

**C-C AND C-N ROTATIONAL BARRIERS IN VINYL KETENE AND
VINYL ISOCYANATE**

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¹ Taken in part from the thesis of A. Al-Saadi that will be submitted to Chemistry Department in partial fulfillment of M. S. degree.

ABSTRACT

The conformational behavior and structural stability of vinyl ketene and vinyl isocyanate were investigated by utilizing ab initio calculations with 6-311++G** basis set at the Density Functional (B3LYP) level. Both molecules were predicted to have the *s-cis* \leftrightarrow *s-trans* conformational equilibrium with the *s-trans* form being the predominant conformer for the two molecules. Full optimization was performed at the ground and transition states in the two molecules. The calculated rotational barriers in the systems were compared to each others and it was found that the barrier of the internal rotation around the C-C single bond in vinyl ketene is much higher than that of the corresponding C-N bond in the vinyl isocyanate. The vibrational frequencies were computed at the DFT-B3LYP level and the calculated infrared and Raman spectra of the *cis-trans* mixtures of the two molecules were plotted. Complete vibrational assignments were made on the basis of normal coordinate calculations for both stable conformers of the molecules.

Keywords: Vibrational spectra and assignments; Rotational barriers; vinyl ketene; vinyl isocyanate.