

ÚSTAV ORGANICKÉ CHEMIE A BIOCHEMIE AKADEMIE VÉD ČESKÉ REPUBLIKY INSTITUTE OF ORGANIC CHEMISTRY AND BIOCHEMISTRY ACADEMY OF SCIENCES OF THE CZECH REPUBLIC

Prague, August 31, 2015

Letter from the PhD. advisor

It is a pleasure for me to recommend the PhD. thesis of Alena Habartová for defense. Alena has been a PhD. student in my group since 2011. Until early this year, she worked under the auspices of Dr. Martina Roeselová, however, after her untimely death I took over as Alena's direct advisor this February. Primarily due to family reasons, Alena started her PhD. after a many year break after finishing her Ms. studies. Nevertheless, she managed to "get back" to science beautifully and did a very good piece of work resulting in a nice thesis.

In her PhD. work Alena focused on molecular dynamics simulations of thin organic layers, investigating their interactions with atmospheric pollutants. The results are very interesting *per se* in terms of exploratory research of structural and dynamical aspects of molecules adsorbed at organic layers. When in accord with experimental findings, as is the case here, such simulations also provide invaluable and detailed interpretation of spectroscopic experiments. At the same time, the obtained results are of a great practical importance for atmospheric modelling providing quantitative data about adsorption and penetration of important pollutants into atmospheric aerosols. Alena presented her results in the form of contributed lectures and posters on several international conferences and also managed to publish the main findings in three papers in prestigious international journals (in two of which she is the first author), with several other manuscripts submitted or in preparation.

In summary, Alena has been a very good PhD. student who diligently carried out high quality original research. She also wrapped it out in a form that clearly demonstrates that she deserves to obtain the title PhD.

With kindest regards

Prof. Pavel Jungwirth

Flemingovo nám. 2 166 10 Prague 6 Czech Republic Tel.: +420-2-20410314 Fax: +420-2-20410320 e-mail: pavel.jungwirth@uochb.cas.cz