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Lab Observations

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A Lab Practice Study, conducted as part of a PhD
in Web Science: Computer Science & Chemistry

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1 Inorganic Chemistry Lab

These lab observations were conducted on 08/02/2016 and involved observing 5 chemists who did not taken part in the focus groups (Participants AA, AB, AC, AD & AE). The following colour key is used for the Participants and Observer:

Observer
Participant AA
Participant AB
Participant AC
Participant AD
Participant AE

1.1 Observations

In this research group setup, there were multiple working environments for the students. There was a computer room where the students had their desks, a main lab area, which was set up for conventional bench chemistry, and finally an x-ray room which was a much smaller room on a different floor with specialised equipment.

At the time of observation, there was a mix of students in the lab and at their desks. Some students were sat at their desks, **Participant AA** was making graphs in Excel, with data obtained from scanning materials with x-rays and retrieving the data off the computer. They were using Excel to plot the graphs and manage the data, with help from their paper lab notebook on the desk. **Participant AB** was also using Excel, in this instance to make complex tables of data, taking data from different data files off their computer and combining them into tables. **Participant AC** was using their computer to order stock but also had Word open on another screen. These activities were all related to data modelling to create material for writing up their experiments.

Inside the main lab room, students were wandering in and out, and wearing lab coats, and performing experiments with their lab books out on the desk. This lab also had a very social atmosphere and the students clearly got on well. There were two computers in this lab that were switched off and did not look like they were in use. After enquiring about these computers, **Participant AD** explained that one was linked to a machine for the purposes of reading data off it, and the other was for inventory. This shows a pattern of computers existing in the lab, but only being used for specific purposes, typically to read data off a machine or in this case for organisational purposes.

When **Participant AD** was asked why they wouldn't want to make notes on a laptop rather than using their paper lab notebook, it lead to this conversation:

Observer:	*'Why wouldn't you use a laptop as you're measuring something rather than making notes in your lab notebook?'.*
Participant AD:	*'My laptop is the only one I have, I wouldn't want to ruin it'.*
Observer:	*'What if you had an excess of cheap tech and it wasn't a case of ruining one precious laptop'.*
Participant AD:	*'If it was cheap and durable maybe'.*
Observer:	*'Do you think that would be better than paper or not?'.*
Participant AD:	*'Paper still seems quicker but you don't know until you try'.*

Participant AE extended an invitation to the x-ray room (which is shown in Figure 1); this room had a lot more computers in it that were actually being used. The computer **Participant AE** was using showed real time data on the screen and then provided the data files once the x-ray had finished. The students who use this x-ray machine often write down the values produced into their lab book, and then transfer them into excel. It was mentioned that these machines will only save the data produced as PDF's which means that they then find it difficult to get the data out of it in a readable form.

As a stark contrast **Participant AE** thought that Electronic Lab Notebooks were a fantastic idea: "it puts everything in one place, there are too many different data files of different formats, for one material there could be up to 8 data files for a basic characterisation, and it gets very frustrating and it's very hard to link together". They then continued to explain how they write up all the important information from their lab book onto their computer. They went into more detail about their industry sponsors, how for work involved with them they are not allowed to use Skype or Dropbox as they are considered insecure, but for non-sponsored work cloud based software is used; following up with the fact that they found navigating through somebody else's lab book very difficult and confusing. **Participant AE** also mentioned that their supervisor was in favour of ELNs and had informed them about their existence.

They set their new sample on the computer for an hour. They filled in the wizard, and set the fields and methods to save as a sequence which runs automatically. The results are shown in real time on the computer but they can be processes later. Some people write down the data points by hand, which can lead to human error when they are typing them into the computer. This data can be saved as a PDF and transferred with a memory stick.

The X-Ray machine is standalone. One has a computer where the parameters can be set and a database can be accessed. Its hard to make something new with this as it wont be in the database. The computer is networked and so the data can be obtained from the PCs upstairs. The raw files and text files that come from this machine can be opened in Excel. **Participant AE** uses their paper lab book to note down characters and these will get written into excel.

- X-ray (computer)
- Synthesis (paper)
- Reactions (masses/settings)

Use of the index in the back of the book to link experiments to files.

