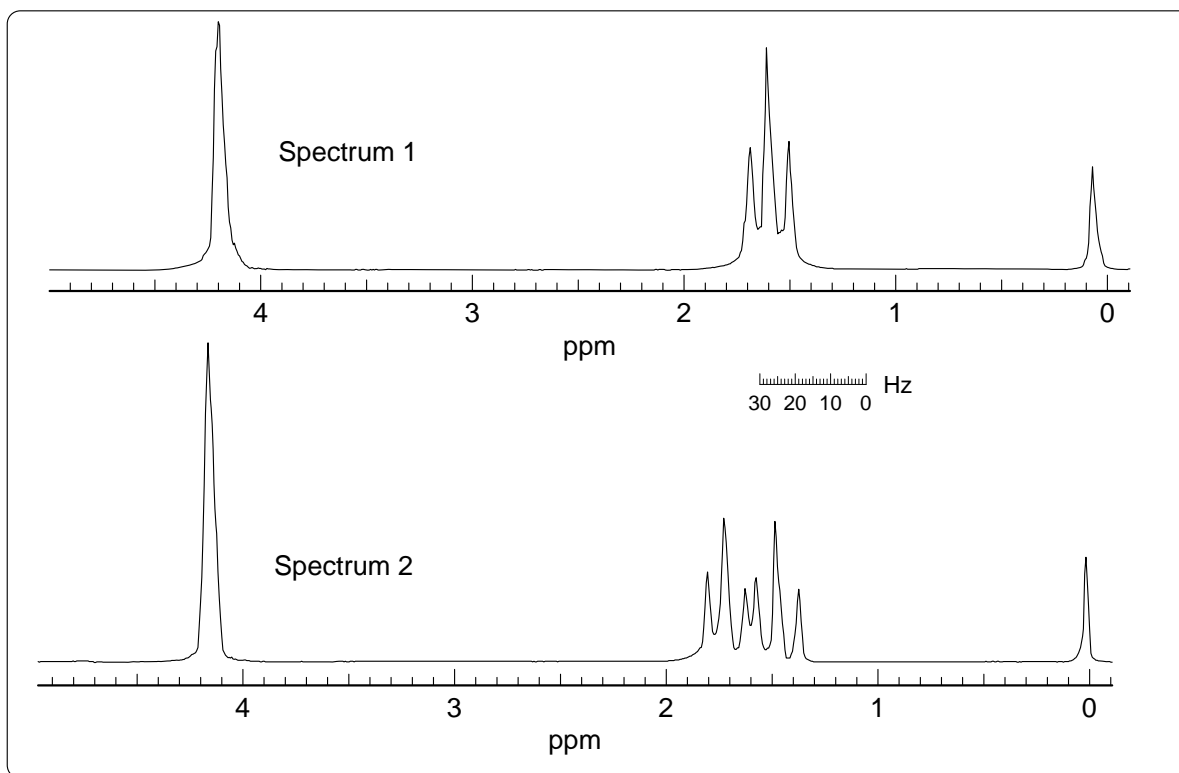
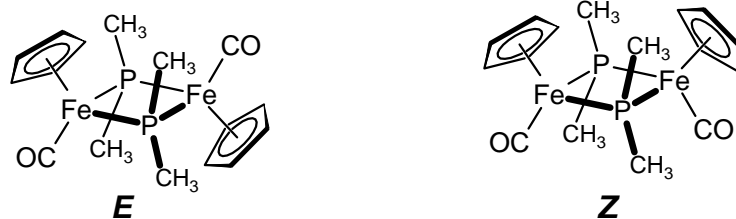


Problem R-11S ($C_{16}H_{22}Fe_2O_2P_2$). Below are the 60 MHz 1H NMR spectra of two stereoisomers (E and Z) of the iron Cp complexes shown (*J. Am. Chem. Soc.* **1963**, 85, 3120).

