Electronic Conferencing on the Internet: The First Electronic Computational Chemistry Conference[1]

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The First Electronic Computational Chemistry Conference (ECCC) was held in November 1994 entirely on the Internet. This paper discusses the design, preparation, organization, and outcome of this conference. The principal aim of the conference was to explore the use of this new medium for holding conferences. The success of the ECCC points toward further implementation of electronic conferences as a means for chemists to exchange ideas.

I. INTRODUCTION

Conferences are an important component of scientific discourse. Scientists gather to present and discuss their most recent results. Contacts are made and collaborations born. Between the meetings of the major chemistry scientific organizations, regional meetings, and specialist meetings, scientists could be away from their laboratories nearly every day of the year.

While the importance of scientific meetings has not diminished, the ability of scientists to attend meetings of interest has declined over the last decade. There are simply more meetings and conferences during the year than time permits. Costs for travel and registration fees have risen substantially, and in an era of decreasing funding for the sciences, most researchers, particularly scientists in developing countries, cannot afford frequent travel. Physically challenged scientists have always had difficulties in attenting conferences where their special needs may be difficult to accommodate.

As an alternative to traditional meetings, we decided to explore the ability of chemists to meet "virtually", present their work, and discuss their science without leaving their offices. The reach of the Internet[2] into scientific laboratories across the world offers an opportunity for "electronic conferences". The recent advances in network software, particularly the advent of the World-Wide Web (WWW or simply the web),[3,4] provides a new communication medium that seemed to us prime for exploration by chemists as a means for holding conferences. This paper describes our efforts in planning, organizing, and hosting the first Electronic Computational Chemistry Conference (ECCC)[5] from November 7, 1995 through November 18, 1995 on the Internet.

II. PLANNING STAGE

The first electronic chemistry conference was *ChemConf '93*, held June 14−August 20, 1993.[6] *ChemConf '93* was dedicated to the application of technology in teaching chemistry. This conference contained 17 papers that were made available to the participants by ftp (file transmission protocol) or electronic mail (email). Ftp is a service that allows computers running TCP/IP (transmission control protocol/Internet protocol) to exchange files. The papers, as ASCII text files, were placed in a directory made available by anonymous ftp, which allowed anyone to access these files. Each paper was open for discussion for a given three day period, during which the author agreed to be available to participate in the discussions. Discussions were implemented by electronic mail directed through a discussion group. A discussion group is a collection of people who exchange mail through a central server. Mail is sent to the server, which then forwards it to all members of the group.

While *ChemConf '93* was a great success, there were many limitations. Graphics were extremely difficult to handle, since the participants were using a wide variety of computer platforms and software, and there is very little standardization in the graphics arena. Since chemistry is a graphics-oriented science—chemists rely on 2D drawings of molecules and 3D structures, spectra, plots, etc.—the absence of graphics severely limits the chemistry that can be easily discussed in a paper. In order to use ftp one must know some arcane commands and have some familiarity with UNIX, yet many participants were novice computer users. Finally, in mid-1993, the reach of the Internet, particularly its penetration into commercial locations, was much smaller than its current scope.

By the summer of 1994, the status of Internet resources had changed dramatically from just a year earlier. The World-Wide Web, stimulated by the remarkable success of the NCSA *Mosaic*[7] browser, had become one of the largest resources on the Internet. We have also seen the commercialization of the Internet. This change has allowed corporate sites access to the Internet. Many chemical companies are now connected to the Internet, and their scientists can now participate in Internet communications.

Encouraged by these developments, we decided in early summer 1994 to organize an Electronic Computational Chemistry Conference, making use of the web as the principle communications medium. In this section we detail our decisions on the operating policy of the conference and the software employed. Section III details the preconference preparations, and in section IV we discuss the actual conference operation. In section V we report the results of the conference survey and our appraisal of the conference. We finish with some conclusions on electronic conferencing.

General Format. Selection of Conference Medium. The first task in organizing an electronic conference is the

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selection of the means for dissemination of information, principally how will participants obtain the papers? For *ChemConf '93*, papers were distributed using an anonymous ftp site or by electronic mail. Both of these procedures have serious drawbacks. Many mail programs have severe limits on the size of the message. Use of ftp is not intuitive, and the participants need to be trained to use this tool effectively. Further, these methods allow the transfer of individual files, so that text and graphics are separate, and there is no standard for text or graphics formats. Some users will not have the appropriate software to view all the different types of files.

The client-server tool Gopher[8] obviates some of these problems. Gopher is a menu-based navigational tool, enabling users to obtain files by simply selecting a menu item. A Gopher server can then replace the need for the ftp server, as long as all participants have the Gopher client software. However, Gopher delivers separate files, so that text and graphics are not integrated, and again there is no format standard for text or graphics files.

The World-Wide Web is a hypertext client-server navigational tool that can deliver text, graphics, audio, and video files. The user selects items of interest by positioning the mouse over highlighted text or graphics (called links) and clicks the mouse button. The server then delivers the new document. Hypertext documents are written in HTML (HyperText Markup Language),[9] which specifies how the text will appear on the screen. HTML allows for graphics in the GIF (Graphics Interchange Format) to appear inline with the text. With the development of a number of different browsers (particular *Mosaic*) and servers, the WWW is an excellent medium for presenting chemical information.

We therefore decided that all papers would be presented using the web. We would provide the web server to deliver the documents, and each participant would have to obtain a web browser. Web browsers are available for free for a wide variety of platforms including Windows, Macintosh and UNIX computers. The use of this system imposes a standard text (HTML) and graphics (GIF) format, so that every participant will see the same document, regardless of their computer platform. Further, since the papers include graphics, which tend to be large files, the participant would need a relatively high-speed Internet connection, essentially precluding those persons who access the Internet by modem. The advantages of the HTML documents with graphics certainly outweighed the disadvantage that some people could not participate due to inappropriate network connections.

Viewing the papers alone would make for a relatively sterile conference. Discussions of presentations is often quite illuminating. To encourage the discussion of the electronic papers, a discussion group would be created. Participants register for the conference by joining the list server. They could then comment on a paper by sending an email message to the server, which would then forward the message to all other participants.

Finally, one advantage of operating a conference in this manner is the potential for very low costs. The software required to operate the conference, and the software each participant required are all available at no cost. To encourage as wide an audience as possible, there was no registration fee for the ECCC.

Scientific Organizing Committee. The ECCC was to be an experiment in the use of the web for distributing chemical information. We felt that this conference would be precedent setting, so to insure the quality of the presentations, a Scientific Organizing Committee (SOC) was formed. The principal function of the SOC was to screen the abstracts and select only those of high scientific merit.

CD-ROM. Conference proceedings are frequently published, including the papers and often an edited transcript of the discussions. The SOC decided to pursue publication of the proceedings and mail discussions of the ECCC. Publication in a traditional journal was discounted since one of the goals of the ECCC was to explore the use of electronic media for disseminating chemical information. The SOC decided to pursue publication of the proceedings on CD-ROM containing the HTML papers and associated files and the mail discussions.