Observer: *Why wouldnt you use the computers in the lab?*

Participant AE: *Ive not been given a chance, paper is just as good and it doesnt matter if it gets dirty. Nearly everything does on the computer. Theres another instrument computer that controls the gas/chromatography machine, it gets a trace and people write down the numbers in their book or can save the traces as PDF. It will only save as PDF or visual results files.*

The x-ray diffraction data comes out as a .CSV (Experiment Name, Parameter, Value. Another computer controls the Quartzy inventory, there is a printed version in a folder but its harder to search.

1.2 Photos

Figure 1: The XRay Room

2 Crystallography Lab

These lab observations were conducted on 10/02/2016 and involved observing 3 chemists, 2 who did not take part in the focus groups (Participants AF & AG) and 1 of the chemists who took part in one of the chemistry focus groups (Participants W) . The following colour key is used for the Participants and Observer:

Observer
Participant AF
Participant AG
Participant W

2.1 Observations

The crystallography lab is in two parts, a prep room with microscopes (Figure 5) where the crystallographers can prepare their samples and then the main lab with the diffractometer machines Figure 3.

In the prep room there is a computer for looking at the microscope on the machine which can also be used to take pictures of the microscope display. The computer has windows on and when I enquired if it could be used for other things as well as operating the microscope **Participant W** said that they have never seen it used for that. The only other thing that they have seen it used for was for users to email themselves the pictures that they had obtained from the microscope.

Participant W uses a paper sample book in the prep room and lab to note down figures to transfer between systems, although they said that some of their colleagues use a computer or keep numbers in their head instead. They put their infomation into the physical sample book and then writes down the information from the computer.

Observer: *Couldnt you do this on a laptop?*
Participant W: *It would be a bit awkward to have a computer in there (the lab) and a laptop in here (prep room), I use the book for a quick reference.*

Participant W has a sample sheet for the crystal sample, which gets filed away. These records exist on paper in the lab. The information that **Participant W** fills in on the sheet is the date they have looked at it, whether it was successful or unsuccessful or not. Then **Participant W** puts it in the finished tray and an admin member of staff logs the info on a computer.

In the prep room, **Participant W** puts the sample they are investigating today on a glass slide. They look at the sample using the microscope that's attached to the computer. They use a pin to isolate the crystal and then takes the sample to the diffractometer. They bring their sample sheet and sample book into the main room.

Participant W then starts using the computer that is attached to the diffractometer, using Crystal Clear Software. They opened a new project and gave it the NCS Reference (National Crystallography Service). **Participant W** is able to see a visualisation of their sample both on the computer screen and on a screen attached to the diffractometer. **Participant W** then writes down the information in the sample book:

- NCS Code
- Computer Project Name
- Code Generated
- Temperature
- Which Diffractometer
- Info off the Sample Sheet

Observer: *Why do you get given handwritten sheets?*
Participant W: *Some are produced on the computer but most are written by hand as its so hard to draw the structures.*

The Crystal Clear software on the computer has an onscreen ruler that can be used to measure the size of the crystal. **Participant W** puts in the molecular formula from the sample sheet into the software project that was created for this sample.

- Mount / Pip
- Morphology
- Measurements from the on-screen ruler (which went into the sample book first to remember them)
- NCS sample reference number (in the notes section)
- Crystal ID (in the notes section)

The information is then saved and associated with that sample code.

The Crystal Clear software gives figures which give an initial idea of how good the crystal is. It displays real time images of the data.

In the crystallography lab there is a paper diary that everyone has to use, they have to write in what they have run on the diffractometer. Everyone writes down what sample they have run and whether it failed or not.

Participant W explains that other people can remote into this machine and if they move the mouse when someone else clicks then it runs the risk of closing the program and having to start all over again. The software (Crystal Clear) is temperamental and crashes under certain circumstances. E.g running one thing and clicking on something else.

Participant W writes down the data from the computer into their sample book to check against. **Participant W** uses the software to go through the images. During this process the software starts lagging and showing the wrong windows for what has been clicked on. **Participant W** explains that they tend to write descriptive notes in their sample book (e.g this took a long time).

The computer crashed and so **Participant W** went back to the office to find **Participant AF**, the person in charge of the crystallography lab who had remote desktoped into the machine. **Participant AF** clicked through the procedure from their computer. **Participant W** wrote some more notes in their sample book. **Participant W** explained that they tend to make more notes than a lot of the other crystallographers.

