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To whom it may concern

RESPONSE

to the dissertation submitted for the degree of candidate of physical and mathematical sciences of Elena Tupikina

"NMR and IR diagnostic of geometry, energy and electronic structure of hydrogen bonded complexes"

The work of Elena Tupikina is devoted to a quite general topic of application spectroscopy methods (NMR and IR) in hydrogen bonded (H-boned) systems. "Hydrogen bonds are quite special bonds: they are strong enough to significantly modify properties of molecules, yet weak enough to be distorted or broken fairly easily by an external stimulus, an incoming reactant or by-passing molecule" - this felicitous sentence was brought out by Hermansson 2017 during XXII International Conference on Horizons in Hydrogen Bond Research. Indeed, due to the abundance and high importance in the molecular world covering biochemistry, biological systems and life processes, the need of better understanding of fine details of H-bonding stimulate research and unabated discussions. Among the most important issues are the creation of effective methods of diagnostic of geometry, energy and electronic structure of H-bonded systems, i.e. those considered in the dissertation of Elena Tupikina.

One of the central problem in H-bond research is the proton location and proton motion pathways. The finding of correlations with the bond strength and with the external factors as well as the reliable spectral benchmarks to monitor them have a fundamental importance. Therefore the tracking of the changes in NMR chemical shifts and spin-spin coupling constants along the proton transfer pathways for complexes with CH···X (X = O, N, F) bonds successfully realized in the present work by Elena has to be noted especially. Furthermore, she has developed the new quantum mechanical approach of outer electronic shells investigations, using ^{3}He atom as a probe, and tested on the fluorine-containing systems, including neutral molecules, cations and anions. Another result, which can be useful from the practical point of view, are easy-to-use correlations linking spectroscopic measurable H-bond parameters with geometry and energy for FH···F, NH···N and CH···X (X = O, N, F) bonds.

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Elena Tupikina has published 7 scientific papers, 4 of them in high ranking international journals as *J. Phys. Chem. A* and *C*. The dissertation is based on 4 original publications, and one paper was recently accepted to *J. Chem. Phys.* (2019). We had several opportunities to get to know the main results of the present research during XX, XXI and XXII International Conferences on Horizons in Hydrogen Bond Research (in Belgium, Antwerp, 2013, Poland, Wroclaw, 2015 and Finland, Jyväskylä, 2017).

Taking into account all formal aspects of dissertation as well as original results of experiments and advanced theoretical developments we can state that the present work of Elena Tupikina meets the main requirements to PhD thesis in Lithuania and in many other European countries. We also think that some treatments developed by Elena Tupikina will find applications in related studies in the Faculty of Physics of Vilnius University and in the future maybe even in joint projects between Vilnius and Saint Petersburg Universities.

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