To widen the acceptability of this new technology and insure the highest quality, the papers would be peer-reviewed, with reviewers selected from the conference participants. All reviewing will be handled electronically and coordinated by the SOC.

WWW Server. At the time of the conference, there were three freeware WWW servers available. We opted to use the *Gn*[10] server since we were using this server to operate the Northern Illinois University Chemistry WWW/Gopher Site.[11] The advantage of this server for the ECCC is the use of *.cache* files to control what files will be made publicly available. Related files and directories can be kept together, and only select files will be served.

The only drawback to the *Gn* server for the ECCC concerns the more complicated URLs (Uniform Resource Locator) that are needed. The *Gn* server is used for the NIU chemistry site since it can act as both a Gopher and WWW server. This feature was not used in the ECCC—papers were made available only by WWW. However, to accommodate both systems, URLs are complicated by the need to include the Gopher file type. For example, the URL for the ECCC home page is **http://hackberry.chem.niu.edu:70/0/ECCC/homepage.html.** The **http** indicates a file transfer via the hypertext transmission protocol. The computer address comes next, and the **:70** indicates use of tcp port 70. WWW defaults to port 80 and gopher defaults to port 70, which we use to serve our gopher clients. The next part of a URL indicates the file path name, but *Gn* requires a preceding number to indicate the file type, in this case **0/** indicates a text or HTML file. This more complicated URL structure meant only that the construction of the links for all papers needed modification by the conference technical staff, but this was transparent to the conference presenters and participants. A different server would probably have made this task easier, but regardless of the server, all links would have to be rigorously checked and confirmed.

Email Discussion Server. Comments and discussion can greatly illuminate a presentation. The ECCC used electronic mail for the exchange of ideas and comments among participants and presenters. To allow all conferees to read all the discussions, we set up a discussion group for the ECCC. We selected the *listserv*[12] program to handle this function. This is a very versatile and robust list server which allows individuals to subscribe and unsubscribe to a list with no human system administrator intervention. *Listserv* accepts mail messages from subscribers and then forwards them to all other subscribers. The program checks for proper mail addresses and duplicate messages. Conferees can select to

obtain the messages as they arrive or in a digest form, where all messages from one day are delivered together.

We configured *listserv* to operate a discussion group called **eccc**. People registered for the conference by subscribing to this discussion group by sending the message **subscribe eccc yourname** to **listproc@hackberry.chem.niu.edu.** Messages to be distributed to the entire list were sent to **eccc@hackberry.chem.niu.edu.** Note that registration was only necessary if you wished to participate in the discussions. The WWW server and the ECCC papers were available to anyone.

Since we anticipated a large number of papers and discussions of these taking place simultaneously, participants were asked to start the subject line of their message with the number assigned to each paper. Participants could then screen messages by the subject line.

The mail messages were archived and made available using the program *hypermail.*[13] *Hypermail* converts mail files into HTML files and creates indexes. We configured a dummy account to receive all mail messages from the ECCC discussion group. Upon receipt of a message, a Perl script[14] determined the paper being discussed by parsing the subject line. *Hypermail* was then directed to convert the message to HTML and archive the file in two locations, one in a directory holding all messages and one in a directory for the particular paper discussed. Thus, every paper had a directory to store all messages related to that paper. Indices of the messages for both the entire archive and each individual paper archive were automatically updated by *hypermail.*

Anonymous FTP Site. Submission of papers was facilitated through an anonymous ftp server. We created a directory called "ECCCsubmissions" and within this directory we created a subdirectory for each paper, with the name "PaperXX" where XX corresponded to the paper number. Presenters then simply deposited their papers in the correct location. The system administrator then checked each paper, correcting the URLs and checking that all aspects of the paper worked properly.

We created a symbolic link within the WWW server directory to the "ECCCsubmissions" directory so that only one copy of the paper needed to be stored. This arrangement also allowed those people with limited Internet access to obtain the papers by anonymous ftp and view them using the local file viewing feature of *Mosaic.*

III. PRECONFERENCE IMPLEMENTATION

Design of the User Interface. The participant enters the conference through the home page (Figure 1). The home page provides links to the conference materials—titles of the papers, titles listed by author name, abstracts, email discussions, and registrant list. Each of these entry points contains links to the others so that the user is free to enter the conference in the manner that best suits their purpose.

The ECCC Titles page (Figure 2) lists each paper by title and author. The title is a link to the abstract of the paper. As an example of how this link is established, a portion of the actual HTML is reproduced in Figure 3. The key feature is that all abstracts are held in one large file, and each paper is given an anchor name. The anchor name is given following the number sign (#) in the URL. Selecting a particular title takes you to that abstract in the ECCC Abstract Page.

The Titles-By-Author Page is an alphabetical listing of every author followed by the title of the paper(s) they submitted. Each title is a link to the abstract in the ECCC Abstract Page.

The ECCC Abstract Page is really the central focus of the conference. Access to the actual papers is obtained exclusively through this page. The abstract page contains each abstract in the order that it was received. Each abstract, see Figure 4 for an example, begins with the paper number and a link to the email discussion of that paper. Next comes the title, which is a link to the actual paper, followed by the author's name, affiliation, and email address. This is followed by the text of the abstract. A sample of the HTML for this page is listed in Figure 5. The anchor name is given by the HTML tag ⟨**A NAME=name**⟩, providing the anchor for the link in the title page. Links are made to the actual paper and to the mail discussions of that paper.

The Email Discussion Page contains links to all the email archives. These archives are HTML versions of the mail messages from the discussion group, as prepared by *hypermail.* The link connects to the index file for the archive of interest.

The Registrants Page is a list of all persons who subscribed to the discussion group. A *C* program reads the *.subscribers* file, generated by *listserv*, and creates an alphabetical list of the names and email addresses of the participants.

Conference Announcement. The preliminary announcement for the ECCC was made on May 17, 1994 on the Computational Chemistry List and on the *sci.chem* Usenet list. The full announcement appeared on June 23, 1994 on the same electronic lists. This announcement included the deadlines for abstract and paper submission and a pointer to general instructions on how the conference would operate.

General Instructions. The general instructions provided a brief philosophical motivation for the conference. The conference would cover all aspects of computational chemistry, and we left it up to the authors themselves to define the field. The remainder of the instructions were how to prepare and submit the abstract, how the abstracts would be reviewed, how to prepare and submit the final paper, and how to register for the conference.

Abstract Submission. While each abstract would be presented in a uniform format, we did not necessarily want to impose a format upon the authors in submitting their abstracts. We therefore developed two procedures for authors to deliver their abstracts without defining a standard format. The first was by electronic mail. We set up an account **conference@hackberry.chem.niu.edu** to accept abstracts submitted by a mail message. Authors then sent their abstract, containing a title and author names and addresses to this account. No format was imposed. Upon receipt of the abstract we formatted the entry for inclusion in the ECCC abstract page.

