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## Solution of a spectral problem for molecules $NH_2NO_2$ , $CH_3NO_2$ and $N_2O_4$ in coordinates $X_{\delta}^0$

## © Alexander V. Belik

Faculty of Chemical Technology and Computing Chemistry. The Chelyabinsk Sate University. Br. Kashiriny St., 129. Chelvabinsk, 454001. Russia. Phone: +7 (351) 799-70-66. E-mail: belik@csu.ru

*Keywords:* molecules NH<sub>2</sub>NO<sub>2</sub>, CH<sub>3</sub>NO<sub>2</sub>, N<sub>2</sub>O<sub>4</sub>, the generalized force constants, coordinates  $X_{\delta}^{0}$ , calculations DFT, vibration frequencies.

## Abstract

Within the framework of approach B3LYP 6-311 ++ G (3df, 3pd) the force field of NH<sub>2</sub>NO<sub>2</sub>, CH<sub>3</sub>NO<sub>2</sub> and  $N_2O_4$  molecules in coordinates  $X_{\delta}^{0}$  for the first time is obtained. Frequencies of normal vibrations were calculated. Comparison of the obtained generalized force constants with those of molecule was carried out.