

# Bittner Group FAQ Sheet

last updated: May 27, 2003

These notes spell out administrative details that will help your research get started as quickly as possible. Most of this is in the "stream of thought" style.

- **Notebook:** The group notebook is used to record research on a day-to-day basis. It is not meant to disrupt or change your style of doing research: it is simply to keep a permanent record of what we all do. It is particularly useful for recording seldom used computer commands, new techniques, etc. If you wish, a copy will be made for you when you leave the group: the original remains here. I will borrow it for a few hours from time to time. Do not do research on scraps of paper! As an alternative to paper copies, electronic notebooks either as Latex or Mathematica notebooks are often more useful especially for graphics, quick-time movies, and data analysis. From time to time I will ask for either electronic or hard copies.
- **Computer Programs:** When a project is completed, a documented version of the code with sample input and output, must be placed in the group archive computer space. In addition, you should make a CDROM archive of important data and codes.

- **Computational Resources:**

1. Electronic Mail: use the UH campus mail server (mail.uh.edu) rather than setting up local mail accounts. This can be accessed either via the web (useful for travel) or as a POP or IMAP server.
2. Group Computers:
  - Various Intel-based Linux and G4-OSX Macintosh computers (k2.chem.uh.edu, )
  - Dual processor Alpha workstation (666MHz/4GB ROM) (montblanc.theory.uh.edu)
  - Dual processor SGI Origin2000 (190 MHz) (everest.theory.uh.edu)
  - 14-node/28 processor Beowulf cluster located in HPC. (hwaet.hpcc.uh.edu)

With few exceptions, all these have Fortran and C compilers and can be used for both development and production. Please try to do development on your local desk-top computer and port the code to the larger (Alpha or Beowulf) for production runs. Since the Beowulf can be used for programs running in parallel, I would like to see movement towards using MPI and other parallel programming paradigms in future codes developed in this group.

3. Programming Languages: I am well versed in Fortran and Mathematica and can do some coding in C. I would encourage you to use whatever language you want knowing that I may not be able to help you in all cases. I would recommend learning C or C++ since this is a useful skill to have.
4. Printers. Pike.chem.uh.edu is the address of the HP4100 laser printer in Fleming 221. Various color ink-jet printers are attached to desktop workstations.
5. Firewall. Most of the computers in Room 221 are behind a common firewall and can be accessed from the outside only via secure shell login to alta.chem.uh.edu. For security reasons, telnet and ftp access are denied to this machine and you should use secure versions: ssh and sftp to access alta. Machines behind the firewall are in the "theory.uh.edu" subdomain which is not available outside the firewall.

6. Group web-page: eiger.chem.uh.edu, a linux server in the common room serves the group web-pages. It is also the repository of papers, code, and other common electronic resources. We are in the process of migrating our web-resources to this computer from k2.chem.uh.edu
7. DHCP. Computers not wired into the office LAN should use the campus DHCP for IP addressing.
8. Wireless LAN. We have a wireless internet port in our office. If you laptop computer has a wireless LAN card, or you would like to borrow one, this is an easy way to connect.
9. Group Laptop: Group members are free to use my older Apple G3 Powerbook for travel, presentations, and the like. I also have a Sony Vaio pocketbook computer which is generally available.
10. Quantum Chemistry packages: g98 and gamess are installed on the G4 Macintosh. Spartan v5 is on the SGI Origin and available in the Fleming Computer Center in the basement.
11. Mathematica is installed on many of the group computers. Also, gridMathematica is on the Beowulf cluster.

- **Helpful People:**

1. Prof. Tony Haymet
2. LaRuth Davis: Chemistry Department secretary. Handles travel requests and reimbursements.
3. The senior member of the group, in my absence, runs all aspects of research.

- **Time Off:** This is usually up to you, but you must let me know your plans well ahead of time. In general, you are expected to be available for me (and others) to talk to you (i.e. doing ALL your research at home is discouraged). For many active groups in Physical and Theoretical Chemistry, both here and around the world, Saturday is often a regular working day.
- **Supplies:** The Research Stores on the second floor of Old Science (just to the east of Fleming) can be used for most supply needs. The exception is that office supplies (pens, note paper, staples, paper clips, file folders) must be obtained from the Chemistry Office.
- **Photocopying:** For library photocopies, you can get a copy card from the Research Stores. We also have a group copy card. Photocopy everything you need and nothing else. It's a good idea to read and take notes before you photocopy, especially since our libraries are so comfortable. We have access to a FAX machine. The Chemistry FAX number is 713-743-2709
- **Telephone:** The group telephones are provided for all kinds of research calls, and incoming local calls. For other (emergency or unavoidable personal) calls, please keep a record of number, time, and duration in case our accountant requires you to refund the cost of the call.
- **Manuscripts:** All research manuscripts, preprints, conference abstracts, group reports, etc., are prepared using the standard group word processing system, which is currently LaTeX or MSWord. Manuals are available, but modifying an existing document is a good way to start. A final draft of the paper will be kept in a common place which can be accessed by the group. My preference is for LaTeX using the APS Revtex package. The TeTeX documentation guide

is a good resource for using more advanced features of latex, especially the “seminar and foils style for preparing presentations. Moreover, I prefer that you use pdflatex (or TeXShop on the Mac) to generate a final PDF version of your paper. If you do use Word, please use the MSWord equation editor rather than MathType.