Participant W went back to the lab to check on things. They wrote down the following pieces of information on the sample sheet:

- **Participant W**s initials
- Which machine the crystal was run on and what day

The vial of the sample is generally labelled with the same code so that they know that they are putting it back with the correct information **Participant W** said that now the crystal can be left for the next 3 hours. The machine will continue adding images to the groups data share and then they are finished they will be copied over to **Participant W**s machine. **Participant W** will then process the images and put the final copy back on the data share, and put the crystal sample and corresponding information into the done box. The length of the data collection for the crystals varies from between 1 hour and 14 hours, so some samples are specifically run overnight. **Participant W** showed me a computer drawn version of one of the structures on a different crystal to sheet to illustrate that some of the sample sheets are produced on a computer.

Participant W went back to their office. In **Participant W**s office there are another 5 people and they all have computers and desks in a standard office layout.

Participant AF is looking at data and molecular 3D structures on their computer. **Participant AG** is writing emails.

Participant W logs into the UK National Crystallography Service Portal on their computer. **Participant W** types in a sample code for the crystal and selects whether this was a full sample analysis or a data collection (in this case it was data collection). They then sent the sample to their account on portal.

Observer: *Will you add the data to this portal?*
Participant W: *No, Ill zip up all the data files and email them over, and then log into portal again and set that Ive done that.*

Participant W then opens a different software program (CrysAlisPro) which is used for processing the crystal data. **Participant W** explains that it doesnt quite transfer all the information from Crystal Clear and that this is why she writes down quite so many things in the sample book as it then needs to be typed into CrysAlisPro in order to process the data. **Participant W** also explains that hopefully the systems are going to be unified at some point so that this transition will no longer be necessary.

Participant W then opened OLEX2 which is for sorting the data and will give you the molecular structure of the crystal and show you how good the data is. For the data collection process **Participant W** only needs to send the processed data out of CrysAlisPro but they use OLEX2 anyway to check that the data works and there havent been any mistakes. **Participant W** then shows me an example of one that has gone wrong because its been put in the wrong symmetry group and therefore doesnt solve properly. For the full structure analysis **Participant W** would need to go through all of the steps across the different software programs that they just showed me, and write up the information into a report.

Participant W explains that the standard day for them is to:

- Prepare a crystal
- Put it on the diffractor
- Process it
- Repeat

Participant W is also working on assessing some crystals for their viability to be processed. They have another paper notebook for that. This is being done using another software program (Mercury which looks at structures and can display symmetry elements).

Observer:	*What happens to the sample sheets once youve filled them in?*
Participant W:	*We put them into the done box, the admin staff fills in the information and files it, and sends it back to the lab. They keep all the handwritten documents, and check that is has been logged on portal.*

Participant W is also doing some other work where they are trying to produce crystals which are written up into an actual Paper Lab Notebook.

[Scenario Example]

Participant W uses excel to maintain multiple tables of crystal data and grids of substitutions. **Participant W** says that they are unable to actually enter data into this spreadsheet in the lab unless they take their laptop in which they said wasnt ideal because of the lack of space.

Observer:	*Why wouldnt you just use Google Sheets and use the computers in the lab?*
Participant W:	*They are attached to the diffractometer so I wouldnt want to use them.*
Observer:	*If you had another computer that wasnt attached to a diffractor would you be interested in using Google Sheets as you could then use it in the lab and at your desk.*
Participant W:	*Yes that would be useful, especially as this has been passed down from different people who all kept a record of these in different ways.*
Participant AF:	*These projects started and they didnt know that they would go anywhere.*
Observer:	*Why wouldnt you have a separate computer in the lab for working on?*
Participant AF:	*Why wouldnt you just use the computers in the lab?*
Participant W:	*But I wouldnt want to use the diffraction computers.*
Participant AF:	*Using a browser wouldnt be an issue.*
Observer:	*I think that using Google Sheets would be really useful then lots of people can contribute to it and also youd be able to use it on any computer with a web browser.*
Participant W:	*When me and Participant Ws colleague both worked on this sheet we had a nightmare trying to keep a master copy.*
Observer:	*How did you do it? Dropbox or email?*
Participant W:	*No wed just compare laptops side by side and try and keep a paper list of what wed changed.*
Participant AF:	*People dont tend to think about these things at the start, they never expected them to turn into such big projects.*

Participant AG: *Some of my lab students have asked why we only learn about ELNs (specifically labtrove) in 3rd year when we could have started with them at the beginning.*

2.2 Photos

Figure 2: The Prep Room in the Crystallography Labs

Figure 3: Main Crystallography Lab

3 Molecular Chemistry Lab

These lab observations were conducted on 22/02/2016 and involved observing 3 chemists, 1 who did not take part in the focus groups (Participant AH) and 2 of the chemists who took part in one of the chemistry focus groups (Participants S & T). The following colour key is used for the Participants and Observer.

