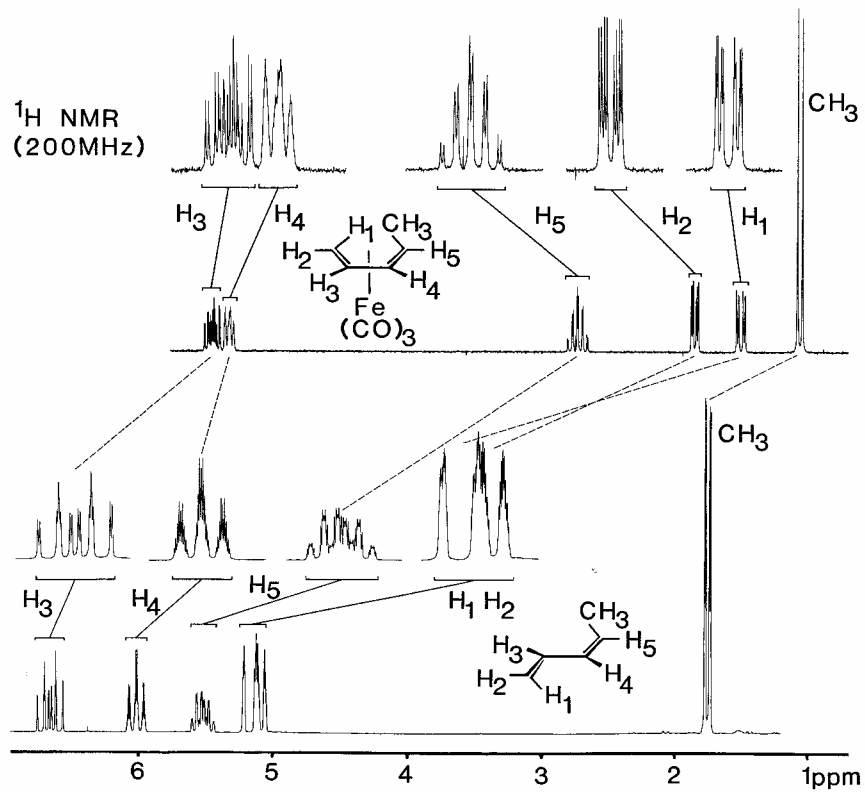
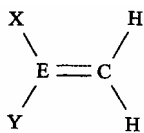


The ^1H NMR spectra of some octahedral iridium **hydrides** (hydride region). Each stereochemistry gives a characteristic coupling pattern.



^1H NMR spectra of $(\eta^4\text{-cis-1,3-pentadiene})\text{Fe}(\text{CO})_3$ and of free 1,3-pentadiene in CDCl_3 at 200 MHz. $\Delta\delta^1\text{H}$ decreases in the order endo (H_1) > terminal, exo ($\text{H}_{2,5}$) > central ($\text{H}_{3,4}$).



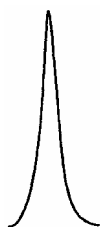
Consider a molecule having two hydrogens in **non-equivalent** environments. In this example, the carbon to which the hydrogens are attached is bonded to another atom by a bond that has hindered rotation as a result of π -bonding.



At **low T**, rotation around this bond is very slow, and the NMR shows two signals: one for each hydrogen. Since the magnetic environments of these hydrogens are different, their corresponding chemical shifts are different.

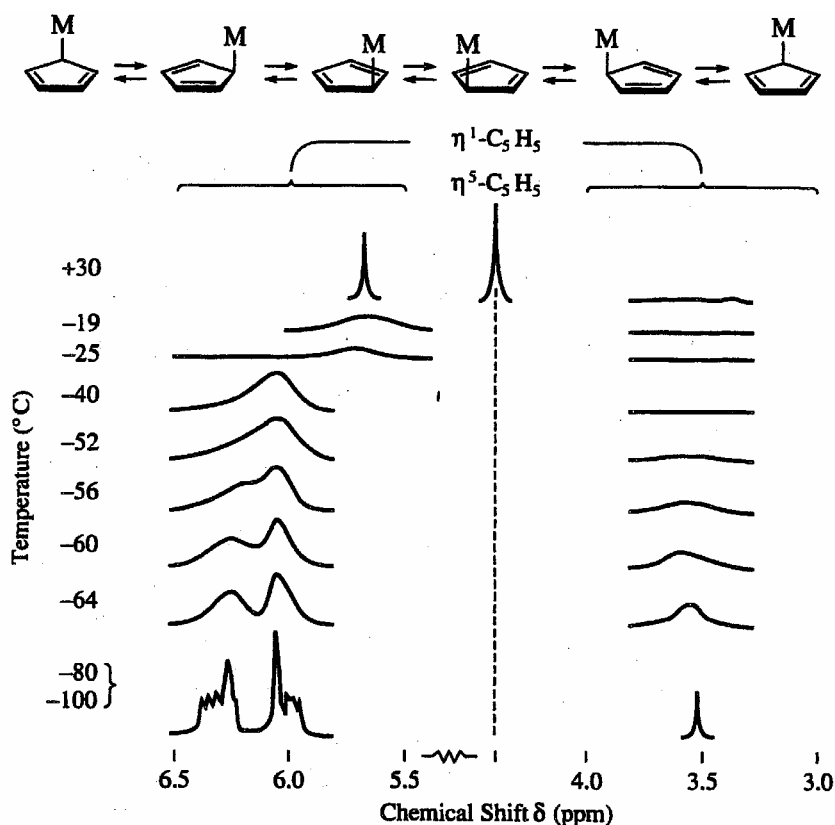


As T is raised, the rate of rotation about the bond increases. Instead of showing the hydrogens in their original positions, the NMR now shows the peaks beginning to **merge** or "**coalesce**".



At **high T**, the rate of rotation about the bond becomes so rapid that the NMR can no longer distinguish the individual environments of the hydrogens; instead, it now shows a simple signal corresponding to the average of the two original signals.

Molecular rearrangement processes.



"Ring whizzer" mechanism and variable-temperature ^1H NMR spectra of $(\eta^5\text{-C}_5\text{H}_5)\text{Fe}(\text{CO})_2(\eta^1\text{-C}_5\text{H}_5)$.