MICROWAVE SPECTRA AND INTERNAL ROTATION OF DIENE-IRON TRICARBONYLS

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In chemistry, attention has been focussed on transition metal carbonyls for two reasons. First, they revealed new bonding situations like the binding of non-polar ligands explained by back donation and second, they are known to have catalytic activity in a variety of important industrial processes and are useful tools in preparitive chemistry. Microwave spectroscopy is the method to obtain most exact structures in the gas phase and therefore is a key for understanding how stable transition metal carbonyls take influence on reactions on the one hand and could be a means to get information about non-stable intermediates in reactions, on the other hand. This would lead to the ability to verify reaction paths, calculate reaction rates and find better catalysts by calculating the energy of such systems. The spectra of tricarbonyl(isoprene) iron and tricarbonyl(2,4-hexadiene) iron are presented and explained. The fine structure of the rotational transitions due to internal rotation of the methyl groups allows the determination of the torsional barrier. By the help of the rotational constants of the ^{56}Fe- and the ^{54}Fe-isotopomer the most uncertain internal coordinates were determined. Furthermore, recent results for tricarbonyl(methylcyclopentadienyl) manganese are given, too.

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