

Density functional calculation of N-N barrier and analysis of vibrational spectra for nitrosoisocyanate and nitroisocyanate

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Source: JOURNAL OF MOLECULAR STRUCTURE-THEOCHEM **Volume:** 536 **Issue:** 2-3 **Pages:** 203-212

Abstract: The structural stability of nitro isocyanate $O=C=N-NO$ and nitroisocyanate $O=C=N-NO_2$ were investigated using ab initio calculations. The calculations were carried out at DFT-B3LYP/6-311++G** level. From the calculation nitrosoisocyanate was predicted to exist predominantly in the trans conformation with high trans-cis rotational barrier. The rotational barrier of the NO group was calculated to be about 6 kcal/mol, while that of the NO₂ group to be of about 2 kcal/mol. The vibrational frequencies were computed, normal coordinate calculations were carried out and potential energy distributions were calculated for both molecule:. A complete vibrational assignment was provided for the normal modes of the two molecules. (