Conformational properties and vibrational analyses of monomeric pentafluoropropionic acid CF_3CF_2COOH and pentafluoropropionamide $CF_3CF_2CONH_2$

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Abstract

*The structural stability of pentafluoropropionic acid and pentafluoropropion-amide was investigated by DFT-B3LYP/6-311+G** and ab initio MP2/6-311+G** calculations. The calculated potential energy curves of the acid were consistent with two distinct minima that correspond to cis (C=O eclipses the C-C bond) and gauche conformers, with the latter being the lower energy form at ambient temperature. The equilibrium constant for the conformational interconversion of pentafluoropropionic acid were calculated at both levels of theory and found to correspond to an equilibrium mixture of about 76 % gauche and 24% cis conformations at 298.15 K. From the calculations, pentafluoroproionamide was predicted to exist only in the gauche conformation. The vibrational frequencies of pentafluoropropionic acid in the cis and the gauche conformers and pentafluoropropionamide in the gauche structure were computed at B3LYP level and complete vibrational assignments were made based on normal coordinate calculations and comparison with experimental infrared data of the molecules.*

Keywords: Conformational and structural stability; Potential energy curves; Vibrational spectra and assignments. Normal coordinate analyses; pentafluoropropionic acid; pentafluorpropionamide

Résumé

*Nous avons étudié la stabilité structurale de l'acide pentafluoropropionique et du pentafluoropropionamide avec des calculs DFT-B3LYP/6-311+G** et MP2/6-311+G** ab initio. Les courbes calculées d'énergie potentielle de l'acide étaient consistantes avec deux minimums distincts qui correspondent aux conformères cis (C=O éclipsant le lien C-C) et gauche, ce dernier étant à la plus basse énergie à température ambiante. La constante d'équilibre de l'interconversion conformationelle de l'acide pentafluoropropionique a été calculée aux deux niveaux théoriques et elle correspond à un équilibre d'une mélange des conformations d'environ 76 % gauche et 24% cis à 298.15 K. À partir de ces calculs, il est prédit que le pentafluoroproionamide existe seulement sous la conformation gauche. Nous avons calculé les fréquences de vibration de l'acide pentafluoropropionique sous les conformères cis et gauche et celle du pentafluoropropionamide dans sa structure gauche au niveau B3LYP et nous avons complété les attributions vibrationnelles en se basant sur des calculs de coordonnées normales et des comparaisons avec des données infrarouges expérimentales de ces molécules.*

Introduction

Recently the investigation of the conformational stability of a series of halopropanals of the general formula R-CHO, where, R is CX_3CH_2, CHX_2CH_2, or CH_2XCH_2 and X is F or Cl were reported [1-4]. We investigated the structures of 3,3,3-trifluoropropanal [1], 3,3-difluoropropanal [2], 3-fluoropropanal [3] and 2,2,3,3,3-pentafluoropropanal [4] to study the effect of coupling between the carbonyl -CHO and the fluoromethyl rotors on the conformational stability of these molecules. The

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