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Computation of vibrational spectra of 5-methoxy-4-nitrobenzofuroxan in coordinates X_δ^0

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Abstract

The presented work is continuation of a cycle of quantum-chemical calculations of the author devoted to memory of the known scientist in the field of chemistry furoxans and furozans Lenor Ivanovich Khmelnitskiy (1927-1995). 1,2,5-oksadiazol-2-oxide compounds possess unique properties which are caused by their internal structure. Research of a structure of such compounds and their physical and chemical characteristics is an actual problem. In work the molecule 5-methoxy-4-nitrobenzofuroxan is considered. The substance formed by these molecules, is interesting to that it easily is exposed to a rearrangement Boulton-Katritzky. It is known that without 5-substituent the rearrangement is not observed, and with 5-methoxy group the rearrangement proceeds easily already at 33 ^oC. The author makes the assumption that such behaviour of substance is connected with features of an vibrational motion of atoms in a molecule and, accordingly, with features of a force field of compound. Therefore, work is devoted calculation of frequencies and forms of normal vibrations of atoms in a molecule 5-methoxy-4-nitrobenzofuroxan. As a method of research within the DFT approach B3LYP 6-311++G(3df, 3pd) is chosen. The connection Force field is calculated in co-ordinates X_δ^0 as the most universal, allowing correctly to solve a spectral problem.

Within the limits of method B3LYP 6-311++G(3df,3pd) the force field of 5-methoxy-4-nitrobenzofuroxan in coordinates X_δ^0 for the first time is received. The generalized force constants are found, frequencies of normal vibrations were calculated and their assignment to certain kinds of vibrations is spent.

It is received that the greatest value of the generalised force constants among bonds N-O in a molecule 5-methoxy-4-nitrobenzofuroxan belongs to bond N-O furoxan rings from nitrogroup and is equal 23.8681 mdyn/Å. The maximum value of the generalised force constants belongs to bond C=N furoxan rings from nitrogroup and matters 25.9473 mdyn/Å. The generalised force constants of bonds C-N and N-O nitrogroup in a molecule 5-methoxy-4-nitrobenzofuroxan are equal, accordingly, 6.3597 and 12.7159 (average) mdyn/Å, received with use of approach B3LYP/6-311++G (3df, 3pd) in co-ordinates X_δ^0. The Most intensive mode in a settlement spectrum of a molecule 5-methoxy-4-nitrofuroxan has frequency of 1661 cm^{-1}.