The alternative method was to fill out an HTML form. Use of this form is restricted to those browsers that are forms-capable and, at the time, *Mosaic*[7] and *MacWeb*[15] were the only forms-capable browsers available. The ECCC Abstract Submission Form contained entries for author name(s), organization and address, email address, and the text of the abstract. When this form was submitted to the NIU server, a CGI (Common Gateway Interface) script was launched which automatically took the entries and formatted them properly and appended them to the ECCC Titles and

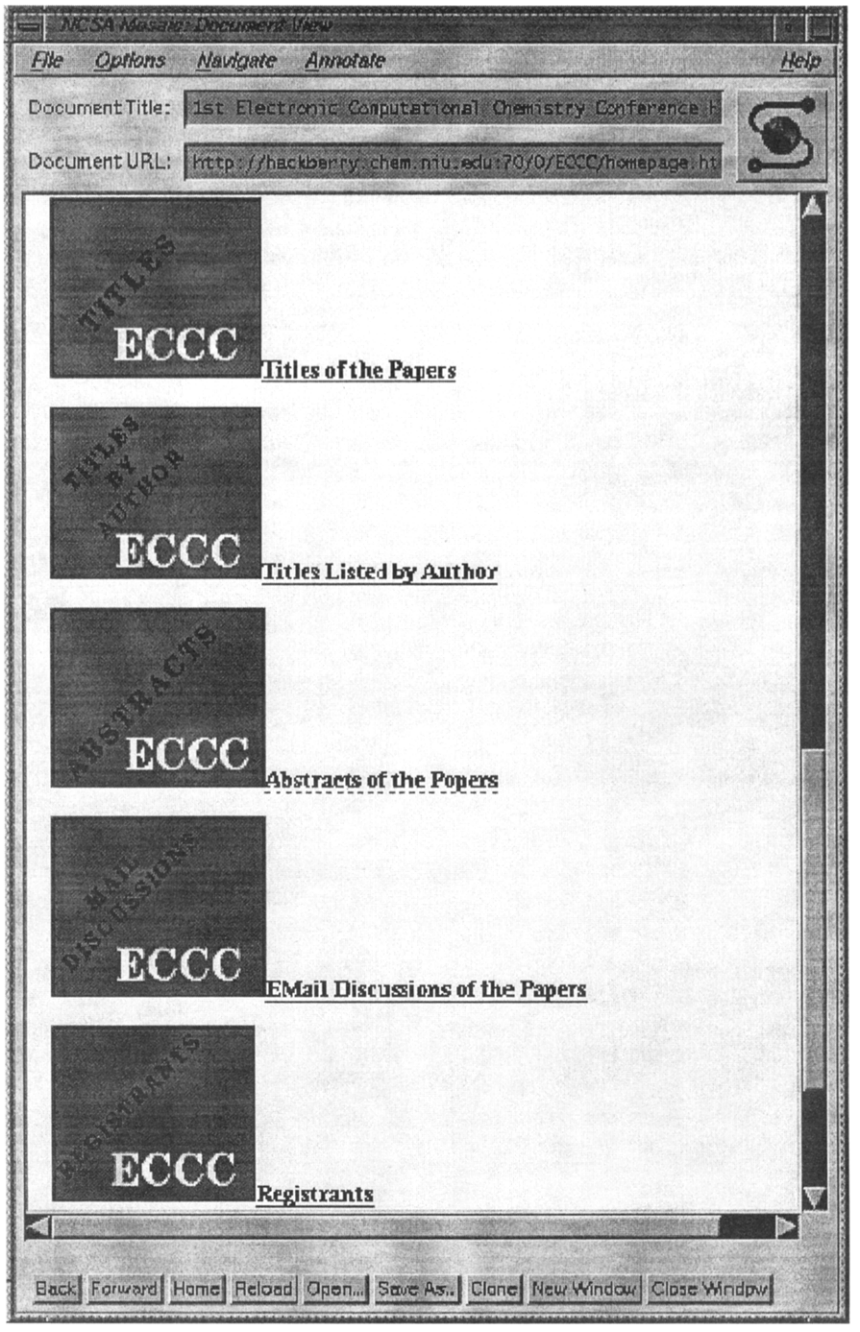

Figure 1. The ECCC home page as viewed using *Mosaic* on a silicon graphics workstate.

Abstracts Pages. This procedure was certainly much less time-consuming and easier for the conference organizers. With the proliferation of forms-capable browsers, form-based abstract submission is strongly recommended.

Abstract Screening. Groups of 12 abstracts were collected and then sent by email to the member of the SOC for review. This review was essentially to judge the suitability of the abstract for the conference, to assure a minimum level of scientific quality, and to assess the use of Internet features that might enhance the conference. The abstracts were screened by the members of the SOC only and were not subject to the rigors of review common for journal publication. The reviews of the abstracts were collected by the conference coordinator, and the authors were then notified, again by email, of the decision on each abstract.

Paper Preparation. All papers for the ECCC were required to be written in HTML, in keeping with the use of the WWW as the exclusive means for communication of the papers. While HTML is not a difficult formatting language, we assumed that most chemists were unfamiliar with its use. Therefore we listed a number of resources on the Internet that could provide useful assistance in preparing the papers. We provided no strict guidelines on the paper presentation since we wanted to encourage as wide an audience as possible and encourage creative use of the medium. Our only suggestions were to limit the amount of text, since large text blocks are not usually effective communications on the web, and to make extensive use of graphics. We suggested that small graphics should be included directly in the document and large images made available through a link. One of the features of web browsers is that after a document is transferred, the browser can spawn the appropriate application to handle that document. For example, a user may select a link that transfers a large JPEG (Joint

