DESCRIPTION FOR THE GENERAL PUBLIC

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Nowadays, nuclear magnetic resonance spectroscopy (NMR) is one of the basic tools that are used to study electronic structure and molecular geometry in chemistry and biochemistry. Moreover, it is applied in medicine in one of the imagining techniques, so called magnetic resonance imagining (MRI). Spectra obtained in NMR experiments are most commonly analysed on the basis of two parameters: shielding constants and nuclear spin-spin coupling constants. At present, quantum chemical calculations of these parameters are becoming widely used to analyse NMR spectra. Unfortunately, not all of the factors that can influence the results have been studied by now.

The project is aimed at implementing a method of precise calculations of spin-spin coupling constants involving highly changed nuclei, for which both relativistic effects (resulting from high speed of electrons) and so-called vibrational effects (resulting from molecular vibrations) are important. So far relativistic and vibrational effects have been calculated separately. Our preliminary investigations indicate that non-relativistic calculations of vibrational corrections for some spin-spin coupling constants of heavy nuclei may lead even to incorrect signs, i. e. lead to worsening, instead of bettering, the quality of the computational results. We are going to implement a method of calculations of vibrational corrections based on relativistic Dirac-Coulomb Hamiltonian and add it to the freely distributed program package Dirac. The method will be tested on several simple examples of molecules containing highly charged nuclei. The subject is important on account of the nuclear spin-spin coupling constants being used as structural parameters. The implemented method will also allow to calculate vibrational frequencies of small molecules using relativistic Hamiltonians. Such calculations have not been performed so far.