

Structural stability and normal coordinate analyses of 1-formylazirine  $c\text{-C}_2\text{H}_2\text{N-CHO}$  and 3-formyldiazirine  $c\text{-N}_2\text{CH-CHO}$ . Badawi, Hassan M.; Altalbawy, Farag M. A. Department of Chemistry, King Fahd University of Petroleum & Minerals, Dhaharan, Saudi Arabia. Asian Journal of Spectroscopy (2005), 9(1-4), 21-35.

#### Abstract

The structural stability and internal rotation of the formyl group in 1-formylazirine and 3-formyldiazirine were investigated by ab initio MP2 and DFT-B3LYP calcns. with 6-311+G\*\* basis set. From the calcns. 1-formylazirine was found to exist predominantly in gauche (carbonyl C=O group nearly eclipses ring C-N bond) conformation, while 3-formylazirine to exist in cis .tautm. trans conformational equil. For 3-formyldiazirine the cis (C=O moiety eclipses the ring) and the trans (C=O moiety eclipses the  $\alpha$ -hydrogen of the ring) conformers were predicted to have a comparable relative stability with cis to trans rotational barrier of about 9 kcal/mol. The equil. const. for the cis .tautm. trans interconversion in 3-formyldiazirine was estd. to be 0.2914 that corresponds to an equil. mixt. of about 23% cis and 77 % trans at 298.15 K. The vibrational frequencies were computed at DFT-B3LYP level for the gauche 1-formylazirine and the cis and trans mixt. of 3-formyldiazirine. Normal coordinate calcns. were carried out and the potential energy distributions PED were calcd. for the stable conformers of each of the two mols.