RING-PUCKERING CONFORMATIONS OF 3-HYDROXYTETRAHYDROTHIOPHENE AND TETRAHYDROTHIOPHEN-3-ONE FROM ROTATIONAL SPECTROSCOPY

CHARLES R. TOROK and MICHAEL J. TUBERGEN, *Department of Chemistry, Kent State University, Kent, OH 44242*.

Rotational spectra of the heterocyclic rings 3-hydroxytetrahydrofuran and tetrahydrothiophen-3-one have been recorded using a Fourier-transform microwave spectrometer. Spectra of the ^{34}S and ^{13}C isotopomers were recorded in natural abundance. The a-, b-, and c-type transitions observed for each species were fit to a Watson A-reduction Hamiltonian, which led to the rotational constants A = 4272.6617 (9), B = 2764.5523 (7), and C = 2250.1361 (4) MHz for 3-hydroxytetrahydrothiophene and A = 5623.697 (1), B = 2431.3551 (4), and C = 1801.4946 (4) MHz for tetrahydrothiophen-3-one. Ring-puckering conformations were determined from fitting the rotational constants as well as from Kraitchman calculations of the atomic coordinates. Ab initio calculations at the MP2/6-31+G** level support the experimental structures.