Abstract Submitted
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Very accurate variational non-relativistic non-Born-Oppenheimer atomic & molecular spectra predictions employing explicitly correlated Gaussian basis functions[1] KEEPER SHARKEY, University of Ariozna — Due to the fast increasing capabilities of modern computers it now becomes feasible to calculate spectra of small atom and molecules with accuracy which matches the accuracy of high-resolution measurements. The algorithms for the calculations are directly derived from the first principles of quantum mechanics. The Hamiltonian operator used in the approach is called the internal Hamiltonian and is obtained by rigorously separating out the center-of-mass motion from the laboratory-frame Hamiltonian. Algorithms for determining the isotopic energy shifts of L=0 and M=0 states of atoms were implemented and tested in the calculations of the ground ^{4}S state of the nitrogen atom. Bound states of diatomic molecules corresponding to the total angular momentum quantum number equal to one (N=1) was derived and implemented and was tested in the calculations of the N=1, v=0, . . . , 22 states of the HD^+ ion and in the calculations of the ortho-para spin isomerization of the hydrogen molecule in its all bound vibrational states. This has lead to the development of a new studying of muonic molecules (dpμ, tpμ and tdμ). The algorithms for calculating rovibrational states of small molecules is currently being extended to H_3^+ using *sin* and *cos* ECGs.

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