Structural stability, vibrational assignments and C-N rotational barrier in vinyl azide.
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Abstract

The conformational behavior and the structure of vinyl azide (CH2:CH-NNN) were investigated by DFT-B3LYP calcns. with 6-311++G** basis set. The mol. was predicted to have the cis trans conformational equil. with very comparable relative stability between the two conformers. Full optimization was performed at the ground and transition states in the mol. The barrier to internal rotation around the C-N single bond in vinyl azide was calcd. to be of about 5 kcal/mol. The vibrational frequencies were computed at the DFT-B3LYP level and the calcd. IR and Raman spectra of the cis-trans mixt. of the mol. were plotted. Complete vibrational assignments were made on the basis of normal coordinate calcns. for both stable conformers of the mol.