Statement of supervisor to the Ph.D. thesis submitted by Mgr. Mária Šoltésová

Prague, August 25, 2013

Mgr. Mária Šoltésová completed the doctoral program under the joint responsibility of the Charles University in Prague (Department of Low Temperature Physics) and the Stockholm University (Department of Materials and Environmental Chemistry) under supervision of Prof. Jozef Kowalewski (Stockholm University) and myself. She has submitted the thesis entitled *Fast Dynamic Processes in Solution Studied by NMR Spectroscopy*.

The thesis describes original results of scientific investigations of several molecular systems with their structures and dynamics significantly influenced by weak intermolecular interactions. The thesis comprises of five scientific papers and a general introduction to the studied systems and experimental methodology and an overview of major results. The candidate clearly and fairly specified her personal contributions to each of the papers. The style and the formal quality of the thesis are at very high level, which conforms to the excellent presentation skills of the candidate.

The molecular systems studied can be divided into three groups: inclusion complexes of cryptophane-Č with chloromethanes, oligo- and polysaccharides and the molecular clusters of ethanol. The selection of these systems arose mainly from the general fields of interest of the two collaborating groups. The major exploited experimental technique was the nuclear magnetic resonance spectroscopy in the liquid state, namely the methods sensitive to molecular mobility and flexibility such as the measurements of several modes of the nuclear spin relaxation, the chemical exchange and the translational diffusion. Interpretation of the experimental data involved application of several theoretical motional models and hydrodynamic calculations.
Ms. Šoltésová undoubtedly demonstrated her full abilities for independent scientific work. She designed, performed experiments and carried out data processing and interpretation at a high level of expertise. I admit her persistence when seeking for a consistent application of motional and hydrodynamic models.

As the most important results of this work I wish to point out achievement of a deep understanding of the structure/dynamics relationship in the case of cryptophane-C inclusion complexes, the interpretation of the trisaccharide dynamics with the new DCM model that is fully compatible with the experiments, and development of a novel method of determination of the average size of the hydrogen bonded clusters present in liquid alcohol.

Ms. Šoltésová demonstrated a very high working flexibility when alternating between Prague and Stockholm at the semester intervals. Despite of the time-costs of such arrangement, she was able to complete the thesis within the regular period of 4 years. She was efficiently operating several different NMR spectrometers in Prague, Stockholm as well as in the international center in Florence. This is a certificate of her organization and experimental skills.

During her doctoral studies she became a key member of the group at Charles University. She also participated in supervising of undergraduate students. Ms. Šoltésová was a principal investigator of the project funded by the Grant agency of the Charles University and she is a team member of several other grant projects.

It follows from the above statements that the candidate has clearly demonstrated her full capabilities of independent scientific work. The obtained results were presented as posters or short lectures at roughly 10 scientific conferences and as 4 papers in high quality international scientific journal (two additional journal contributions exist as manuscripts). I recommend, therefore, awarding Mgr. Mária Šoltésová with the Ph.D. degree upon successful defense of the dissertation thesis.

Jan Lang
Stockholm, August 27, 2013

Statement of supervisor to the PhD thesis submitted by Mgr. Maria Soltesova

Mgr. Maria Soltesova completed the doctoral program under the joint responsibility of Charles University in Prague (Department of Low Temperature Physics) and Stockholm University (Department of Materials and Environmental Chemistry). I was the supervisor of her thesis work in Stockholm, while Doc. RNDr. Jan Lang was supervising her work in Prague. She is putting forward a PhD thesis entitled *Fast Dynamic Processes in Solution Studied by NMR Spectroscopy*. As stipulated by the agreement between the two universities, the thesis defense will take place in Stockholm and is scheduled for September 25, 2013.

The thesis consists of an introduction to the methods and systems under consideration, followed by five scientific papers, four of which are already published in international journals, and the fifth one is a manuscript. The personal contributions from Ms. Soltesova to all papers are clearly specified in the thesis. The introductory part, written by the candidate alone, is very well organized and formulated.

The papers deal with three types of systems. The first two studies are concerned with host-guest complexes between the cage-like molecule, cryptophane-C, and chloromethanes. Papers 3 and 4 describe work on oligo- and polysaccharides. Paper 5 presents a study of ethanol clusters. The investigated dynamic phenomena include chemical exchange (papers 1 and 2), rapid molecular rotational motions, studied through spin relaxation measurements (papers 2,3,4), and translational diffusion (paper 5). The cryptophane articles and the ethanol work contain also structural considerations and have weak intermolecular interactions as a common theme. Papers 3 and 4 are oriented towards modeling of internal motions in oligo- and polysaccharides. All works contain experimental parts, in the form of sophisticated NMR measurements, and theoretical considerations. The latter can be quantum chemical (DFT) calculations, hydrodynamic calculations, stochastic model development or testing of the models.

Ms Soltesova demonstrated in her thesis that she acquired the skills necessary to perform independent scientific research, including both theory and experiments. She has spent about half of her time at each of the two universities and was able to handle the difficulties connected to her moving between the two countries. Even more important, she proved also capable to take advantage of the changes in her environment. Besides Stockholm and Prague, she also visited two laboratories in Italy (Florence, Padova), in connection with the work described in papers 3 and 4. Moreover, she participated in about ten conferences, presenting her work as posters or lectures. Her scientific talks demonstrate clearly that she is a very skilled communicator. In summary, I warmly recommend awarding Mgr. Maria Soltesova the PhD degree upon successful dissertation defense.

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