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DFT Parametrized Spin Hamiltonians for Simple Paramagnetic Molecules

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This work will first present our results from the computational studies of the spin properties of selected paramagnetic molecular species, and then briefly study the combination of these results with analytical methods to compute the exact solutions of the studied systems. The molecular species we will work with are nitrogen monoxide and diboron, both of which are paramagnetic. First, Density Functional Theory (DFT) is used to evaluate parameters such as the **g**-tensor values, including the diamagnetic correction, orbital Zeeman and spin-orbit coupling contributions. For this purpose, the Gaussian 09 software is used. Subsequently, a model Hamiltonian, specifically a spin Hamiltonian, which consists of the dominant magnetic interactions within the systems, is constructed. This Hamiltonian relies on the previously obtained parameters. The parametrized calculations of the diagonalized Spin Hamiltonian are performed using Wolfram Mathematica 11.

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