Observer
Participant AH
Participant S
Participant T

This chemistry lab fitted with the image of a conventional lab with students in white coats performing experiments, and bore similarities to the Inorganic chemistry labs. One of the participants in this lab, **Participant AH** told me that they had used LabTrove for some crystallography experiments and quite liked it.

Interestingly after comments in the focus groups about not wanting to take laptops into the lab, this lab seemed to have it's own personal laptop. **Participant AH** had their phone in the lab and was using their lab notebook and the lab computer. They put their samples into the fluorometer which is hooked up to a desktop computer, which measures fluorescence decay of a compound, and this computer is only used to process the results from this machine. When asked why they used a USB to transfer the results to their lab computer rather than using any cloud based software I was informed that the computer didn't actually have internet access. I enquired as to why and the general consensus was that there was a concern that the computer would be more accessible to viruses if it had internet access.

Upon explaining Google Sheets to **Participant AH**, they said they thought it was a good idea. They said that the laptop in the lab has internet but they would still need to move the files over from the computer hooked up to the machine. I asked them what happens after the file transferal, they said that they would then make the graphs to put into their reports which will be written in Word.

I observed **Participant T** (from the focus group) in the NMR room which was another room consisting of large machines and computers linked up to them. I was warned that the computers and indeed any pieces of technology needed to be kept a certain distance from the machines as they contained powerful magnets. They put their compounds on the machine. The computers have paper books by them for logging all of the experiments that have been done. They can open all the files by IP address on the computer but they arent saved onto those machines.

Observer: *What file formats do you get data in?*
Participant T: *iconNMR*

The computers ran iconNMR and ACD labs which were used in conjunction with the lab book for these experiments. **Participant T** has all the codes from their samples, they note them into the logbook and then logs into the group account on the software and enters all the codes for the samples there. All the chemists use different variations of codes. **Participant T** opened their data using ACD Labs, which transfers NMR data from frequency to peaks with needed information.

We went back to the laboratory and **Participant AH** is still waiting for their transport runs to finish. They take 16 minutes, they are watching the progress on the graph on the screen.

Upon exiting the lab, I spoke to **Participant S** (from the focus group also) who was working at their computer because their experiment hadn't worked. They told me that they were working on an abstract for a conference which was being written in word. They kindly took me through their notes and files on their computer and I was amazed at the sheer amount of different files associated with their experiments.

They stored all of their data digitally split into different types. They showed me their Lab book some of the compounds they have made. They showed me a scheme they had set up for a reaction, where they used the Lab book number and page number to link to the appropriate data.

Before going into the lab they will write down the following information:

- Reactants
- Quantities - How much
- Properties - Mass/Density
- Safety data - whether they need gloves / to use the fume cupboard
- Will do COSHH assessment for dangerous chemicals

At the end they will write down:

- The yield after weighing it out
- References of analytical things run on it

The entries were very organised and formulaic. Which definitely seems like the type of layout that could work with a templated design. They also make use of ACD labs and other software packages to visualise their data.

Their NMR data is all stored on the NMR data server that uses FTP. The spectrums are in a group folder, and can be found by date and initials. **Participant S** showed me a spectrum in ACD which contained the raw spectrum data. They use iconNMR for automated process running, and in TopSpin they can manually change settings, which runs on the machine they do experiments on, but find ACD prettier.

These lab observations were very interesting as this was the first (and only) lab situation I encountered where there was an actual space where computers and technology couldn't be, although admittedly this was a small space and didn't stop the presence of computers in that room. These observations emphasised like the previous one that there are so many different files and software packages that there is clearly a need for some form of unification.

