



DEUTSCHER AKADEMISCHER AUSTAUSCHDIENST
RISE WORLDWIDE



Report about the internship in Microwave Spectroscopy

at the University of Newcastle upon Tyne, England

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Abschlussbericht

Über die Stipendienzeit

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Im Einklang mit Ziffer 10 der „Allgemeinen Bedingungen für deutsche Stipendiatinnen und Stipendiaten des DAAD“ kann dieser Bericht ohne Nennung meines Namens, meiner Anschrift, meiner Telefonnummer und E-Mail-Adresse an künftige Stipendiaten des DAAD zur Information weitergegeben werden.

☒ Ich bin auch mit der Weitergabe meines Namens und meiner E-Mail-Adresse an künftige Stipendiaten des DAAD einverstanden, um eine eventuelle Kontaktaufnahme zu ermöglichen.

26.10.16

Datum

J. Heitkämper

Unterschrift

1 Introduction and acknowledgment

I decided to write this report in English, knowing that I was the first DAAD student in this working group and therefore I want to seize the chance to give my supervisor a collected overview in written form about my stay in Newcastle. Since this is my first scientific report in English I would like to apologise for any mistakes based on grammar or language.

Because I am endless thankful that I got the possibility to have such a great experience, I would like to take the chance to thank the people who enabled this:

I want to thank the DAAD to provide a programme like 'RISE worldwide' to afford important experiences abroad on the one hand from a financial point of view and on the other hand offering a platform to match undergraduate students to projects abroad. I also want to thank for the care about individual problems and the quick and helpful answers per mail.

Of course, I want to thank Nick Walker for taking the time to provide an individual internship for an undergraduate student and always being intent to create my stay as comfortable, diversified and educational as possible. I always felt welcome and like a part of the working group and every concern or request I've had fell always on sympathetic ears.

Also, I owe a lot to Chris Medcraft, supervising me and always taking the time to answer my questions patiently and in detail. The knowledge I've learned from him will be a great help in my future work.

Further I want to thank John Mullaney, always having a great time with him. He made me feel a lot more comfortable with my non-native-speaking English by being motivated to learn German and asking me about the German vocabulary and general German things all the time.

I want also thank the whole working group for the time apart from the working hours, showing me Newcastle and its pubs and having a great and funny time.

I think I was influenced a lot by working in this group and I will take this experience to improve the work I will do in the future.

2 Project

2.1 My project

Nick Walker and his group are working with an unique broadband microwave spectrometer, which measures the rotational spectrum of molecules in plasma. It is a complex device comprised of many different components, but in the end one receives a spectrum with signals at different frequencies, based on absorption to excite a molecule to a rotational state with a higher quantum number. Microwave spectroscopy enables to determine rotational constants out of a recorded spectrum and gives therefore accurate information about bond lengths and angles in a molecule or complex. The main work is based on analysing the recorded spectra rather than spending much time in the laboratory, because the spectrometer runs approximately a day on its own to record one spectrum.

Special computer programmes allow to fit an Hamiltonian to the recorded absorption signals and display quantum numbers and rotational constants. With these and the information about isotopic substituted species one is able to calculate coordinates of the parent molecule and at least bonding distances and angles of them.

For me it was helpful that I've heard the lecture 'Applied Quantum Chemistry' and 'Quantum Mechanics for Chemists' in my previous semester. But the working group introduces detailed into the work they do and therefore this knowledge isn't necessarily expected. However, it was helpful for me personally.

Before I went to Newcastle I contacted Nick Walker and he suggested to join 'Research Gate' before my arrival. There I could access papers the working group previously published and reading them was a good preparation for me so I could imagine what to expect.

During the first week I became acquainted with the most important programme 'Pgopher' to fit the Hamiltonian to a recorded spectrum. After Nick Walker introduced me into the features of the programme, I fit a few spectrums of previously measured compounds with known rotational constants to practise the use of it. During that time I also read a lot of papers to appropriate the knowledge I needed to work in this field. At the beginning it took a while because I needed a long time to read and get english scientific texts but it got better from time

to time.

