THESIS SUPERVISOR'S REPORT

IDENTIFICATION DATA

Thesis title:	Deep learning for computational chemistry with differentiable background knowledge
Author's name:	Emir Hodžić
Type of thesis :	master
Faculty/Institute:	Faculty of Electrical Engineering (FEE)
Department:	CS
Thesis reviewer:	Gustav Šír
Reviewer's department:	CS

II. EVALUATION OF INDIVIDUAL CRITERIA

Assignment   **extraordinarily challenging**

How demanding was the assigned project?

This was basically a research assignment, requiring to obtain a solid knowledge of state-of-the-art in graph deep learning, computational chemistry, and neural-symbolic integration, all beyond the scope of standard study curriculum.

Fulfilment of assignment   **fulfilled**

How well does the thesis fulfil the assigned task? Have the primary goals been achieved? Which assigned tasks have been incompletely covered, and which parts of the thesis are overextended? Justify your answer.

Completely fulfilled as intended.

Activity and independence when creating final thesis   **A - excellent.**

Assess whether the student had a positive approach, whether the time limits were met, whether the conception was regularly consulted and whether the student was well prepared for the consultations. Assess the student's ability to work independently.

The student had a background in chemistry and approached the remaining parts very proactively. He was able to independently study state-of-the-art models and methods, and develop in a complex neural-symbolic framework.

Technical level   **A - excellent.**

Is the thesis technically sound? How well did the student employ expertise in his/her field of study? Does the student explain clearly what he/she has done?

I see the technical approach as highly innovative and overall excellent. The final results are not particularly good, which I account to a lack of time left for the final experimentation stage (my fault), but the overall approach is exactly as it should have been.

Formal level and language level, scope of thesis   **A - excellent.**

Are formalisms and notations used properly? Is the thesis organized in a logical way? Is the thesis sufficiently extensive? Is the thesis well-presented? Is the language clear and understandable? Is the English satisfactory?

The thesis is thoughtfully structured and nicely written, with a lot of instructive examples, which are important given the complex nature of the studied models. I commend highly especially the custom diagrams and figures.

Selection of sources, citation correctness   **A - excellent.**

Does the thesis make adequate reference to earlier work on the topic? Was the selection of sources adequate? Is the student's original work clearly distinguished from earlier work in the field? Do the bibliographic citations meet the standards?

Appropriate (just bibliography should not be an appendix I believe).

Additional commentary and evaluation (optional)

Comment on the overall quality of the thesis, its novelty and its impact on the field, its strengths and weaknesses, the utility of the solution that is presented, the theoretical/formal level, the student's skillfulness, etc.

See the final evaluation.

III. OVERALL EVALUATION, QUESTIONS FOR THE PRESENTATION AND DEFENSE OF THE THESIS, SUGGESTED GRADE

Summarize your opinion on the thesis and explain your final grading.

As a supervisor who designed and went through the project with the student in close detail, I don't have any further comments or questions.

Overall, this is a nice thesis targeting a timely and advanced topic the results of which, after a bit of extra experimentation/tuning to target the overfitting problem, we plan to publish.

The grade that I award for the thesis is **A - excellent.**

Date: **31.5.2023**   Signature: