STRUCTURES AND NUCLEAR QUADRUPOLE COUPLING TENSORS OF A SERIES OF CHLORINE-CONTAINING HYDROCARBONS

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Rotational spectra for *gauche*-1,2-dichloroethane (12DCE), *gauche*-1-chloro-2-fluoroethane (1C2FE) and both *anti*- and *gauche*-2,3-dichloropropene (23DCP) have been observed using chirped-pulse Fourier-transform microwave (FTMW) spectroscopy in the 6-18 GHz region. Although the *anti* conformers for all three species are predicted to be more stable than the *gauche* forms, they are nonpolar (12DCE) or nearly nonpolar (predicted dipole components for *anti*-1C2FE: $\mu_a = 0.11$ D, $\mu_b = 0.02$ D and for *anti*-23DCP: $\mu_a = 0.25$ D, $\mu_b = 0.02$ D); nevertheless, it was also possible to observe and assign the spectrum of *anti*-23DCP. Assignments of parent spectra and ^{37}Cl and ^{13}C substituted isotopologues utilized predictions at the MP2/6-311++G(2d,2p) level and Pickett's SPCAT/SPFIT programs. For the weak *anti*-23DCP spectra, additional measurements also utilized a resonant-cavity FTMW spectrometer. Full chlorine nuclear quadrupole coupling tensors for *gauche*-12DCE and both *anti*- and *gauche*-23DCP have been diagonalized to allow comparison of coupling constants. Kraitchman's equations were used to determine r_s coordinates of isotopically substituted atoms and r_0 structures were also deduced for *gauche* conformers of 12DCE and 1C2FE. Structural details and chlorine nuclear quadrupole coupling constants of all three molecules will be compared, and effects of differing halogen substitution and carbon chain length on molecular properties will be evaluated.