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¹³C, ³¹P and ¹H NMR Investigations of Rh(I)-(2S,4S)-2,4-Bis(Diphenylphosphino)Pentane (Bdpp)-Diene Complexes

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^{13}C , ^{31}P AND ^1H NMR INVESTIGATIONS OF $\text{Rh(I)}-(2\text{S},4\text{S})-$
2,4-BIS(DIPHENYLPHOSPHINO)PENTANE (BDPP)-DIENE
COMPLEXES

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Although transition metal-phosphine-diene complexes can be conveniently studied by ^{31}P NMR occasionally other nuclei such as ^{13}C or ^1H can provide more valuable information.

Here we report on the liquid state stereostructure and conformational behaviour of $[\text{Rh}(\text{NBD})(\text{S,S-BDPP})]^+$, $[\text{Rh}(\text{COD})(\text{S,S-BDPP})]^+$ and $[\text{Rh}(\text{NBD})(\text{S,S-BDPP})\text{Cl}]$ complexes. The stereochemistry of these precursors is of interest from the point of homogenous catalytic reactions such as hydrogenation. In the square-planar cationic complexes the phosphine chelate show C_2 symmetry whereas in the spectra of the five-coordinated neutral species this symmetry is lost when recorded in aromatic solvents (C_6D_6 , toluene- d_6) or at lower temperature (^{31}P , CD_2Cl_2 , 195 K). At the same time the ^1H and ^{13}C spectra indicate pairwise non-identity of the diene atoms.

Our measurement underline the critical role of the phenyl rings in the observed enantioselectivity of such chiral phosphines.