MICROWAVE AND INFRARED SPECTRA, ADJUSTED R_0 STRUCTURAL PARAMETERS, CONFORMATIONAL STABILITIES, VIBRATIONAL ASSIGNMENTS, AND AB INITIO CALCULATIONS OF CYCLOBUTYLCARBOXYLIC ACID CHLORIDE

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The FT-microwave spectrum of cyclobutylcarboxylic acid chloride, c-$C_4H_7C(O)Cl$, has been recorded and 153 transitions for the ^{35}Cl and ^{37}Cl isotopologues have been assigned for the gauche-equatorial conformation. The ground state rotational constants were determined from these assignments with following values for ^{35}Cl [^{37}Cl]: A = 4349.84294(48) [4322.0555(56)], B = 1414.80319(36) [1384.50581(105)], C = 1148.24114(18) [1126.35465(101)]. From the determined microwave rotational constants and ab initio MP2(full)/6-311+G(d,p) predicted structural values, adjusted r_0 parameters are reported. Variable temperature (-70 to -100°C) infrared spectra (4000 to 400 cm^{-1}) were recorded in liquid xenon and gauche-equatorial conformer is the most stable form with an enthalpy differences of 91 $\pm$ 9 cm^{-1} (1.09 $\pm$ 0.05 kJ/mol) with gauche-axial and 173 $\pm$ 17 cm^{-1} (2.07 $\pm$ 0.04 kJ/mol) with the trans-equatorial conformer. The relative amounts present at an ambient temperature are 54% gauche-equatorial, 35 $\pm$ 1% gauche-axial and 12 $\pm$ 1% trans-equatorial. The conformational stabilities have been predicted from ab initio calculations utilizing several different basis sets up to aug-cc-pVTZ from both MP2(full) and density functional theory calculations by the B3LYP method. Vibrational assignments have been provided for the observed bands for all three conformers which are supported by ab initio calculations to predict harmonic force constants, vibrational wavenumbers, infrared intensities, Raman activities and depolarization ratios. The results are discussed and compared to the corresponding properties of some related molecules.