When I felt a bit more confident in handling the programme, my task was to fit a mysterious species or state similar to Imidazole and its single 1-D-substituted Isotope. Out of the resulting rotational constants I calculated the coordinates of the unknown parent species and tried to figure out what it could be. Unfortunately, we couldn't figure out the solution until now and it's still an open question but this work was a great exercise to learn about programmes which calculate molecular properties like bond length out of isotopic substituted information.

Afterwards we measured the spectrum of Urea and Imidazole to find a dimer of these two. Previous computational calculations told us possible geometries of conformers and we tried to find them and the C-13-isotopic substituted species in the spectrum. At least we've found two different conformers and their Isotopes.

We then recorded the spectrum of 2-Methylimidazole and I fitted the C-13 and N-15 Isotopes, which appeared in natural abundance next to the parent molecule. I used these information to calculate the structural parameters like bond lengths and bond angles of the parent molecule with different programmes. This took me a while because I had to get into the programmes deeply to choose the input adjustments carefully.

After a while I got access to a national cluster and was then able to run computational calculations. After introducing me into the handling of computational calculations I tried to calculate different conformers of molecules that could have been formed out of 2-Methylimidazole in plasma in the spectrometer, for example 2-Methylimidazole and water, 2-Methylimidazole and Argon or a dimer of 2-Methylimidazole. Using the rotational constants from previous DFT-calculations I found a dimer of 2-Methylimidazole and water and 2-Methylimidazole and Argon in the spectrum. Structural calculations gave information about for example where the argon is placed.

In my last week we measured the spectrum of 2-Methylimidazole and Urea to find a dimer of these two molecules. I ran some computational calculations for possible geometries of conformers but at this point I had to leave and therefore I couldn't go on working.

In my third week my supervisor organised the possibility to work in another group for one week to get also an insight in other research areas. This working group dealt with photochemistry and catalysts to oxidate water. During this week I measured cyclic voltammetry scans of five different cobalt-salen-complexes at a specific pH. It was totally different from the work I did in Nick Walkers group because I spent all day long in the laboratory and therefore it was a great possibility to see a different field. Nick Walker was very anxious that I have a great time during my internship and he would have organised another week in another working group if I had wanted to. But I liked the work I did in his working group and this was the reason why I

decided to stay there for the rest of my time in Newcastle.

I was also invited to many seminars and talks from visiting scientists for PHD students and staff and also to the lecture ‘Astrochemistry’ taught by Nick Walker himself and so I had a diversified time and learned a lot about many different areas in chemistry.

2.1.1 Computer programmes

During the intership I got in touch with a lot of different computer programmes which are necessary for analysing the recorded data. I want to list a few to give a deeper insight in what I did and learned:

- Pgopher: Fits the Hamiltonian to a recorded spectrum and gives rotational constants, centrifugal distortion constants and nuclear quadrupole coupling constants
- Kra: Calculates coordinates of an atom out of information about isotopic substitution
- Eval: Calculates internal values out of cartesian atom positions
- strfit: Fits bond lengths and angles to measured rotational constants of substituted species
- Spyder/Python: Runs written scripts for example to Fourier-transform a measured spectrum from the time to the frequency domain or to calculate the rotational constants of an isotope
- molden: Visualises molecules and outputs of computational calculations
- gview: Visualises molecules and outputs of computational calculations; creates input-files for a computational calculation with Gaussian

3 Challenges

The biggest problems for me were based on the challenge to use the English language in a scientific environment. Because I hadn't had English lessons in school since class ten I did two language courses at university, but it was still exhausting for me to use English all day long. Especially in the laboratory, when the other group members were talking to me and I didn't know a specific technical term I needed to understand the content of the statement. It is annoying to ask them to describe something more detailed every time. As I was the only non-native English speaking person in the working group I was sometimes ashamed that my English didn't sound very professional in some situations. And the more I thought about that, the worse my English got.

