1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: The Fine and Hyperfine Structure in Molecules – Calculations in the Explicitly Correlated Gaussian Functions

1.1. **Project goals** Determination of relativistic corrections causing splitting of molecular states, leading to the fine and hyperfine structure of the molecule, using very precise ab initio calculations. Testing the level of accuracy of the determined splitting. Comparison of calculation results with experimental data.

1.2. **Outline** Calculations in the bases of explicitly correlated Gaussian functions allow obtaining accurate values of the non-relativistic energy of the atomic system, taking full account of the effects of electronic correlation. Currently, this is achievable for several-electron systems. These calculations can be performed by treating atomic nuclei as quantum particles, i.e. going beyond the Born-Oppenheimer approximation. The very accurate functions describing molecular states obtained in this way allow the determination of precise energy corrections representing relativistic or QED effects. A special class of relativistic corrections is created by operators dependent on the electron spin and/or nuclear spin, which generally lead to the splitting of molecular states. Magnetic interactions between spin-orbit and spin-spin electrons cause the so-called fine structure, while magnetic interactions between the nucleus and electrons lead to the hyperfine structure.

1.3. **Work plan** Derivation of matrix elements for operators representing relativistic

corrections to first-order energy in molecules leading to fine and hyperfine structure. Implementation of these expressions as a module into an existing Fortran program. Performing test calculations. Performing calculations for selected several-electron molecules. Writing a doctoral thesis.

1.4. Literature *(max. 10 listed, as a suggestion for a PhD candidate*

- *Angular Momentum Theory for Diatomic Molecules, BRIAN R. JUDD (1975)*
- *Operator Techniques in Atomic Spectroscopy, BRIAN R. JUDD (1998)*
- *Optical Spectroscopy of Lanthanides, Magnetic and Hyperfine Interactions, Brian G. Wybourne, Lidia Smentek (2007)*

1.5. Required initial knowledge and skills of the PhD candidate Knowledge of quantum mechanics and programming. Knowledge of Racah algebra preferred.

1.6. Expected development of the PhD candidate's knowledge and skills acquiring extended knowledge in the field of quantum mechanics and relativistic quantum mechanics. Efficient use of tensor operator algebra. Development of programming methods, mainly in Fortran