



## THESIS EVALUATION OPPONENT EVALUATION

Author name: Petr Myslík

Thesis title: Komplexace anilidu atomy bromu

Opponent: inž Stanislav Waclawek, Ph.D.

Opponent workplace: Technical University of Liberec

- A. Abstract quality, keywords matching ..... Excellent (1)
- B. Research scope and processing ..... Excellent (1)
- C. Level of theoretical part ..... Excellent (1)
- D. Appropriateness of the methods ..... Excellent minus (1-)
- E. Results elaboration and discussion ..... Good (3)
- F. Students own contribution ..... Very good (2)
- G. The conclusion statement ..... Very good (2)
- H. Fulfillment of Thesis tasks (goals) ..... Fulfilled
- I. Structure, correctness and fulness of references ..... Excellent minus (1-)
- J. Typographical and language level ..... Very good minus (2-)
- K. Formal quality ..... Excellent minus (1-)  
(text structure, chapters order, clarity of illustrations)

Comments, remarks:

Major comment:

"1 eV = 23,06 kJ/mol": here, I think you mean kcal/mol; thus, the conversion factor is wrong.  
Therefore, the whole section 3.4 (and other sections where these values are compared to your work)  
could be wrong.

Minor comments:

Section 3.1: "pricemž se pri se pri novém" - repeated words.

Section 3.4: "mnohem vyšší.[8]" - citation in a wrong place.

Section 4.4: "další další funkcionál" - repeated words.

„Tabulka 7.1” you should provide units as well.

+

... continue on page 2





Overall assessment:

Petr Myslík in his thesis, has examined the complexation of bromide by various N (3,5-bis-trifluoromethylphenyl)-dichloroacetamide conformers. In order to reach the thesis goals, he has performed computations primarily based on the density functional theory (DFT). The thesis is written primarily correct except for one major and several minor mistakes, which I have marked in the comments section.

However, in the reviewer's opinion, it meets the standards of the bachelor thesis. The research is promising and, as such, could be continued. The stated objectives mainly were accomplished, and overall I consider the thesis to be of good quality.

Questions for the defense:

1. Please explain how did you apply the conversion factor for kJ/mol  $\rightarrow$  eV (for values taken from Müllerová et al. and your study)?
2. Your computed results are in a good correlation with the experimental results that could be found in the literature. Thus, do we still need experimental methods that are laborious and cost so much money?
3. Please explain Intrinsic Reaction Coordinate (IRC) method. Could it be beneficial for your study?

**Overall classification and recommendation:**

Work meets the Bachelor degree requirements and therefore I recommend it for the defense  
I suggest to classify this work by grade: Excellent minus (1-)

By signing I certify that I am not in any personal relationship with the author of the thesis

In Liberec

date 20.01.2022

