



Thesis review: NMR and IR diagnostic of geometry, energy and electronic structure of hydrogen bonded complexes

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The thesis addresses the problem of evaluation of characteristics of hydrogen bonded complexes from spectral data. It consists of an introductory section and three chapters. The first chapter is dedicated to an overview of the scientific landscape of modern hydrogen bonds investigations. The second chapter presents a new method of fluorine atom lone pairs localization – using of ^3He atom as a numerical probe. The third discusses simple correlation equations linking hydrogen bonds characteristics (energy, geometry) with its spectroscopic observables, consists of both theoretical and experimental data.

Overall, the thesis is well written and has systematic structure. The results are presented clearly and are discussed in detail. The methods used for this research are well justified. This thesis is a self-sufficient scientific work, obtaining results can prove to be important for the development of methods of spectral diagnostics of hydrogen bonded complexes.

As a suggestion for the future studies, it would be interesting to investigate in detail the physical background of an unusual growth of spin-spin coupling constant $^1J_{\text{CH}}$ upon slight elongation of r_{CH} interatomic distance. It could be quite challenging, but very helpful in the further interpretation of experimental spectral data.

It is apparent from this work, publications and conferences list that Elena Tupikina is a valuable member of the scientific community and has contributed original and thoughtful research. In summary, I can conclude that this thesis represents a high-quality research from a scientific point of view and that Elena Tupikina meets all the criteria required for obtaining PhD degree.

A. Filarowski

Prof. Dr. Sc. Aleksander Filarowski

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