GAS PHASE STRUCTURE DETERMINATION OF FERROCENE CARBOXALDEHYDE USING FOURIER TRANSFORM MICROWAVE SPECTROSCOPY [a]

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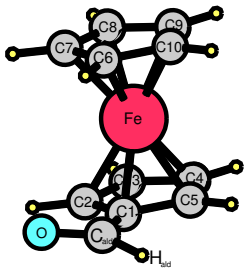

Microwave molecular spectra for six isotopomers (^{56}Fe,^{54}Fe, ^{57}Fe, $^{13}C_{ald}$, $^{13}C_1$ and ^{56}Fe, D_{ald}) of Ferrocene Carboxaldehyde were measured using Flygare-Balle type pulsed beam Fourier Transform Microwave Spectrometer system. The main isotopomer (^{56}Fe) was fitted by employing seven adjustable parameters while other less abundant isotopomers were fitted using only three parameters, namely three rotational constants (A, B and C). A total of eighteen rotational constants and four adjustable parameters were used to obtain the gas phase structure. The structural parameters will be compared with the values obtained from Kraitchman analysis and Density Functional Theory calculations. Structural fit results indicate that the aldehyde group droops towards the iron atom and twists with respect to the Cp plane. More over, the inductive Hammett parameters will be correlated with the structural parameters obtained from this study and previous gas phase microwave results for various substituted Ferrocenes.

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