

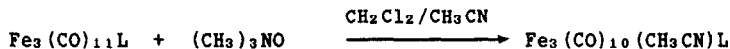
IRON CLUSTERS CONTAINING THE TRIFLUOROMETHYL
ISOCYANIDE LIGAND

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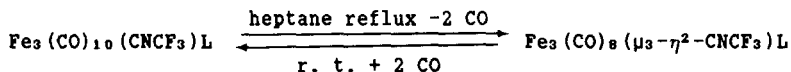
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Dodecacarbonyltriiron is a highly fluxional molecule, which in solution undergoes rapid exchange of the carbonyl ligands even at $-150\text{ }^{\circ}\text{C}$ [1].

$\text{Fe}_3(\text{CO})_{11}(\text{CNCF}_3)$, which can be prepared from $\text{Fe}_3(\text{CO})_{12}$ and CNCF_3 , however, possesses a rigid bridging trifluoromethyl isocyanide ligand even at ambient temperature and becomes completely rigid on the nmr time scale at $-100\text{ }^{\circ}\text{C}$ [2]. Nevertheless the assignment of the ^{13}C nmr resonances of the eleven different carbonyl carbon atoms is ambiguous.



$\text{L} = \text{P}(\text{CH}_3)_3, \text{P}(\text{C}_2\text{H}_5)_3, \text{P}(\text{OCH}_3)_3, \text{CN-t-C}_4\text{H}_9$



To facilitate the assignment of the carbonyl resonances phosphine and phosphite substituted derivatives have been synthesized. The structures of $\text{Fe}_3(\text{CO})_{10}(\text{CNCF}_3)\text{P}(\text{CH}_3)_3$, two isomers of $\text{Fe}_3(\text{CO})_{10}(\text{CNCF}_3)\text{P}(\text{OCH}_3)_3$, and $\text{Fe}_3(\text{CO})_8(\text{CNCF}_3)\text{P}(\text{OCH}_3)_3$ have been investigated by X-ray crystallography. The variable temperature nmr spectra of the compounds and possible migration mechanism of the ligands will be discussed.

1 F. A. Cotton and D. L. Hunter, Inorg. Chim. Acta, **11**, L9 (1974).

2 I. Brüdgam, H. Hartl, and D. Lentz, Z. Naturforsch., **39b**, 721 (1984); D. Lentz, Z. Naturforsch., **42b**, (1988) 839.