But I was very pleased with the other group members who never gave me the impression that this was a problem and explained things patiently when they recognized that I didn't understand anything.

They rather tried to learn German sometimes and asked for the German expression of different things and that helped enormously to feel more comfortable and to think less about my lacking English.

The second challenge I had to deal with was to find my project as it was not exactly defined at the beginning. During my first few days it was hard to figure out what my work will be in the next ten weeks, what my project was and what I was supposed to do. Because in Germany I am used to have an exactly defined topic for example for a bachelor thesis, this situation was new for me. I think this is based on the fact, that on the one hand the molecules which are measured and therefore the work that has to be done aren't defined a long time in advance as this is more like a process of figuring out what molecules and complexes can be of interest rather than having a strict plan what molecules have to be measured in the future. On the other hand Nick Walker is keen to create an individual project, based on the interests of the intern. As this turned out to be a perfect possibility to work on exactly what one like, it was hard in the first few days, especially because I've never worked in a scientific project and it was therefore harder to get into it without a special goal or plan. In the end this was a great chance for me to work exactly in the field I wanted, because at every moment I was totally free to

spend more time in the laboratory or to analyse the data.

4 Living in Newcastle and cultural experiences

Because England is a part of the European Union, I didn't have problems with getting a visa etc. I flew from Stuttgart to Manchester and took the bus (megabus) to Newcastle. I lived in a staff and visitor accommodation offered and managed by the university (<http://www.ncl.ac.uk/accommodation/staff-and-visitors>), because all the student residences were closed during the semester breaks or it was not allowed to stay for such a short period.

Nick Walker recommended the above mentioned service. The rent in England is quit expensive in general, but the room in a shared flat was a very clean place to stay with a very friendly staff ,everything included (Wifi, bedding, television, cleaner etc.). It is also located right on the campus. I shared the flat with a few other interns and this was really helpful to talk about the experiences we collected during the time. There were also a lot of PHD students from all over the world and therefore it is a very nice international place to stay.

Even if England and its culture is not too far away from the German one, it was very important for me to get in contact with local people and learn more about the country and its habits.

I wanted to join a football team, but as I stayed there during the semester break it was hard to find one, because a lot of sports is connected to the university in England. At last I found a rugby team and decided to try this new kind of sport. Even if it was really hard to learn its complicated rules I had great training sessions and eventually I had the possibility to play a real match.

Unfortunately, I spent the first few weekends learning maths because I had to redo an exam on 19th September. But I had enough time to discover the region around Newcastle on the weekends. For example, I visited the coast, the historical cities York and Durham, the famous Castle Alnwick and a fishing town called Seahouses. I spent a lot of time with a German PHD student and also with members of my working group and we went to two football matches of the local football team Newcastle United.

5 Conclusions and what I've learned

As we didn't work much with special computer programmes at university I learned a lot about the general handling, the writing and creating of input-files and interpret output-files. During my internship I learned to become acquainted with computer programmes quicker. Then I needed more and more special programmes and I was more and more able to learn to work with them without needing help from someone else. I think this is an important step towards a self-reliant research skill.

This internship is also an unique possibility to work with such an unique spectrometer and therefore I learned a lot about the technical aspect of working with such a complex instrument. I spent sometimes more and sometimes less time in the laboratory but I got to know the spectrometer because from time to time we had to fix different components and that gave me a comprehensive picture of the whole spectrometer. I think an important skill of a scientist is to fix things which don't work how they should and it was interesting to see how this works and what different spontaneous alternatives there are.

I enjoyed the work in this field of chemistry and I was sad to leave at the end. In my opinion spectroscopy is one of the most interesting themes because it includes a lot of quantum mechanics, but is like an applied form of it. I can imagine to work in this field later because I really had a lot of fun doing the work in this project.