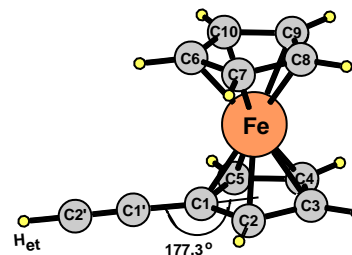


## THE STRUCTURE OF ETHYNYLFERROCENE USING MICROWAVE SPECTROSCOPY<sup>a</sup>

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Structural parameters for ETHYNYLFERROCENE and other singly-substituted ferrocenes have been determined, using microwave spectroscopy and DFT calculations. For ethynylferrocene twenty-four rotational constants have been determined by fitting the measured frequencies of a- and b- type transitions, for various isotopomers. The distance between the Fe-atom and the center of the cyclopentadienyl ring is 1.648(5) Å and the distance between the carbon atoms of the cyclopentadienyl ring is  $r_{CC} = 1.432(2)$  Å. The ethynyl group is bent away from the Fe-atom and out of the plane of the adjacent carbon atoms by  $2.75^\circ$ . The DFT calculations and analyses of fits including  $^{13}\text{C}$  isotopic substitution data indicate that the molecule is in an eclipsed conformation. Trends in microwave experimental values for the distance between the Fe-atom to the center of the cyclopentadienyl ring for a series of substituted ferrocenes have been analysed. This analysis provides an estimate of the gas phase distance between the Fe-atom to the center of the cyclopentadienyl ring for ferrocene of 1.65(1) Å.



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