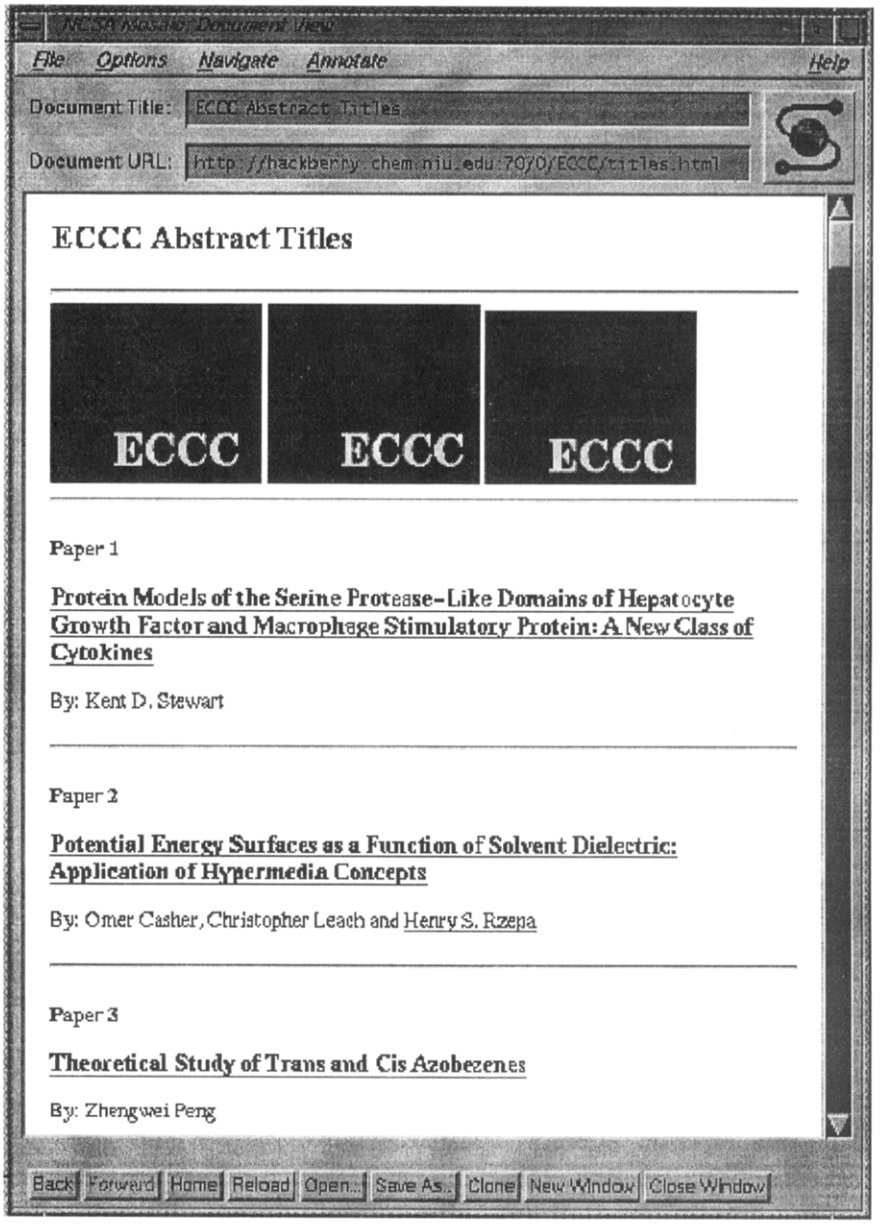

Figure 2. The ECCC titles page as viewed using *Mosaic* on a silicon graphics workstate.

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<TITLE>ECCC Abstract Titles</TITLE> <H1>ECCC Abstract Titles</H1><P>
<HR>
<A HREF="/0/ECCC/homepage.html"><IMG SRC="/I/ECCC/ECCChome.gif"></A>
<A HREF="/0/ECCC/abstractshome.html"><IMG SRC="/I/ECCC/ECCCabstract.gif"></A>
<A HREF="/0/ECCC/titlesbyauthor.html"><IMG SRC="/I/ECCC/ECCCtitlesbyauthor.gif">
</A> <HR>
<H3>Paper 1</H3>
<H2><A HREF="/0/ECCC/abstracts1.html#link1">Protein Models of the Serine Protease-Like
Domains of Hepatocyte Growth Factor and Macrophage Stimulatory Protein: A New Class of
Cytokines</A></H2> By: Kent D. Stewart<P>
<HR>
<H3>Paper 2</H3>
<H2><A HREF="/0/ECCC/abstracts1.html#link2">Potential Energy Surfaces as a Function of
Solvent Dielectric: Application of Hypermedia Concepts</A></H2> By: Omer Casher,
Christopher Leach and <A HREF="http://www.ch.ic.ac.uk/rzepa.html">Henry S.
Rzepa</A><P> <HR>
<H3>Paper 3</H3>
<H2><A HREF="/0/ECCC/abstracts1.html#link3">
Theoretical Study of Trans and Cis Azobezenes</A></H2> By: Zhengwei Peng<P>
<HR>
<H3>Paper 4</H3>
```

Figure 3. A portion of the HTML file for the ECCC title page.

Photographic Experts Group) image. Upon completion of the transfer, the browser automatically launches a viewing program with the image as the input file. We encouraged the use of these external programs, which we discuss further in the section on *Chemical MIME-type*.

HTML Resources. Our instructions listed two types of resources for assisting in the preparation of HTML files. The first set were primers and style guides on writing HTML. This list included the documentation[16] written by the developers of *Mosaic*.

The second set was a list of converter utilities, which take word processor documents and convert them into HTML documents. Since most scientists are experienced with a word processor, the use of a converter is the simplest path toward creating an HTML file. Converters are available for RTF (Rich Text Format),[17] Microsoft Word for Windows,[18] LaTex,[19] and Word Perfect[20] documents. Many authors did make use of these converters to prepare their papers.

Chemical MIME-Type. As described above, one of the features of web browsers is their ability to launch helper applications. This ability is made possible by the use of MIMEs (Multipurpose Internet Mail Extension).[21] Every document transmitted by a web server has a MIME-type assigned to it. The web browser can be configured to recognize certain MIME-types and then launch a particular application when that MIME-type is encountered. This feature is widely used on the web for viewing large graphics images. These are sent with the appropriate MIME (such as image/jpeg to indicate a JPEG graphic), and the local

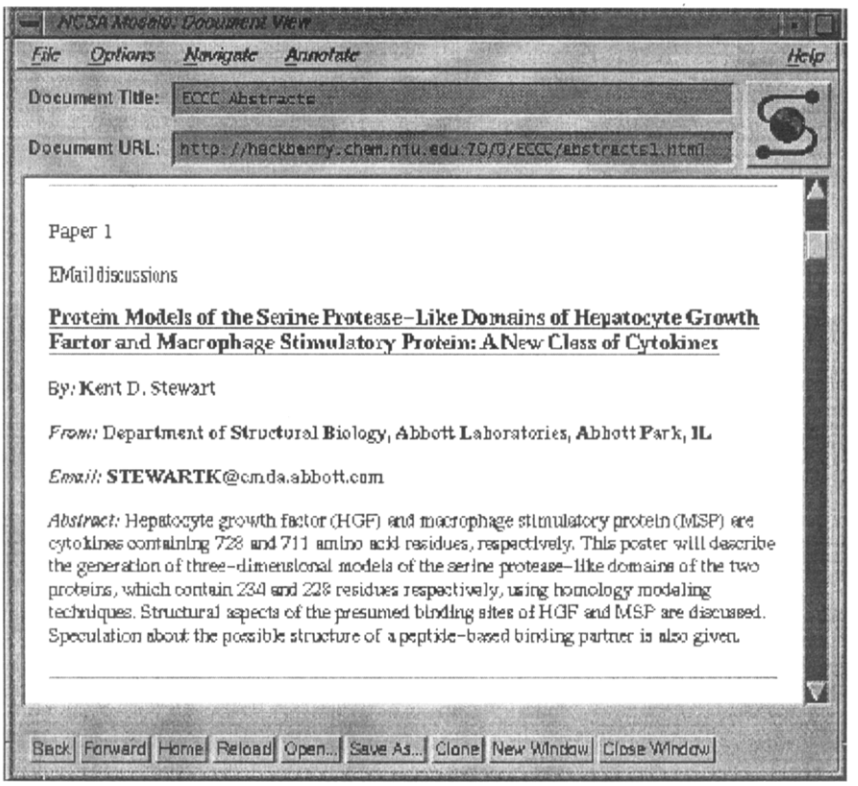

Figure 4. An abstract from the ECCC abstracts page as viewed by *Mosaic* on a silicon graphics workstation.

