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## Executive Committee Meeting Minutes

Division of Computers in Chemistry  
Boston, Massachusetts

August 17, 2002  
Convened at 3:30

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### Present

Bill Jorgensen (Chair), Curt Breneman (Treasurer), Jeff Evanseck (Secretary), Peter Gund (Councilor), Peter Jurs (Councilor), Michelle Francl (Councilor), Michelle Lamb (Newsletter Editor), Ralph Wheeler (Program Chair), Lisa Balbes (Web Master), Wendy Cornell (Assistant Program Chair), Dominic Ryan (Guest), Andy Holder (Editor, JGM), Alex Tropsha (Alternate Councilor)

### Chair's Report

- Bill presented a summary of the Yale Retreat, Ann. Rep. Comp. Chem., and e-mail access. The discussion is as presented below.
- David S. reported that the Ann. Rep. Comp. Chem. is making good progress. The intention is to make it the same in spirit as that provided by the MED CHEM Division.
- David will be the Editor. If Academic Press publishes, then the Division should receive royalties.
- Wendy C. asked if ARCC should impact other journals, such as the Journal of Computational Chemistry?
- Bill said that it should not be an issue. The distribution for JCC is small, but ARCC should be much greater. He stressed that we should use the MED CHEM publication as a model, since it has shown long term success.
- Andy H. Asked about area editors?
- Bill stated that the details have not yet been worked out.
- Bill stated that Peter Grootenhuis is pursuing the e-journal options for the Division. We have to wait until the next meeting for an update. PG is looking for sources of funding. It has been estimated that we need \$10/person for both JMGM and JCC.

- Michelle F. stated that allocations for the Division may increase next year.
- Bill stated that JCC is actually \$160/person. However, if we can make a deal of \$10/person with a journal, then raising the membership dues should not be a problem. Value-added is important to the membership,
- Bill stated that if dues are raised, then members should vote on which journals they would want. The question becomes, how many can we afford?
- Bill suggested that a questionnaire of the membership may be the right approach.
- Bill suggested that the next Retreat should be in the winter. This would allow for more separation in time between the retreat and the national meetings.

## **Secretary's Report**

- Jeff E. reported that the membership declined by 11% (317) members as compared to the same time last year. David S. commented that it is difficult to make such a comparison. Members pay their dues at different times, and it is best to compare the membership at the end of the year.
- Jeff E. described the Innovative Project for Divisional Enhancement submitted. The title of the submitted proposal was "Undergraduate Research Combining Computers and Experimental Investigation". The idea is to promote greater interaction between COMP and other divisions by creating summer undergraduate fellowships. Obviously, the undergraduates would benefit, but could we attract experimentalists to join COMP as a consequence?
- Jeff E. gave a preliminary assessment of the pending election. Everything went as planned and is on schedule. The deadline is September 1<sup>st</sup>. The positions of Chair-Elect and Councilor are too close to call. For the Treasurer position, Curt B. has a commanding lead over George Clooney.
- Jeff E. stated that electronic elections issue was unclear. He has made several attempts to get the story straight, but is getting different views from the ACS. It seems that a task force has been established to investigate electronic elections. The COMP division will have to wait until National gets it straight.

## **Treasurer's Report**

- From the final 2002 report submitted to the ACS, Curt B. reported that the COMP division is in good financial shape.
- Curt B. Reported that the CCG Travel Awards for students will be increased from 6 to 10 next meeting.
- Curt B. asked if our current donors could advertise at the Sci-Mix and COMP poster session. Tripose supported everything asked of them over the last year.
- Ralph commented that advertising during the poster session is not allowed.
- Andy H. suggested that an acknowledgement could be accomplished by thanking the symposium supporters by using the overhead before the symposium and during intermissions.
- Curt B. said that Pam Newton is the new Account Manager (CCG). Ralph W. will hand out the CCG awards at the poster session.

## Councilor's Report

- Michelle Francl went into more detail concerning ACS Stop/Gap funding. The Divisions will receive more money. In addition, membership and programming will receive more financial assistance. The bylaws are being changed to correct the current situation.
- Last year the Division received approximately \$4K. Curt B. said it was \$6.6K.
- COMP needs to respond on how the previous stop/gap money was utilized; otherwise no money will be made available next time.
- Michelle F. said that a \$15-20K increase has been proposed for COMP. There currently exists a current division in money allocation between local sections and divisions. In rough terms, the division gets \$600 per 100 division members, while a local section gets \$4K per 100 local members.
- The changes in local/division funding is expected to be implemented over the next 4-5 years.
- Peter J. said the Publications Division desired to have more cooperation with JCICS.
- The Publications Committee decide upon ACS Editors. There are 8-10 editorial board members for JCICS.
- Should there be a stronger connection between JCICS and COMP?
- Peter J. reported that the journal is doing fine. Yet, there is a sense that it is not serving the community as well as it could.
- The papers currently accepted by JCICS must be practical. If only theoretical, then JCICS will not publish.
- Peter G. reported on the Committee of Science. The programming is currently active. The ACS President chooses a theme each year. In 2003, it was "communication between government, society and engineering." At the New Orleans Meeting, it was "nontraditional sources of funding", and at NYC it will be the 125<sup>th</sup> year anniversary of the Journal of the American Chemical Society.
- Peter G. stated that the NRC (as a follow on) will support a "computing and communications" half-day symposium. There will be a workshop in Washington on data information, simulation and modeling, design tools, process models and multiscale codes. Peter brought up the idea of COMP co-sponsorship. He also asked if there was any programming conflict during the Fall of 2003?

## Program Chair's and Vice-Chair's Report

- Was covered in the preceding Programming Meeting. Jeff E.'s plane was 3 hours late into Boston, as a consequence he missed the Programming Meeting.
- Andy H. presented a proposal for the MJS Dewar Symposium (see Supporting Information).
- Andy's tentative first symposium target is within the next three national meetings.
- The idea is to hold the Dewar Symposium every two years.
- National needs to agree to the terms of the proposal, so that the Division isn't agreeing to something it cannot support.
- The COMP members agree in principle to the proposal, as long as the national ACS agrees.

## **JMGM Report**

- Andy H. reported that from January to date, 35 papers have been received by the US Editor. Since assuming the editorship in May 2001, a total of 60 papers have been received.
- All six 2002 issues have been published.
- One special issue by Davis Winkler is in the processor. Others are being considered.
- As of 2002 (Vol. 21) color pictures and a new cover design have been introduced.
- As of May 2002, JMGM is one of the top 30 journals to have articles downloaded by electronic subscribers.

## **Web Site**

- Lisa B. reported that all the changes described at the Yale Retreat have been made.
- Lisa asked if the meeting abstracts should be posted. Most agreed that this would be a good idea, and that we should look into posting the abstracts for the next meeting.
- Lisa would like to update the demographics of the Division that are posted on the web. Jeff E. will provide the data.
- The sponsorships have been posted, but should numbers be added as well? Peter asked if the numbers per year or over a three year period. Essentially, the more names the better.
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