THE MOLECULAR STRUCTURE OF CHLORO-FERROCENE DETERMINED FROM MICROWAVE DATA

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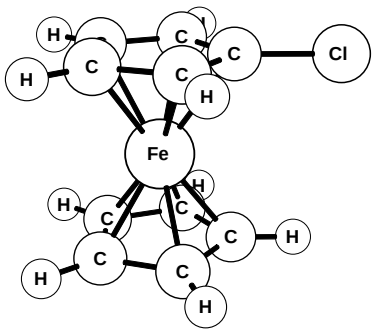
Microwave rotational transitions for 8, new, low-abundance isotopomers of 1- chloroferrocene were measured using a Flygare-Balle type microwave spectrometer. There are no previous reports of structural data for mono-substituted haloferrocenes from diffraction or microwave work, so further refinement of the microwave structure provides the only insight into subtle structural modifications resulting from substitution of the electronegative chlorine atom.



A refined gas-phase structure of chloroferrocene has been obtained through analysis of the microwave spectra for ten isotopomers. New data for ^{54}Fe, ^{57}Fe, ^{37}Cl and six unique ^{13}C isotopomers were combined with data from previous work. This large data set, which contained 30 rotational constants, was used to determine many new structural parameters for chloroferrocene. The carbon atoms in the chlorinated Cp ligand ($\eta^5 - C_5H_5$) show distortions from five-fold symmetry of approximately 5%. The C-Cl bond is bent away from the plane of carbon atoms by nearly 7°. The two Cp ligands are eclipsed, in contrast to the staggered conformation obtained from X-ray and neutron diffraction data for unsubstituted ferrocene.