Conformational equilibrium and normal coordinate analyses of ketenecarboxylic acid O=C=CH-COOH. Badawi, Hassan M.. Department of Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia. Canadian Journal of Analytical Sciences and Spectroscopy (2006), 51(1), 9-16.

Abstract

The conformational and structural stability of ketenecarboxylic acid O=C=CH-COOH were investigated by DFT-B3LYP and ab initio MP2 calcns. with the 6-311+G** basis set. From the calcns. ketenecarboxylic acid was predicted to exist predominantly in a mixt. of cis (the CO and the CHCO groups eclipse each other) and trans conformations with the trans being the lower energy form. The C-C- and C-O rotational barriers in the mol. were calcd. to be about 10 and 12 kcal/mol, resp. The equil. const. for the cis .tautm. trans conformational interconversion of ketenecarboxylic acid was calcd. to be 0.4117 that corresponds to an equil. mixt. of about 29% cis and 71% trans at 298.15 K. The vibrational frequencies of the mol. in the cis and trans conformations were computed at the DFT-B3LYP level. Complete vibrational assignments were made on the basis of normal coordinate analyses of cis and trans ketenecarboxylic acid.