4 Organic Chemistry Lab

These lab observations were conducted on 15/03/2016 and involved observing 3 chemists who did not take part in the focus groups (Participants Y, Z & AI). The following colour key is used for the Participants and Observer:

Observer
Participant Y
Participant Z
Participant Z

4.1 Observations

This chemistry lab was similar to that of the inorganic chemists. Students in white coats performing experiments with chemicals and compounds, and making notes in their lab books. There was a friendly atmosphere and a feeling of camaraderie as all the students seem to get on and be happy to help each other and discuss their work. Students come and go frequently, popping in to change something in their experiment, or popping back out to make a note of something at their desk or send an email. There was a very obvious paper feel to the lab, not only due to the presence of multiple paper notebooks. There was a folder with all of the COSHH forms, and a table stuck up on the wall for people to fill in if they wanted to add more chemicals to the database, and all the labels on the glass doors were written in pen that could easily be wiped off and written over. Additionally it was very obvious why certain chemists had stated that they wouldn't want to take their technology into the lab. A lot of the lab coats boasted chemical stains and all of the students were wearing gloves to touch any of the chemicals they used in their experiments.

A friendly student (**Participant Y**) engaged with me and we conversed about the current note taking practice; Participant Y writes on a paper lab notebook to be quick and then writes it up neatly at their desk as they said that they wouldnt want to bring their office laptop into the lab. Theyd always have to take off their gloves to use it whereas they have a specific lab pen.

Observer: *When you write up your notes out of the lab what do you use?*
Participant Y: *My Supervisor gave me access to Enovalys but I dont use it because I want it to be written in my own style not using someone elses template.*
Observer: *Do you use any domain specific software?*
Participant Y: *ChemDraw and ACD Labs*

The lab had several computers scattered around, and I enquired as to their purpose, and their seeming lack of usage. One holds their chemical database, and is mostly used for searching for chemicals, although it was mentioned that it was also linked to 'Flow Chemistry' and one of the students not present in the lab at the time used that to program their reactions frequently. There was another computer that nobody seemed to know what was for, and the only piece of technology that seemed to exist in the lab aside from these was a calculator for aiding in performing calculations in the lab book.

Observer: *Does anyone use the computer to take notes instead of the lab books?*
Participant Y: *No.*

Participant Y also showed me the computer that they used in the instrument room (a room full of computers and equipment). They told me that this computer was used for their gas chromatography machine, and that it had replaced a Windows XP machine that had recently stopped working. I was astonished to see that this machine was running Windows NT. **Participant Y** described that currently the students have to make notes by hand to capture the results and values generated on the machine, because that was currently the only way they could do things. Before the XP machine died they were getting PDFs from the machine and using memory sticks to transfer that data, now they have to use floppy disks! **Participant Y** has a separate lab book for Gas Chromatography.

Participant Y has two lab books currently, one that theyve finished recently and a new one that they have started. **Participant Y** is doing a reaction similar to one they have done in their old lab book so they are using that as a reference.

Observer: *Are these the books with the white pages you can rip out for backup copies?*
Participant Y: *No theyre annoying.*

Participant Y explains that everything they do is written up in word documents so she would be okay if she lost her lab book. They use dropbox to backup their work.

Observer: *So you already do something like an Electronic Notebook, so what put you off using an ELN bar the templates?*
Participant Y: *Once youve done it one way you dont want to change it, and you wouldnt want to change how you do something midway as it would mess up your experiment numbers.*
Observer: *Have you ever used one?*
Participant Y: *I worked in industry for a year and used one there, I didnt mind it but when it crashed you couldnt do anything (this was Contour ELN).*

What was very interesting was that despite not using an ELN, **Participant Y** showed signs of working within this environment. They took paper notes in their lab book, and then wrote them up neatly on the computer at a later date, and therefore clearly wasn't resisting an ELN because of the potential duplication of data that so many people take issue with, and indeed one could argue that in an environment where those types of notes are already performed this would be the perfect environment to introduce an ELN to.

Another student (**Participant Z**) had actually brought their laptop into the lab, but was merely using it for music, whilst still making notes in his lab book by hand during their experiment. This student seemed particularly resistant to the idea of ELNs and said that they much preferred to make notes by hand as and when they were doing things as part of their experiment. **Participant AI** was less against the idea, having used one in an industrial placement, although did comment that whilst they didn't mind it, when it crashed it brought all work to a resounding halt.

4.2 Photos

Figure 4: Inorganic Chemistry Lab

Figure 5: Computers in the Inorganic Chemistry Lab