Density functional calculations of vibrational wavenumbers and derived potential energy distributions for fluoro- and chlorocarbonyl ketenes

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Abstract: The structural stability and conformational behavior of fluorocarbonyl ketene and chlorocarbonyl ketene were investigated by utilizing ab initio calculations with the 6-311++G** basis set at the density functional (B3LYP) level. Both molecular systems were predicted to exist in the planar s-cis and s-trans conformations with a relatively high-energy barrier. Full geometrical optimization was performed at the ground and transition states in the two systems. The vibrational frequencies were computed at the DFT-B3LYP/6-311++G** level and the calculated vibrational infrared and Raman spectra of the cis-trans mixtures of fluoro- and chlorocarbonyl ketenes were plotted. Complete vibrational assignments were made on the basis of normal coordinate calculations for both stable conformers of the molecules.