



FACULTY
OF MATHEMATICS
AND PHYSICS
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Review of supervisors of the Ph.D. thesis submitted by Mgr. Mikuláš Peksa

The Ph.D. programme of Mgr. Mikuláš Peksa was initially designed as bi-nationally supervised doctoral thesis between the University of Leipzig (supervisor PD Dr. Frank Stallmach) and Charles University (supervisor doc. RNDr. Jan Lang, Ph.D.) and Mr. Peksa was enrolled as Ph.D. student at the both universities. Within four years of the joint programme, the candidate completed all experimental and most of theoretical work. However, he failed to submit the thesis within the period presumed by the international agreement. In 2019, when the thesis were ready for submission, it turned out that circumstances had changed and officers at University of Leipzig did not support revival and update of the bi-national agreement, and they suggested to carry out the thesis defence solely at the Charles University. Nevertheless, in order to acknowledge the actual bi-nationality of the project this review is signed by the both supervisors.

The thesis entitled “Ordering, transport and rotational dynamics of adsorbed carbon dioxide in metal-organic framework $Zn_2(BDC)_2(DABCO)$ ” deals with in-depth investigation of CO_2 binding and mobility in a microporous crystalline framework consisting of 1D channels. Mr. Peksa accepted his key role in the project with full responsibility. He covered a broad range of activities, starting from the experimental ones such as preparation of NMR samples (including sometimes activation, gas filling and final flame-sealing), advanced NMR measurements of diffusion and relaxation, solid state static as well as magic-angle-spinning experiments and spectra processing. Next, Mr. Peksa carried out molecular dynamics simulation trajectory processing in order to derive NMR-related quantities such as diffusivity and relaxation times. For this purpose he extended the theory of nuclear magnetic relaxation such that it is applicable for mobile (adsorbed) CO_2 molecules in an anisotropic environment. He also developed a theory that explains the linear dependence of the width of ^{13}C static lineshape of adsorbed CO_2 on temperature. For this purpose, he introduced the model of harmonic oscillations of CO_2 in the binding sites of the MOF. Furthermore, these oscillations were found later in MD simulation trajectories when deriving the correlation function for spin-rotation interaction. Thus, the candidate displayed excellent abstract and mathematical

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skills when devising models for experimentally observed dependencies. He was struggling very successfully with hand-on chemistry and physics, which were clearly more difficult for him than theoretical derivations and computations.

The submitted thesis represents a well-balanced and targeted scientific report. We would like to point out that the NMR theory part is presented in a very condensed but a thoughtful manner. It provides a complete basis for the candidate's own work description. The most valuable results in our opinion are a very detailed description of adsorbed CO₂ dynamics including translational self-diffusion, a high level of consistence between experimental and computed results and an unusual derivation of the correlation functions for three relaxation mechanisms in Cartesian coordinates. Especially his derivation of the correlation functions suits much better to uniaxial symmetry of the investigated MOF system rather than the ordinarily utilized spherical coordinate system. It should be noted that the analysis of the relaxation data is yet unpublished because we have been seeking for a better experimental demonstration of the forecasted extremely long ¹³C relaxation rates of adsorbed CO₂.

To conclude, Mgr. Mikuláš Peksa completed a single broad but closed scientific project. He was its central personality and he himself performed a very broad range of the key activities in very active and skilful way. As result of his work in the respective research projects at our institutions, he contributed as co-author or even as first author to seven papers published in scientific journals with peer review system. It is just a pity that Mr. Peksa decided to leave a scientific carrier which also delayed the submission of his thesis. We gladly recommend awarding Mgr. Mikuláš Peksa with the Ph.D. degree upon successful defense of the submitted dissertation thesis.

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