- **Latex:** The OSX Macs and the Linux machines all should have the Latex package installed. On the Macs, TexShop is a *very* useful application for writing papers in Latex and comes with a number of templates for papers, letters, etc. Also, you can download a Latex equation editor, which has some “point and click” menus for helping you to write complex equations. Also, I have an on-line documentation for “teTEX”, which is the standard Linux/OSX implementation of Latex. ([k2.chem.uh.edu/Latex](http://k2.chem.uh.edu/Latex))
- **Divisional Seminars /Group Meetings:** These meetings are the heart of science, and are mandatory. Please be on the look out for seminars in other departments, especially Physics, because they do not always advertise well. Inform other group members of potentially interesting talks. At present, you should definitely attend Physical Chemistry Seminar at Noon on Wednesday, and Departmental Seminar on 2:30 on Tuesday.
- **Library:** It is very important to keep up with the current literature. Journals and books of relevance are in the MD Anderson Library. Most of the relevant physics and chemistry journals can be accessed and searched on line. For this you will need to set up your web-browser to use the UH Librarys proxy server (c.f. <http://info.lib.uh.edu/remote/instructions.htm/>). Articles can be saved as either PDF or printed out on the group laser printer. We also have CAS SciFinder Scholar installed on at least one group computer. Please use this as much as possible to keep abreast with whats going on and what has been done in the past.

I also subscribe to a number of pre-print alert services. To sign up, you need to first go to each journal’s web-site and browse a bit. Science, Nature, PRL, JCP, Chem. Phys. and a few others provide this service. Also, from time to time I will send you an email link to an article I think you should know about and read.

- **Shared Resources:** Currently, the Bittner and Haymet groups share common office space in Fleming 221 and share various pieces of equipment, such as the laser printer in 221, some computing resources, and the microwave and coffee maker. In order to engender harmony and good will, it is important to share certain responsibilities in system administration, and housekeeping.
  - Keep the shared areas clean. Pick up your mess.
  - The coffee makers are yours to use. Just keep the area clean.
  - Replenish the paper supply for the printer. We have a rotating schedule for group members directly responsible for this. If it is your turn, do your part. Even if it is not your turn, be a good citizen and replenish the paper. Packages of paper can be obtained from the Chemistry Office.
  - Limit large downloads or printing jobs to off-hours.
  - nice your computing jobs if the system load is high.
  - Be alert for unauthorized access to either our physical space or to our computers. We have had thieves and hackers in the past break into our group.

- **Research:** I am available at anytime to discuss research, except during (a) scheduled seminars, (b) University meetings and (c) my classroom teaching hours. If you have a choice, grab me in the afternoon rather than morning. Use electronic mail to send me news of breakthroughs / disasters, and to arrange a meeting time if you cannot find me. If at anytime you are uncertain about what you should be doing, or which of many lines of investigation you should pursue first, it is very important to talk to me or exchange e-mail as soon as possible. Whatever happens, you should talk to me at least once a week, if only to tell me “I am stuck and I want to be left alone to figure it out”. It is a good idea to ask yourself always: ”Why am I doing what I’m doing?”
- **Computer Security and Responsibilities** The computer resources are the life-blood of our group. It is your responsibility to make sure they are up and running. It is also your responsibility to insure that the workstation or computer that you do most of your work on is secure from outside hackers and is used only for legitimate purposes.
  1. Never give your password to anyone.
  2. Never write it down.
  3. Make sure your password is not a word in the dictionary.
  4. NEVER NEVER NEVER login as root from a remote site. If you need to perform an administrative task from a remote terminal, use ssh to connect to the computer and then use either ”su” or ”sudo” to perform the task. I prefer the ”sudo” route since it forces you to realize that you’re performing an administrative task. When in doubt, ask first.
  5. Use the campus mail server rather than the mail command on your computer. Download ALL your mail from the campus mail server and never download an attachment from any server other than the campus server. This is the #1 way viruses are spread. The UH mail server is pretty aggressive in filtering attachments that look like viruses. So, take advantage of this protection. The Mac and Linux machines are less vulnerable than the MS Windows machines.
  6. UH has a site license for Virex. Download it, install it, and keep it updated. On the OSX Macs, I have a cron command which periodically updates the list of known viruses.
  7. Educate yourself on basic Unix/Linux/OSX system-level tasks. The web is a powerful resource for this. Check out the following websites:
    - (a) Linux-Newbie guide: <http://linux-newbie.sunsite.dk/>
    - (b) OSX Guide: <http://www.osxguide.com/>
    - (c) Mac OSX hints (also good for general Unix): <http://www.macosexhints.com/>

## Bittner Group Phone List

Name	Office Phone	Home Phone	Email address
Prof. Eric Bittner	3-2775	713-839-9421	bittner@uh.edu
Dr. Stoyan Karabunarliev	3-5101	713-630-0654	karabunarliev@uh.edu
Sean Derrickson	3-5101	713-278-9681	sderrick101@uh.edu
John Glenn Ramon	3-5101	832-867-6562	john-glenn.ramon@mail.uh.edu
<i>Other numbers</i>			
Prof. Tony Haymet	3-2781	713-807-8117	haymet@uh.edu
Chemistry office	3-2701		lesposito@uh.edu
FAX Number	713-743-2709		

For on-campus calls, omit the 713-743- prefix.

For local calls, dial 9- then 10-digit number

For long-distance, 9-1-(area code)-number # (access code—ask me).