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Computation of vibrational spectra of furozan and nitrofurozan molecules in coordinates X_δ^0

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Abstract

For the furozan and nitrofurozan molecules, the force coefficients in the X_δ^0 coordinates within the density functional (DFT) method in the valence-split basis with the correlation functional of Lee, Yang and Parr, represented by the famous acronym B3LYP 6-311++G(3df, 3pd), are determined for the first time. The data obtained allowed to estimate the values of generalized force coefficients of bonds, to calculate the wave numbers (or the frequencies of normal vibrations of atoms in molecules) and to carry out their assignment to certain types of vibrations.

So for molecules furozane obtained that the generalized force coefficients of bonds C-N and C-H in the molecule is, respectively, 18.6189 mdyn/Å, 15.7142 mdyn/Å and 7.0115 mdyn/Å obtained with the B3LYP/6-311++G(3df,3pd) in the coordinates X_δ^0. Coordinates X_δ^0 proposed (first time) L.S. Mayants and G. B. Shaltuper. They allowed to carry out the correct solution of the spectral problem for objects with any combination of atoms (these are molecules with covalent bonds, various complexes, complex supramolecular formations, etc.), while maintaining the "chemical visibility" of the results. It became possible to operate with the old concept of "force constant of bonds", which in this study makes sense of the generalized force coefficient.

For molecules nitrofurozane obtained that the generalized force coefficients of bonds C-H, C-N, and N-O on the opposite side of the nitro group is, respectively, 7.0442 mdyn/Å, 18.8364 mdyn/Å and 15.2080 mdyn/Å obtained with the B3LYP/6-311++G(3df,3pd) in the coordinates X_δ^0. The generalized force coefficients of the C-N and N-O bonds on the nitrogroup side are 18.7374 mdyn/Å and 16.3715 mdyn/A. The force coefficient of bond C-NO_2 is 6.5774 mdyn/Å. (With respect to nitromethane "the rigidity of the connection of the" C-N increased by 0.2917 mdyn/Å). The power coefficient of bond N-O of the nitro group located in the direction of the relationship C-H equal 12.6461 mdyn/Å. The force coefficient of the bond N-O of the nitrogroup located in the other direction is 13.1909 mdyn/Å. the Average value of the force coefficient N-O of the nitrogroup is close to that in the molecule of nitromethane.

The most intense band in the furozan spectrum has a value of 866 cm^{-1}, which can be attributed to the wagging vibration of the C-H bonds with respect to the ring plane.

The most intense band in the spectrum nitrofurozan has a value of 1627 cm^{-1} which can be attributed to asymmetric stretching vibrations of the nitro group relationships N-O.

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