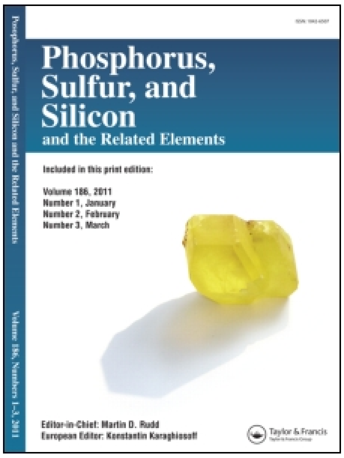

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# $^{57}$Fe Mössbauer and $^{31}$P NMR Spectroscopic Characterisation of $Fe(CO)_3L_2$ Complexes (L=Phosphite and Phosphine)

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# $^{57}$Fe Mössbauer and $^{31}$P NMR Spectroscopic Characterisation of $Fe(CO)_3L_2$ Complexes (L = Phosphite and Phosphine)

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A series of mixed ligand complexes of the type $[Fe(CO)_3L^1L^2]$ ($L^1$ = triphenylphosphite and $L^2$ = phosphine or phosphite) have been prepared to study the Fe-P bond. The $^{57}$Fe Mössbauer spectra of trans-$[Fe(CO)_3L^1L^2]$ showed a quadrupole splitting doublet characteristic of the disubstituted iron carbonyls in trigonal bipyramidal symmetry. The linear dependence of the quadrupole splittings on the isomer shifts with a positive slope has revealed that the iron-to-phosphorus σ-donation is offset by the phosphorus-to-iron π-back donation. The $^{31}P\{^1H\}$ NMR spectra showed a couple of doublets assigned to the coordinated phosphite and the coordinated phosphine. The doublet of the phosphite site was generally observed at the down field compared with that of the phosphine site. The coordination shifts increase with the Mössbauer isomer shifts, suggesting that the iron-to-phosphorus π-back donation plays an important role in the Fe-P bond of trans-$[Fe(CO)_3L^1L^2]$. The relatively large coupling constants due to $^2J(P,P)$ have demonstrated that there exists a strong interaction between trans phosphorus ligands through the $d_\pi$ orbitals of the central iron. The coupling constant is a measure of the bond strength between Fe-P, while the Mössbauer isomer shift reflects the electron density at the iron nucleus. Thus, a linear correlation has been established between these two spectroscopic parameters.