```
<HR>
<COMMENT start of new abstract>
<H3>Paper 1</H3><h4><A HREF="/0/ECCC/ECCCMail/1/index.html">EMail
discussions</A></H4>
<A NAME="link1"><H2><A HREF="/0/ECCC/Papers/Paper1/Paper1.html">Protein Models of
the Serine Protease-Like Domains of Hepatocyte Growth Factor and Macrophage Stimulatory
Protein: A New Class of Cytokines</A></H2><P> <H3><I>By:  </I>Kent D.
Stewart</H3><P>
<H3><I>From:  </I>Department of Structural Biology, Abbott Laboratories, Abbott Park,
IL</H3><P>
<H3><I>Email:  </I>STEWARTK@cmda.abbott.com</H3><P>
<P>
<I>Abstract:</I>
Hepatocyte growth factor (HGF) and macrophage stimulatory protein (MSP) are
cytokines containing 728 and 711 amino acid residues, respectively.  This poster will describe the
generation of three-dimensional models of the serine protease-like domains of the two proteins,
which contain 234 and 228 residues respectively, using homology modeling techniques.
Structural aspects of the presumed binding sites of HGF and MSP are discussed.  Speculation
about the possible structure of a peptide-based binding partner is also given. <P> <HR><P>
<COMMENT start of new abstract>
```

Figure 5. A portion of the HTML file for the ECCC abstracts page.

browser will then launch a viewing application, such as *xv*.[22] The applications to view graphics, PostScript files, and movies for UNIX, Windows, and Macintosh computers were collected from various anonymous ftp sites and placed in the anonymous ftp site for the ECCC. Participants in the conference were urged to obtain these applications and configure their browsers appropriately.

Recently, Rzepa and co-workers have advocated the adoption of a chemical MIME-type.[23] The chemical MIME-type would be used to designate files of special interest for chemists. These include X-ray structure coordinates in the protein data bank[24] and crystallographic[25] format, output from quantum mechanical programs such as GAUSSIAN[26] and MOPAC,[27] molecular description files like MDL Molfile[28] and SMILES,[29] and the JCAMP format for describing IR[30] and NMR[31] spectra.

Rzepa has developed the concept of "hyperactive molecules" whereby the coordinates of a molecule are transferred by a web server using the chemical MIME-type.[32] The browser reads the MIME and then launches a molecular viewing program with the coordinates as input. The user can then manipulate the structure, for example, rotating the molecule to view from a different orientation. We actively promoted the use of the Chemical MIME-type in the ECCC. Participants were encouraged to obtain a molecular viewer such as *XMol*[33] or *RasMol*.[34] Authors were encouraged to include coordinate files in their papers. As a result, nearly one-quarter of the ECCC papers included "hyperactive molecules", in the form of output from a calculation or crystal structure.

Paper Submission. Submission of the final papers could be accomplished in two ways. The choice was dependent on how the author wished the paper to be served. The simplest procedure was to deposit the paper with the official ECCC web server. Every paper was assigned a number, in the order in which the abstracts were received and approved. The anonymous ftp server for the ECCC was set up to accept the papers. Authors deposited, by anonymous ftp, their papers and associated files into the appropriate directory. The authors then sent a note to the coordinator informing him that all files had been transferred. The coordinator then created the *.cache* file to make the files publicly available, tested the links, and added the URL for the paper to the ECCC Abstract Page.

The alternative was for the author to serve the paper on a local WWW server. In this case, the author sent an email message to the coordinator with the correct URL for the paper. The coordinator accessed the paper to insure that it was available and then created the link to this URL on the ECCC Abstract Page.

Registration. Registration for the conference was necessary only if a participant wished to take part in the mail discussions. All presenters were required to register for the conference. Registration was accomplished by subscribing to the *listserv* as described above. Registration was allowed throughout the conference.

IV. CONFERENCE ACTIVITY

Operations. The conference officially began on November 7, 1994 when the ECCC Abstract Page with links to the final papers was publicly released. For the month prior to this date, the ECCC Abstract Page was available, but it did not have the links to the papers. The discussion list had also been operational before the start of the conference, but traffic was limited to announcements and reminders sent by the conference coordinator.

Once the conference began, there was very little work required of the coordinator. The design of the conference was such that the conference was operating with no human intervention. The *Gn* server handled all web requests, the *listserv* program handled delivery of the mail, and *hypermail* archived the messages. The organizer's duties during the conference were to backup the files, insure that the computer and the network were operating properly, and maintain the logs. The *Gn* server logs all requests and files delivered. These records are kept in a log file. The traffic during the conference was sufficiently large that daily log files needed to be created.

There were only two changes to the operation of the conference that occurred during the ECCC. First, participants from Europe complained of the long transfer time to obtain the ECCC Abstract Page. The ECCC Abstract Page was 138K bytes. On the third day of the conference, this file was broken into eight parts, each containing 10 abstracts, and a new abstract home page gave access to these new abstract pages. Transfer times were substantially diminished.

The other change was an extension of the conference. The original plan was to terminate the conference on November 18, 1994. Termination of the conference essentially entailed turning off the list server. However, there were many requests from participants to continue the conference to give everyone more time to digest the papers and continue discussions. Therefore, the conference was extended to November 30, 1994. Although accessing of conference materials and sending email messages during the extension was fairly light (see below), the flexibility of this electronic medium allowed for the extension, which would be virtually impossible at a normal meeting.

Papers and Discussions. The ECCC attracted 81 abstracts and actually carried 73 papers. The topics of these papers were extremely varied, truly spanning a very broad definition of computational chemistry. The topics covered included, for example, use of *ab initio*, density functional theory, and semiempirical methods for understanding reactions, molecular modeling studies of proteins, development of new procedures for QSAR and drug design, protein dynamics, studies of the use of the Internet in chemistry, and the use of computers in chemical education. A complete list of titles is presented in Table 1.

Mail discussions centered on just a few of the papers. Most papers were not discussed at all. However, very active discussions occurred on the topics of solvation modeling and the use of the WWW for distributing chemical information.

An alternative to email discussions was presented in one paper, which covered networked virtual environments. A multiuser interactive environment was established in which conference registrants could participate by having discussions in real-time. A number of informal sessions were held, and one organized gathering to discuss a paper was conducted during the conference. One difficulty with interactive sessions is that participants are located around the world, so scheduling a time when everyone (or even most participants) are awake, let alone available, is problematic.

