

Review report on PhD thesis of
Ing. Barbora Hanulíková
Electronic properties of polysilylenes studied *in silico* on oligomers
in various conformations

This thesis deals with theoretical studies of polysilylenes with focus on the influence of molecular structure and conformational defects on electronic properties of these materials. Theoretical modelling of fundamental electronic properties of advanced materials belongs to promising and perspective areas of materials research. It is therefore a current topic that is of interest not only in terms of basic research, but which also has prospective application potential.

The work presented consists of reprints of three papers published in refereed journals and two other articles already submitted, prefaced by an introduction to the problems treated, methodology used, and achieved results. This section is primarily focused on recapitulation of results described in more detail in the enclosed papers. In this doctoral dissertation, Barbora Hanulíková used a density functional theory in order to study the geometry and electronic properties of several oligosilylene structures. The main contribution and the novelty of the research is based on description of the influence of conformational disorder on electronic properties of oligosilylenes. This thesis is clearly written and well documented. There are only minimum of typing errors and the text is well written in clear and concise manner. The figures and schemes are shown properly as well, however sometimes the small font used makes the figures unclear.

Overall, the thesis is well written; nevertheless some parts are quite short. Notably, the detailed description of the current state of the art in the research area, which can provide the broader contemporary context of the results presented in the thesis, is missing. Also, in the sections dedicated to the description of the results achieved (chapters 6, 7 and 8) there is no description of the author's contribution to the results. As follows from the list of publications (page 41) the authors share in published papers ranges from 40 to 60 percent. However there is no clear differentiation of the author's contribution with respect to the work done by other co-authors of the presented papers.

Question for the defence:

- 1.) Please clarify your contribution to the results presented in the thesis and enclosed papers
- 2.) Could the author compare their work with the results achieved by other teams in the field of study and characterization of oligosilylenes and polysilylenes?
- 3.) Can be your results achieved by theoretical modelling compared or verified with the experimental results?

Conclusion

In summary, it is clear that the student has done a large amount of high quality work. The presented results represent a coherent and conceptually well-constructed research. The conclusions as well as presented results confirm that the formed objective of the work was successfully finished. The author of the dissertation thesis has demonstrated the ability to work independently and creatively in the specific field. The thesis meets the standard requirements imposed on the dissertation thesis in the field. Therefore I clearly recommend its acceptance.

Brno, 13 th June 2016

prof. Martin Weiter, Ph.D.
Faculty of chemistry
Brno University of Technology