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EE/RPPF

For use from May/November 2018

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International Baccalaureate
Baccalauréat International
Bachillerato Internacional

Candidate personal code:

Extended essay - Reflections on planning and progress form

Candidate: This form is to be completed by the candidate during the course and completion of their EE. This document records reflections on your planning and progress, and the nature of your discussions with your supervisor. You must undertake three formal reflection sessions with your supervisor: The first formal reflection session should focus on your initial ideas and how you plan to undertake your research; the interim reflection session is once a significant amount of your research has been completed, and the final session will be in the form of a viva voce once you have completed and handed in your EE. This document acts as a record in supporting the authenticity of your work. The three reflections combined must amount to no more than 500 words.

The completion of this form is a mandatory requirement of the EE. It must be submitted together with the completed EE for assessment under Criterion E. As per the 'Protocols for completing and submitting the Reflections on planning and progress form' section of the EE guide, a mark of 0 will be awarded by the examiner for criterion E if the RPPF is blank or the comments are written in a language other than that of the accompanying essay.

Supervisor: You must have three reflection sessions with each candidate, one early on in the process, an interim meeting and then the final viva voce. Other check-in sessions are permitted but do not need to be recorded on this sheet. After each reflection session candidates must record their reflections and as the supervisor you must indicate the month that the reflection session took place, the candidate's year of DP study at that time and initial this form.

First reflection session

Candidate comments:

I knew I wanted to write my extended essay in Quantum Mechanics due to my interest in physics. I discussed the idea with my chemistry teacher who informed me that it would be quite difficult and I must be sure of it. My teacher introduced me to an individual working in the field of click-chemistry, and he taught me how to use Gauss View 98 application for my simulation research as well as introduced me to the field of Click Chemistry. I had tested out reactions with catalysts on the program and wondered whether quantum mechanical methods could be used to differentiate between a catalyst and non-catalyst reaction. I researched a paper written by Fahmi et al where Methyl Azide and Proyne reaction was being investigated using quantum mechanical methods. I then decided to use those molecules and that paper as my reference to the research and ended up with my research questions.

Month:

DP year (1 or 2):

Supervisor initials:

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**Interim reflection**

Candidate comments:

Researching throughout the months was proven to be difficult due to results which I did not understand and the extra studying required to keep up with the essay. Using Gauss View 98 to do my simulations was very difficult as I had to learn code and advanced level mathematical definitions. 30-40 simulations have been conducted, some of which took over 3 hours. In certain cases the results were infuriating as they did not match the predicted results and would take days if not weeks to realize why. The only thing keeping me on the project was my motivation and excitement towards what I was doing. I am unsure about how to write an essay with a scientific structure, therefore, I asked my supervisor (Chemistry teacher) and she recommended I take a look at other papers within similar fields and try to understand their structure. Explaining the theory behind my essay is the most difficult part as I do not fully understand it, however, the more difficult the essay is becoming to write the more motivated I become to finishing it.

Month: DP year (1 or 2): Supervisor initials: **Final reflection - Viva voce**

Candidate comments:

I have worked on the essay for 9 months and I needed to learn a lot of complicated chemistry and mathematics to understand what exactly I was doing. I am very proud of my achievements along the road of writing this essay, especially for being able to write in a topic far beyond my expertise. Doing this research proved to me that I am very passionate about writing scientific papers and doing research, and would certainly love to do in the future. Though my essay was the most difficult and infuriating thing to deal with, if someone were to ask me if I would do it all over again, my answer would definitely be yes. This essay not only taught me about the significance of scientific papers but also life lessons such as the importance of patience.

Month: DP year (1 or 2): Supervisor initials:

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Supervisor comments:

Supervisor: By submitting this candidate work for assessment, you are taking responsibility for its authenticity. No piece of candidate work should be uploaded/submitted to the e-Coursework system if its authenticity is in doubt or if contradictory comments are added to this form. If your text in the box below raises any doubt on the authenticity of the work, this component will not be assessed.

The student was fully determined that he wanted to do his EE using applied chemistry and there was no way of changing his mind. Since I did my PhD using applied chemistry, I knew that it is possible for a high school student to do such work but that it would mean many more hours than appropriate for an EE. To start with he would need to learn the basis of QM and then how to use the methods, this before even thinking about the research question. I contacted a post-doc if he had time to help my student to understand the theory and how to use the software. I also contacted the professor to make sure that it was ok that my student used their calculation time, also after the learning period. After a month or so of doing research on the method and doing calculations understanding the methodology, the student had a fair understanding what chemical reactions were possible to study using QM (for example that it is not appropriate to use QM on systems with more than 300 atoms). Now the student was no longer supervised by the post-doc.

During the viva voce, we discussed how he came up with the research question and that he wanted to study reactions with and without catalysts. He explained that he could not study any system since this would require too many atoms. Instead he built his study on an already existing study. However, throughout the study, he changed his research question many times in order to get the question more focused. During the viva voce, I also found out that he had the same struggle as all chemists that work using applied QM. Reactions can happen in many different ways, how do you know when you have found the correct pathway? It is even a larger struggle since we had not yet covered organic chemistry and he therefore did not understand the basis of how different reactions occur. But it is amazing how much you learn from studying all the reactions through QM, which was evident when I introduced the organic reactions. The student had a much larger understanding compared to the other students.

Even though it was a large struggle for the student, I noticed how much he loved the research. Every time he saw me in the corridor, he wanted to ask me to tell me something about his research. Every chance he got, he was at the university performing calculations. Also under the viva voce, I understood how much he had understood especially the chemistry. He also admitted that there were many parts in the QM that he did not understand. This was however reassuring - since I know he does not have the mathematical background in order to understand it. These parts he told me that he was very brief about in the report, for example basis sets.

All in all, the student has done an amazing job, and really gotten a much better understanding for how chemical reactions occur that exceeds the IB-curriculum.