Statistics. One can gather a sense of the success of the ECCC by examining of the level of participation.

Registrants. At the start of the conference, there were 297 subscribers to the discussion list. We allowed registration to occur during the conference, and we also allowed people to unsubscribe. The number of subscribers totaled 321 at the end of the conference. It should be noted that there were a few people who unsubscribed from the list.

A breakdown of the country of origin, determined by the domain name of the email address, of the subscribers at the start of the conference is listed in Table 2. While the conference was dominated by American scientists, there were participants from six continents. Of particular note is the participation of chemists from former Soviet bloc nations.

Papers. There were 73 final papers in the ECCC. There were 8 withdrawn papers. As stated above the papers covered a variety of topics. A breakdown of author's countries is given in Table 3. Once again, we wish to point out the international makeup of the authors.

Nearly one-third (22) of the papers we delivered by local WWW servers, while the rest were delivered by the NIU Chemistry WWW Server. Chemistry MIME-types were utilized in 15 papers, while five papers incorporated video. While HTML was the standard format for the papers, five papers did not make significant use of this language. Instead, they were either flat ASCII files or made heavy use of PostScript.

There were 247 mail messages during the course of the conference. The paper that drew the most comments (30 messages) was Paper 56, entitled "WWW—Chemists' Friend or Foe? Problems with Electronic Chemical Data Exchange".

Accesses. A summary of the number of accesses of ECCC files is listed in Table 4. We define an access as a delivery of any file. Access of the ECCC files was very strong early in the conference, and it declined throughout. Nevertheless, there was significant activity during the extension period. (The low access numbers for No. 24 and 25, 1994 are probably due to the Thanksgiving holiday in the U.S.)

Authors who served their own papers were asked to submit their access numbers. We report the accesses for eight of the 22 external papers. Projecting for the additional 14 papers, the total number of conference file accesses was about 63 000.

V. POST-CONFERENCE

Survey Results. At the end of the conference, the participants were encouraged to complete a survey covering many aspects of the conference. The survey was handled using a form-based HTML page. The survey entailed 22 questions, eight directed toward authors and the rest for all participants. The response was in the form of radio buttons ranked 1−5 where 1 indicated strongly agree with the comment and 5 indicated strongly disagree with the comment. A section for general comments was available at the end of the survey. We received 66 replies to the survey.

We present here some of the results of the survey. For the comment "The concept of electronic conferencing inspired me to participate as a presenter of a paper", 31

Table 1. Titles and Authors of Papers in the ECCC

Protein Models of the Serine Protease-like Domains of Hepatocyte Growth Factor and Macrophage Stimulatory Protein: A New Class of Cytokines By: Kent D. Stewart
Potential Energy Surfaces as a Function of Solvent Dielectric: Application of Hypermedia Concepts By: Omer Casher, Christopher Leach, and Henry S. Rzepa
Theoretical Study of *trans*- and *cis*-Azobenzenes By: Zhengwei Peng
Preliminary Solution Structure of the Cytochrome *c*551 from Ectothiorhodospira abdelmalekii by Homonuclear NMR and Distance Geometry By: K. Boulez, M. Budesinsky, J. Martins (#), F. Fant, W. Vranken, and F. A. M. Borremans
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On the Limitations of the Density Functional Theory in Electronic Structure Calculations By: Isaac B. Bersuker
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Multiple Metal Additions to C_{60}. An ab Initio Study of $[M(PH3)2]_nC_{60}$ (M = Pt and Pd; n = 1, 2, and 6) By: Carles Bo, Miquel Costas, Jose Carlos Ortiz, and Josep M. Poblet
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Ab Initio Study of the Diels−Alder Reaction of Phosphaethene and Phosphaethyne with Butadiene By: Debbie C. Mulhearn and Steven M. Bachrach
A Comparison of Some Commercially Available Structural Descriptors and Clustering Algorithms By: Robert D. Brown, Mark G. Bures, and Yvonne C. Martin
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The Hyperfine Structure of Muons in Silicon and Diamond Crystals By: H. U. Suter, N. Paschedag, D. M. Maric, and P. F. Meier
Conformational Sampling of Glycerolphosphatidylcholine Using Distribution Biased Monte Carlo and Langevin Dynamics Methods By: Barry J. Hardy
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Impulsive Energy Transfer During Unimolecular Reaction via Reactive Cylinders in Phase Space By: Joanna R. Fair, Karin R. Wright, and John S. Hutchinson
Ab Initio Study of the Chemisorption of Alkali Metals on the Si(111) Surface By: A. Clotet, J. C. Ortiz, J. M. Ricart, J. Rubio, and F. Illas
A Tool for Negotiating through Structure−Activity Relationship Space: The Hypersurface Iterative Projection Method By: DOnald B. Boyd
Self-Consistent Reaction Field Study of Dual Fluorescence in *p*-DMABN By: Peter Gedeck
A Software Toolkit for de Novo Ligand Design By: Z. Zsoldos, A. P. Johnson, V. Gillet, G. J. Myatt, and D. Bayada
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Comparison of Reactivity of Thiophene, Thiophene 1-Oxide, and Thiophene 1,1-Dioxide as Diene for Diels−Alder Reactions. An AM1 Semiempirical Study By: Branko S. Jursic and Don Coupe
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An Update to the NCI Drug Information System 3D Database By: Daniel W. Zaharevitz, Xinjian Yan, Shaomeng Wang, and G. W. A. Milne
Application of Genetic Algorithm to the Calculation of Bound States and Local Density Approximations By: Yehuda Zeiri, Eyal Fattal, and Ronnie Kosloff
Locating Transition States Using Double-Ended Classical Trajectories By: A. Matro, D. L. Freeman, and J. D. Doll
Stability, Local Geometry and Resonant Vibrations of Cu(+) Impurity in Alkali Halides. By: V. Luana, M. A. Blanco, M. Florez, and L. Pueyo
Strategies for Determining Interionic Potentials from ab Initio Calculations of Ionic Crystals By: M. A. Blanco, E. Francisco, J. M. Recio, A. M. Pendas, and V. Luana
Modeling Enantioselective Chromatographic Separation of α-Pinene Racemates on Permethylated β-Cyclodextrin By: Delbert R. Black, Craig G. Parker, S. Scott Zimmerman, and Milton L. Lee
Calculations of the Phi-Psi Conformational Contour Maps on *N*-Acetyl-*N*′methylalanineamide (Blocked Ala) and of the Characteristic Ratios of Poly-L-Alanine Using Various Molecular Mechanics Force Fields By: Chui Hong Lee and S. Scott Zimmerman
A Quantum Chemical Study of Mechanism and QSAR Analysis of Dopamine-β-Hydroxylase Inhibitors Using PM3 Method By: Emadeddin Tajkhorshid, Massoud Mahmoudian, and Daryoush Khodaverdi
A Localized Projected Atom Approach to Large and Extended Systems By: Jack A. Smith
Proposed Topography of Compounds Acting at the rho1 Receptor By: H. R. Capper, M. Collins, M. B. Gillies, and G. A. R. Johnston
Intramolecular Vibrational Energy Redistribution and Torsional Isomerization: A Model Classical and Quantum Study By: Dr. Harold W. Schranz
Computer Support for the Isoinversion Principle By: Stefanie Kethers
Theoretical Electronic and Vibrational Study of $B_n(CO)_m$ (n,m = 1,2) with the Density Functional Method: Preliminary Results By: Pullumbi Pluton and Bouteiller Yves
Water Clusters—a Speculation By: Dr. Bernd R. Eggen
Molecular Dynamics Study of Peptide Flexibility By: Yan Wang and Krzysztof Kuczera
