# EXPERIMENTAL MEASUREMENT OF 1,1'-DIMETHYLFERROCENE GAS-PHASE STRUCTURE AND DETECTION OF 1,2'-DIMETHYLFERROCENE STRUCTURAL ISOMERS USING PULSE BEAM FOURIER TRANSFORM MICROWAVE SPECTROMETER[a]

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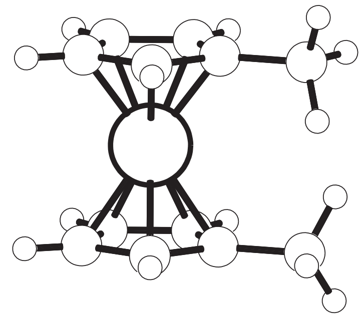

We now report results from the first gas-phase structural study of dimethylferrocene. This research is part of the continuing interests to understand the relation between structure and reactivity of substituted ferrocene. In the present work, we have obtained the microwave spectra of two structural isomers of dimethylferrocene, namely 1,1'-dimethylferrocene and 1,2'-dimethylferrocene. The asymmetric-top spectra of both isomers were measured in the frequency range of 4-12 GHz using a Flygare-Balle type of spectrometer. Overall 74 rotational transitions (R branch) of the normal isotopomer were observed. 30 transitions were assigned to 1,1'-dimethylferrocene and the rest to 1,2'-dimethylferrocene. The least-squares fit to the observed transitions suggests that the structure of 1,1'-dimethylferrocene is nearly rigid. The deviations in the least-squares fit for 1,2'-dimethylferrocene are significantly larger, suggesting some possible fluxional behavior associated with this isomer. 7 out of the 44 transitions for 1,2'-dimethylferrocene clearly exhibits very small splittings that were not observed for 1,1'-dimethylferrocene. These small splittings, which are being analyzed, are most likely due to torsional motion of the methyl group. The rotational spectrum of both isomers will be presented along with the results of the latest fit.

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