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Theoretical research of the force field of chlorotrinitromethane in the coordinates X_δ^0

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Abstract

At present, nitro compounds are widely used in industry and medicine. This necessitates a more thorough study of their specific properties and the construction of theoretical models for their prediction. A special role in this process is given to IR and Raman spectroscopy. However, model calculations are needed to interpret vibrational spectra. This work is devoted to quantum-chemical studies of the force field of the $ClC(NO_2)_3$ molecule and the solution of the direct spectral problem for the selected object.

The Becke-Lee-Yang-Parr B3LYP method with a hybrid potential of 6-311++G(3df, 3pd), as the most promising, was used as the main approach for the study. In addition, in this paper, as an alternative to chemical (natural) coordinates, new coordinates X_δ^0 were chosen, it lets talk about the correctness of the calculations. The calculations presented in this article were implemented using Gaussian and GaussView computer programs designed to calculate a number of molecular properties and characteristics of chemical reactions.

Using the chosen method, in this work, the geometry of the trinitrochloromethane molecule was optimized, the geometric parameters of the compound under study were examined, in particular, were calculated the values of valence angles, dihedral angles, and bond lengths characteristic of the equilibrium configuration of the compound under study. For the first time, generalized force coefficients were obtained for the $ClC(NO_2)_3$ molecule in the X_δ^0 coordinates, which were proposed by L.S. Mayants and G.B. Shaltuper, as universal coordinates in which it is possible to correctly solve the spectral problem. An assessment of the "rigidity" of the chemical bonds of the test compound was carried out. The wave numbers (frequencies of normal vibrations) for the studied molecule in the harmonic approximation are calculated and analyzed. A comparison of the obtained wave numbers with experimental data is given. The results obtained demonstrate a satisfactory agreement between theory and experiment. A general view of the vibrational spectrum of trinitrochloromethane obtained by calculation is presented.

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