A Check on Basis Functions in Density Functional Calculations By: Daniel P. Joubert
Application of Genetic Algorithms to the Determination of Protein 3D Structure from NMR Spectroscopy Data By: Jarmo T. Alander and Jari Ylinen
The Performance of Generalized Gradient Approximation DFT Methods with Gaussian Basis Sets: Sulfur and Chlorine-Containing Molecules By: Gabor I. Csonka, N. Anh, and J. Reffy
The Ability of the MP2 Method to Model the QCSID(T) Basis Set Extension Effects for the Hydrogen Atoms in Molecules By: Gabor I. Csonka and N. Anh
The Evolution of Lactate Dehydrogenase Conformation during Molecular Dynamics Simulations By: C. A. Letner and G. M. Alter
On the Computation of Functions of Matrices By: Herbert H. H. Homeier
Fluctuating-Charge Molecular Dynamics of Liquid Water By: Steven J. Stuart

Table 1 (Continued)

Relativistic Molecular ab Initio Electronic Structure Calculations with the MOLFDIR Program Package By: W. A. de Jong, F. Dijkstra, L. Visscher, P. J. C. Aerts, W. C. Nieuwpoort
WWW—Chemist's Friend or Foe? Problems with Electronic Chemical Data Exchange By: Bernard Blessington and Don Parkin
From Electronic Structure to Phase Stability through Topological Arguments: The Alkali Halide Example By: A. Martin Pendas, V. Luana, J. M. Recio, M. A. Blanco, E. Francisco, and M. Florez
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The Electronic Structure of Singlet and Triplet Nitrenium Ions from MCSCF and DFT Calculations By: Sharon E. Worthington, Christopher J. Cramer, Frederic J. Dulles, and Joey W. Storer
Lone Pairs and the Molecular Electrostatic Potential of Water By: David Young and James F. Harrison
Atomic and Functional Groups Origins of Nonlinear Response Tensors in Urea and Thiourea By: Keith E. Laidig
Networked Virtual Environments and Electronic Conferencing By: John Towell, Paul Hansen, Eric Mercer, Martin Leach, Irit Rubin, Jaime Prilusky, and Gustavo Glusman
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Triflic Acid as a Model for the Acidic Site of the Superacid Catalyst Nafion: An ab Initio Study of Its Hydrogen Bond Propensity By: G. Ricchiardi and P. Ugliengo
The Reactions of Methyloxirane and Methylthiirane with Nucleophiles By: Scott Gronert and Joseph M. Lee
Ab Initio Studies of Carbene—Fluoroalkane Complexes By: Jean M. Standard
Study of Addition Reaction To Form Cyclic Urea Derivatives By: Joerg R. P. Heuer and Harald G. Schweim
Theoretical Study of the Mechanism of Recombinative Hydrogen Desorption from the Si(100) Surface By: Petr Nachtigall, Carlos Sosa, and Kenneth D. Jordan
Electrostatic Fields over Ionic Surfaces and into Zeolitic Cavities: Comparison between LCAO Periodic Calculations in the Hartree Fock and the Density Functional Approximations By: M. Causa
Torsional Dependence of the Methanol—He Interaction Potential By: Han Thai and Stephen L. Davis
Langevin Dynamics of Simplified Protein Models By: John M. Troyer, Fred E. Cohen, and David Ferguson
Conformational Analysis of 2-Aminoethanal and Methylated Derivatives By: Luis Carballeira and Ignacio Perez-Juste
Insights into the Mechanism of the Asymmetric Reduction of Ketones with Diisopinoampheyl Boron Chloride By: Mark D. Mackey and Jonathan M. Goodman
Quantum Control of Molecular Dynamics with Tailored Light Pulses By: Jianwei Che, Jeffrey L. Krause, Bern Kohler, Michael Messina, Rob M. Whitnell, Kent R. Wilson, Vladislac V. Yakovlev, and Yijang Yan
Multimedia Chemistry and Education By: Eric A. Fernandes, Mike Messina, Bret J. Naylor, Daniel A. Olshove, Amandeep K. Shergill, Robert M. Whitnell, and Kent R. Wilson
Klotho By Brian Dunford-Shore, Francis Fabrizio, Jason Holcomb, William Wise, and Toni Kazic

Table 2. Distribution of Registrants by Country

country	no.	country	no.
U.S.A.	152	Belgium	2
United Kingdom	26	Finland	2
Germany	22	Hong Kong	2
Australia	18	Iran	2
Spain	11	South Africa	2
Netherlands	10	Brazil	1
Italy	9	Croatia	1
Canada	6	Czech Republic	1
France	6	Hungary	1
Austria	5	Jamaica	1
Switzerland	4	Japan	1
Poland	3	Mexico	1
Sweden	3	Slovakia	1
Turkey	3	Soviet Union	1

Table 3. Distribution of Authors by Country

country	no.	country	no.
U.S.A.	38	Italy	2
Spain	8	Belgium	1
United Kingdom	5	Finland	1
Germany	4	Iran	1
Netherlands	3	Israel	1
Australia	2	Poland	1
France	2	South Africa	1
Hungary	2	Switzerland	1

people strongly agreed and nine agreed out of 43 respondents. Comments dealing with preparation and submission of the papers indicated that less than half experienced any real problems.

For question 10 "I had no difficulty in viewing the papers", 21 strongly agreed and 21 agreed, with only eight responding negatively. Fifty-nine people answered positively that the web was an appropriate medium for holding a conference. The variety of papers was found to be interesting to 46

Table 4. Number of Access of ECCC Files on the NIU Server

official conference period		extended period	
date	no.	date	no.
Mon 11/7/94	6321	Sat 11/19/94	785
Tue 11/8/94	5796	Sun 11/20/94	501
Wed 11/9/94	4907	Mon 11/21/94	1923
Thu 11/10/94	5289	Tue 11/22/94	1119
Fri 11/11/94	3379	Wed 11/23/94	892
Sat 11/12/94	879	Thu 11/24/94	157
Sun 11/13/94	1253	Fri 11/25/94	560
Mon 11/14/94	3693	Sat 11/26/94	187
Tue 11/15/94	2924	Sun 11/27/94	303
Wed 11/16/94	2160	Mon 11/28/94	1200
Thu 11/17/94	3749	Tue 11/29/94	995
Fri 11/18/94	2846	Wed 11/30/94	982
total	43196	Thu 12/1/94	904
		Fri 12/2/94	792
		total	11300
NIU total	54496		
external total[a]	3136		
grand total	57632		

[a] Statistics gathered for eight of the externally served papers.

participants. To the question "The mail discussions contained useful comments" 12 strongly agreed, 30 agreed, 15 were neutral, and nine disagreed or strongly disagreed. The majority of participants were neutral concerning the lack of real-time interactions detracting from the conference.

The final two questions concerned the overall impression of the conference. To question 21 "The ECCC was a successful conference" 35 people replied strongly agree, 22 agree, seven neutral, one disagree, and one strongly disagree. To the final question "I plan to participate in the second ECCC" 39 participants replied strongly agree and 20 agree.

The written comments were generally quite positive. There were two general themes regarding concrete advantages of the electronic conference over traditional conferences. The first is the ability of the participant to read and contemplate the science without the time constraints of a rushed meeting. For example:

> "When the conference started the email traffic increased with a delay of about two to three days. (Replies to) the discussion came with a low frequency. This seems to indicate that people actually think and do some homework before opening their mouths."

> "One benefit of the electronic conference over a real conference that I had not expected was the chance to take time to think about scientific material that is part of the poster. So many times in a real life poster session, the hustle and bustle of the crowd means you really can't think about the poster. In the case of the electronic posters, I could take all the time I wanted. In fact, I devoted 5 full hours to looking over the posters—something I never would have been able to do at, for example, an ACS meeting poster session."

The second major advantage of the electronic conference was the ability for many people to attend and participate, who could not normally attend meetings. The fact that the conference was free and spread over a two-week period meant that those chemists with limited funds or time could still participate:

> "With the high cost of travel and my heavy teaching load I would have been unable to attend *any* conference this fall without the ECCC."

> "The conference fits well with our special inconvenient economical situation here."

Another person commented that

