

**Density functional calculation of N-N barrier and analysis of vibrational spectra for nitrosoisocyanate and nitroisocyanate.** Badawi, H. M.; Forner, W

**Abstract**

The structural stability of nitrosyl isocyanate (I), O:C:N-NO, and nitril isocyanate, O:C:N-NO<sub>2</sub>, were investigated using ab initio calcns. The calcns. were carried out at DFT-B3LYP/6-311++G\*\* level. From the calcn., I was predicted to exist predominantly in the trans conformation with high trans-cis rotational barrier. The rotational barrier of the NO group was calcd. to be about 6 kcal/mol, while that of the NO<sub>2</sub> group to be of about 2 kcal/mol. The vibrational frequencies were computed, normal coordinate calcns. were carried out and potential energy distributions were calcd. for both mols. A complete vibrational assignment was provided for the normal modes of the two mols.