Theoretical potential functions of halocarbonyl ketenes and halocarbonyl isocyanates and vibrational spectra of the bromides

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Abstract: The conformational behavior and structural stability of bromocarbonyl ketene were investigated by DFT and MP2 calculations using the 6-311++G** basis set. From the calculations, the molecule was found to have the s-cis double left right arrow s-trans conformational equilibrium with the trans being the lower energy form. For comparison purposes, the potential scans and functions of halocarbonyl ketenes CXO-CH=C=O and halocarbonyl isocyanates CXO-N=C=O (where X = F, Cl or Br) were calculated at the B3LYP/6-311++G** level. Full energy optimizations were carried out for the transition states and the minima at B3LYP/6-311++G** and MP2/6-311++G** levels, from which the rotational barriers were calculated for the molecules, The vibrational frequencies were computed at the DFT-B3LYP level and the vibrational assignments for the normal modes of both bromocarbonyl ketene and isocyanate in their stable cis and trans conformations were made on the basis of normal coordinate calculations.