> "The main benefit is my attendance at an international conference in an area which is not my main line of work. Physical attendance would have been difficult to justify."

Lastly, one conferee noted that electronic conferences allow persons with physical disabilities to fully participate:

> "In my own case, I am physically handicapped, the format of the meeting was especially pleasant, no accessibility issues, and...everything was legible in a sitting position, usually not true at conventional poster sessions."

Comments from participants on problems with the conference tended into two areas: the email discussions and the organization of the papers. A number of people objected to the quantity of mail messages (although only 16 people agreed or strongly agreed with the survey comment "The amount of mail traffice was overwhelming"). The comments suggested that the amount of traffic was either too much or not of interest to them. Many offered some solutions:

> "You should not use a mail exploder (listserv) to send everybody's email comments to everyone else; it quickly becomes so overwhelming that nobody can participate even in those discussions that might interest them. I suggest you establish a tree of messages."

> "I was somewhat annoyed by the frequency of mail traffic relating to the conference, much of which was either personal in nature or dealing with issues and/or papers that I was not particularly interested in. Some kind of filtering mechanisms that would allow a participant to "tune out" discussion related to particular papers would be nice."

> "The amount of mail was a bit much. Perhaps folks could have the ability to take themselves out of certain mail discussions?"

The other major complaint was about the organization of the conference. Access to the full papers was obtained solely through the abstracts page. The large ECCC Abstracts Page meant long waits for the overseas participants, though this was somewhat alleviated by breaking this file into smaller pieces. Nevertheless, a couple of people suggested that a mirror site would be helpful.

Also, the abstracts were not ordered in any fashion. A number of people suggested that they would like to see a index or grouping of the abstracts by subject.

Taking this sentiment further, two people commented that they would like to see a greater specialization of the conference, represented by the comment:

> "In my opinion it would be helpful if the conference (would be a) little more specialized on some particular topic."

VI. CONCLUSIONS

The ECCC exceeded the expectations of the organizer in many respects. Since the conference involved use of a new medium, the World-Wide Web and HTML, there was no basis for predicting the degree of participation. Fortunately, we selected a medium with a relatively low learning curve. The success of the conference is best judged by the participation—73 papers and over 300 conferees!

The WWW is a rapidly developing technology that already contains many useful features for electronic chemical communication. Documents can contain both text and graphics. Links allow for quick access to references and related materials. MIME-types allow for transmitted data to be directed to other programs, streamlining the transmission of audio and video files. An excellent example of the application of this tool to chemistry is hyperactive molecules—enabling the end-user to manipulate chemical structures. Further developments of web technology will undoubtedly make document preparation easier and enable more advanced data manipulations.

Nevertheless, there is room for improvements. There are a number of technical issues that need advancement. The version of HTML available at the time of the conference did not support subscripts, superscripts, tables, or the Greek alphabet. The first three of these have now been adopted by the latest version of *Mosaic*[7] (and the recently released browser *Netscape*[35] supports tables), which will certainly enhance chemical documents. Adoption of the Greek character set should occur within another year.

As chemists become more familiar with the web and HTML, they will surely become more adept at making use of the features they command. For the time being, very detailed instructions on how to make use of these features, particularly the use of the chemistry MIME-type should be included in any announcement of future electronic conferences.

Transfer rates for large documents is a problem for intercontinental transmissions. While the optimal solution is increased bandwidth of the overseas connections, an appropriate short-term solution is to have mirror sites in Europe and Asia.

Mail discussions were perhaps the most disappointing aspect of the conference. For many conferees there was just too much traffic, while for others, the degree of discussion was disappointing. There are a few potential remedies. The first is simply educating participants on how to manage potentially large volumes of mail. Participants should be informed of the need to include a subject line that provides a good indication of the content. Conferees can then scan the subject lines and decide which messages should be read and which can be deleted outright. If a list server (sometimes called a mail exploder) is used, the digest feature whereby all mail correspondence for a day is sent in one message, should be publicized.

List servers with topic screening should be explored and developed. The ability of *hypermail* to create indexed mail archives suggests that perhaps a mail exploder is unnecessary. Mail could be sent to a central account and then processed by *hypermail*. Conferees then read the mail exclusively through the web pages, easily following threads and skipping uninteresting discussions.

However, the diversity of topics of the ECCC probably was the main cause for disappointment in the mail discussions. Discussions on topics outside one's specialty was viewed as uninteresting and a waste of bandwidth. The diverse interests of the conferees suggested that there were few people interested in any given topic, so that the "critical mass" needed to engender detailed and exciting discussions did not exist. Electronic conferences devoted to a specialized topic, by definition a conference that will not be as general as ECCC, might gather enough experts to create a truly exciting discussion. Since mail discussions inherently are not spontaneous, these discussions could very well be quite detailed and well-thought out. Just as there are general meetings, such as the National ACS Meetings, that cover a wide variety of topics, and specialized meets, such as the Gordon Research Conferences, electronic conferences can relate to both needs.

Perhaps the most obvious drawback to electronic conferences is the lack of personal (face-to-face) interaction between conferees. Traditional meetings afford the opportunity to meet people in both a formal and informal setting and add a "human" side to scientific interactions. Virtual meeting space and videoconferencing are potential solutions, but the technology is still lacking for effective use of these media.

The advantages of electronic conferences are many-fold. The cost of participation is quite low, opening up the conference to a potentially much larger audience than any traditional meeting. The reach of the Internet to most nations allows for a truly international meeting. The ability of each conferee to access the meeting on their own schedule allows conferees to attend without committing to a particular time frame and absence from regular daily schedules. Physically challenged scientists can participate without limitations. The Internet offers an ideal means for scientists to come together and present their most recent results. The Electronic Computational Chemistry Conference has provided a glimpse of the future of electronic conferencing.

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