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Computation of vibrational spectra of *p*-nitrotoluene and 2,4,6-trinitrotoluene in the coordinates X_δ^0

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Abstract

In the framework of the density functional methods B3LYP 6-311++G(3df,3pd) first derived force field for *p*-nitrotoluene and 2,4,6-trinitrotoluene in the coordinates X_δ^0. Determined generalized force coefficients for the relations in the coordinate X_δ^0 calculated frequency (wave number) of normal vibrations and carried out their assignment to certain types of vibrations.

Our results show that for *p*-nitrotoluene the most intense band in the vibrational spectrum has a value of 1374 cm^{-1}. Preferably in this vibration involves the atoms of the nitro group. It is a valence fluctuation of C-N bond and symmetric vibrations of the two bonds N-O, which are in opposite phase to C-N. Following the intensity band is mostly "owned" as nitrogroup. It matters 1577 cm^{-1}. This vibration involves the atoms of N and O. This is asymmetric vibrations of the two bonds N-O.

In the molecule of 2,4,6-trinitrotoluene has a characteristic intense bands involving nitro groups. The most intense band has a value of 1375 cm^{-1}. It could be attributed to the stretching vibrations of the nitro group. This is mainly the vibration of the bondC-N in position 4 and, in antiphase to that vibration, the symmetric vibrations of the two bonds N-O. The second intensity band with a value of 1604 cm^{-1} corresponds to (mainly) the nitro groups in positions 2 and 6. This asymmetric vibrations of N-O in each of the nitro groups that have coordinated movement relative to each other. Wave number 1385 cm^{-1} corresponds to the following intensity bond and is interpreted as asymmetric vibrations of nitro groups in positions 2 and 6 of the ring.This means that the C-N bond changes in the opposite phase each against the other. Inside each of the nitro groups N-O bonds change symmetrically.

The obtained generalized force coefficients of bonds in molecules of *p*-nitrotoluene and 2,4,6-trinitrotoluene in the coordinates X_δ^0. So the generalized force coefficients for the relations C-N and N-O nitro group in the molecule, and *p*-nitrotoluene was found to be 6.6509 mdyn/Å and 12.7008 mdyn/Å (average) in the coordinates X_δ^0, respectively. The generalized force coefficients for the relations C-N and N-O nitro group in the molecule 2,4,6-trinitrotoluene equal, respectively, 6.4682 mdyn/Å and 12.8707 mdyn/Å (middle).

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