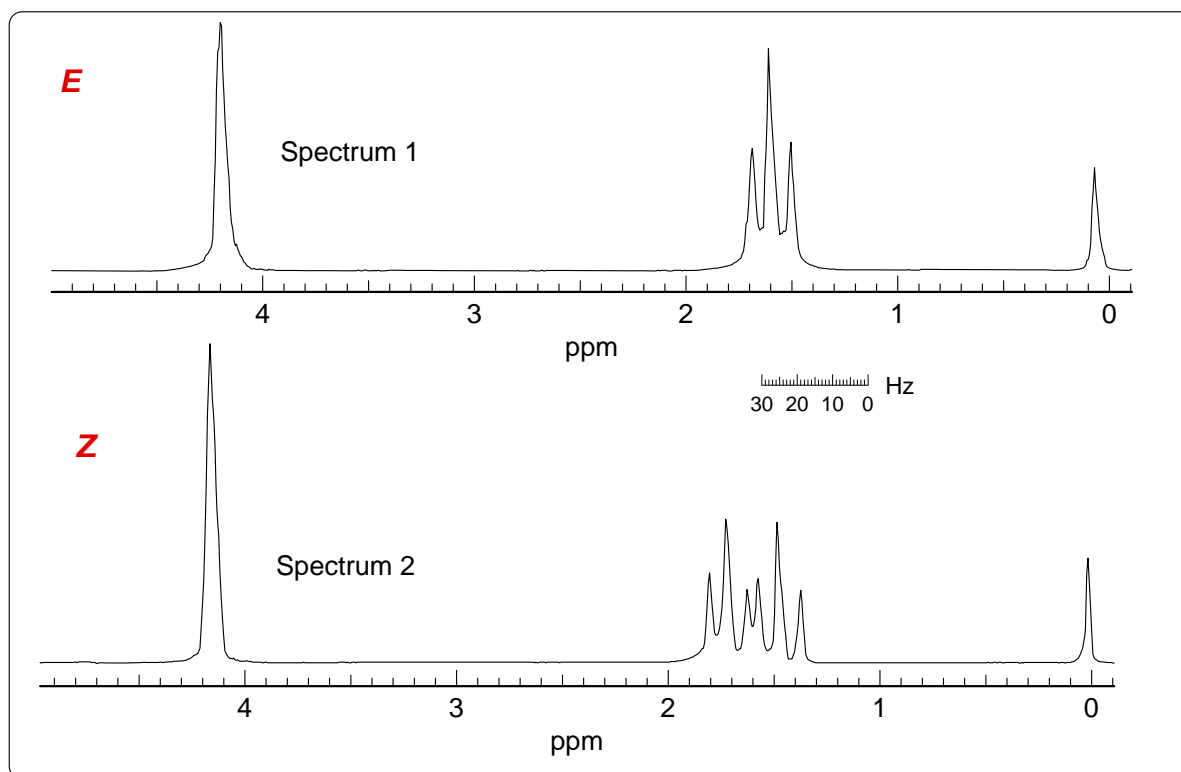


(a) Which isomer corresponds to Spectrum 1 _____, and which to Spectrum 2 _____? Explain

(b) Explain the appearance of the multiplet at δ 1.6 (i.e. why does it look like this).

(c) Would you expect the spectrum to look significantly different at 300 MHz (instead of the 60 MHz of the spectra shown)?

Problem R-11S ($C_{16}H_{22}Fe_2O_2P_2$). Below are the 60 MHz 1H NMR spectra of two stereoisomers (E and Z) of the iron Cp complexes shown (*J. Am. Chem. Soc.* **1963**, 85, 3120).



(a) Which isomer corresponds to Spectrum 1 E, and which to Spectrum 2 Z? Explain

This is a simple symmetry argument - in the Z isomer the PM_e_2 group is diastereotopic, so two triplets are seen. In the E they are identical (related by a C_2 axis).

(b) Explain the appearance of the multiplet at δ 1.6 (i.e. why does it look like this).

In the absence of other effects, the methyl groups should be coupled to one ^{31}P nucleus, hence a doublet. If the 4-bond coupling to the remote P was large enough, one would expect to see a dd. One sees a triplet because there is a large J between the two ^{31}P nuclei, so anything coupled to them will show "virtual coupling" effects - i.e. the methyl group appears to be coupled equally to both P nuclei.

(c) Would you expect the spectrum to look significantly different at 300 MHz (instead of the 60 MHz of the spectra shown)?

Apart from a larger separation between the two triplets in Spectrum 2, there would be no difference - the chemical shift between the P nuclei is zero at all fields, so the "virtual couplings" effect will always be there.