

**C-C and C-N rotational barriers in vinyl ketene and vinyl isocyanate.** Badawi, H. M.;  
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### **Abstract**

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