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Preliminary communications

EXPERIMENTAL OBSERVATION OF DIASTEREOTOPY OF CARBONYLIC LIGANDS IN TRANSITION METAL COMPLEXES CONTAINING A CHIRAL GROUP

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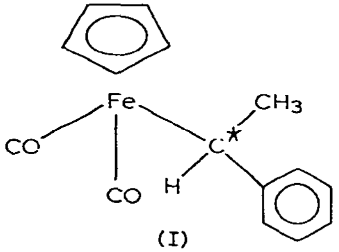
Summary

Diastereotopy of carbonyl ligands in π-$C_5H_5Fe(CO)_2CH(CH_3)C_6H_5$ was observed with ^{13}C NMR spectroscopy.

Carbonyl ligands in the dicarbonyl transition metal complexes containing a chiral group bound to the metal are diastereotopic. However, no experimental evidence on the carbonyl ligand diastereotopy in such complexes has been yet reported. We synthesized the complex π-$C_5H_5Fe(CO)_2CH(CH_3)C_6H_5$ (I). Complex I contains a chiral centre at the carbon atom bound to the iron, and the phenyl group thus its carbonyl ligands are diastereotopic.



(I)

Using ^{13}C NMR we found a non-equivalence of chemical shifts of carbon nuclei in the carbonyl ligands of I. The ^{13}C NMR spectrum of the complex is shown in Fig.1, from which it can be seen that the carbon nuclei in carbonyl ligands give rise to two singlet signals at δ 217.1 and 217.5 ppm. $\Delta\delta$ 0.4 ppm. We note that in the spectrum of π-$C_5H_5Fe(CO)_2CH_2C_6H_5$ the carbonyl carbons only produce a singlet at 216.7 ppm.

Complex I was obtained from sodium salt of cyclopentadienyliron dicarbonyl and α-phenylethyl chloride. The structure of I was confirmed by elemental analysis, IR, PMR and mass spectra.

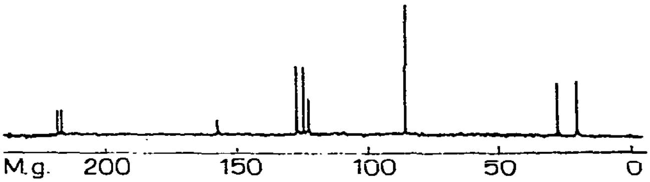


Fig.1. The ^{13}C NMR spectrum of complex π-$C_5H_5Fe(CO)_2CH(CH_3)C_6H_5$.

The ^{13}C NMR spectrum was taken on HX-90 Brueker instrument at 22.63 MHz with the use of a wide band ^{13}C—H decoupler. $CHCl_3$ was employed as an internal standard and solvent. The ^{13}C NMR chemical shifts of complex I are listed below (δ ppm from TMS): 20.51 (CH_3), 28.31 (CH), 86.53 (C_5H_5), 123.11 (*p*-C_6H_5), 125.58 and 127.85 (*o*-, *m*-C_6H_5), 157.48 (key atom), 217.06 and 217.52 (carbonyl groups).

As far as we know this is a first example of experimental evidence to diastereotopy of the carbonyl ligands in transition metal complexes.