Kizilyalli);
- Atlanta, USA (Gole);
- Chicago-area, USA (Nordine with Northwestern University and/or Argonne);
- Cleveland, USA (Jacobsen);
- Grenoble, France (Chatillon and Ansara);
- Moscow, Russia (Voronin);
- Petras, Greece (Papatheodorou);
- St. Petersburg, Russia (Stolyarova);
- Uppsala, Sweden (Carlsson);
- Vienna, Austria (Mikula).

Spear and the new committee will refine this list and Spear will solicit proposals early in 2001 so that selection can be made in 2001 or 2002.

There was some discussion of whether HTMC-XII should be held in 2005 or 2006 with the tenor of the discussion favoring continuing the 3-year cycle and holding HTMC-XII in 2006.

22. The regular Ankara meeting 18 and 19 September, 2000 (Chairman/Kizilyalli)

The official off-year meeting of the Commission will be held in Ankara, Turkey in September. Kizilyalli has reserved a conference room at the University for Monday and Tuesday, September 18 and 19. Participants should plan to work though the day on Tuesday and not leave Ankara until Wednesday. Kizilyalli needs to know who will attend before the end of June and will send out an e-mail announcement to that effect.

Kizilyalli needs an official letter from IUPAC asking her to host the meeting. The Commission Chairman (Chatillon) and/or Division President (Corish) will provide such. [**Added note.** Corish sent this to Kizilyalli shortly after the meeting.]

23. Closing Remarks (Chairman)

Chatillon thanked all for attending and for the progress made, looks forward to receiving project proposals and to all attending at Ankara, and rushed off to catch a train.

Respectfully submitted,
Gerd M. Rosenblatt, acting secretary