

The cyclooctadiene ligand in [IrCl(COD)]₂ is hydrogenated under transfer hydrogenation conditions: a study in the presence of PPh₃ and a strong base in isopropanol

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SUPPORTING INFORMATION

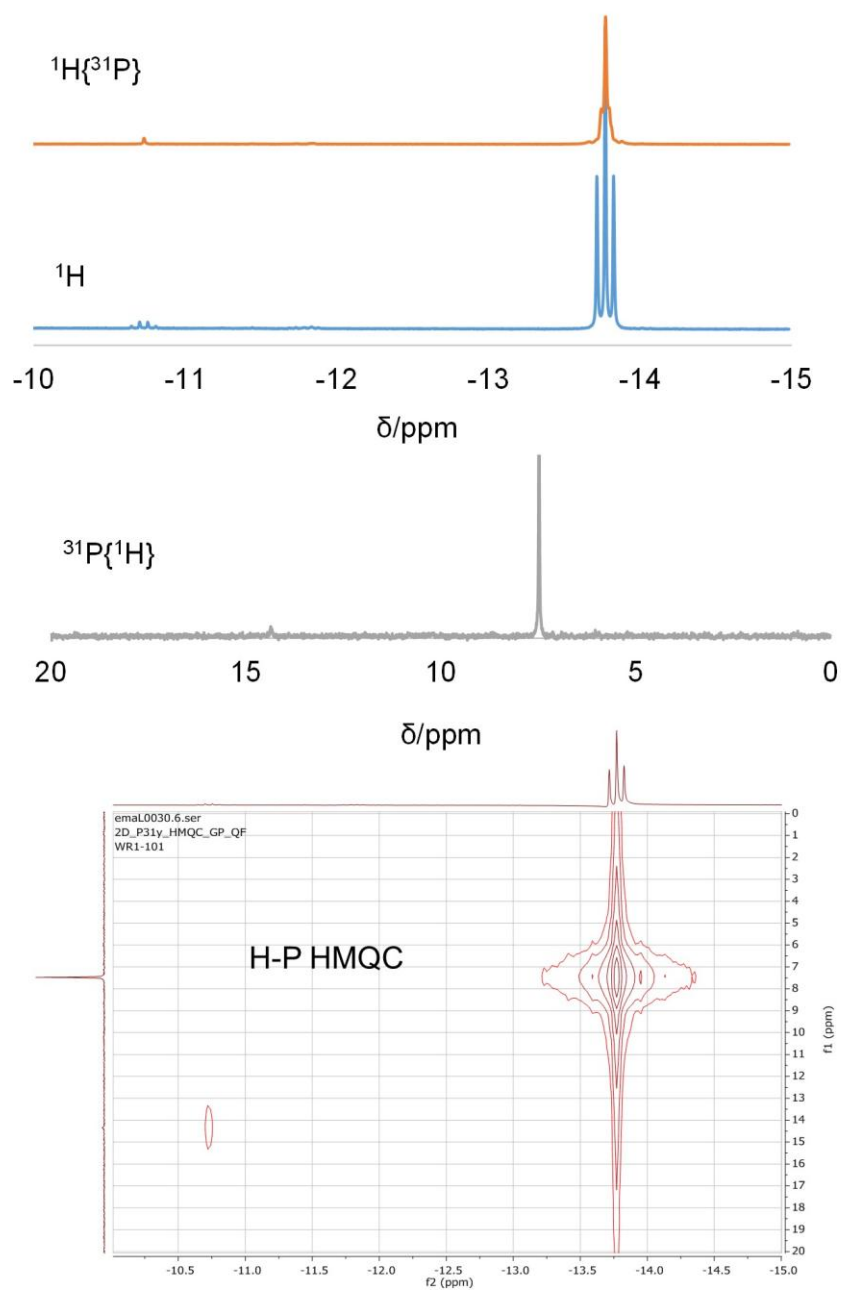


Figure 1S. NMR characterization of the $[\text{IrCl}(\text{COD})]_2/\text{PPh}_3(4 \text{ equiv})/\text{KO}t\text{Bu}$ reaction in isopropanol at room temperature. The solution was evaporated to dryness and redissolved in CDCl_3 .

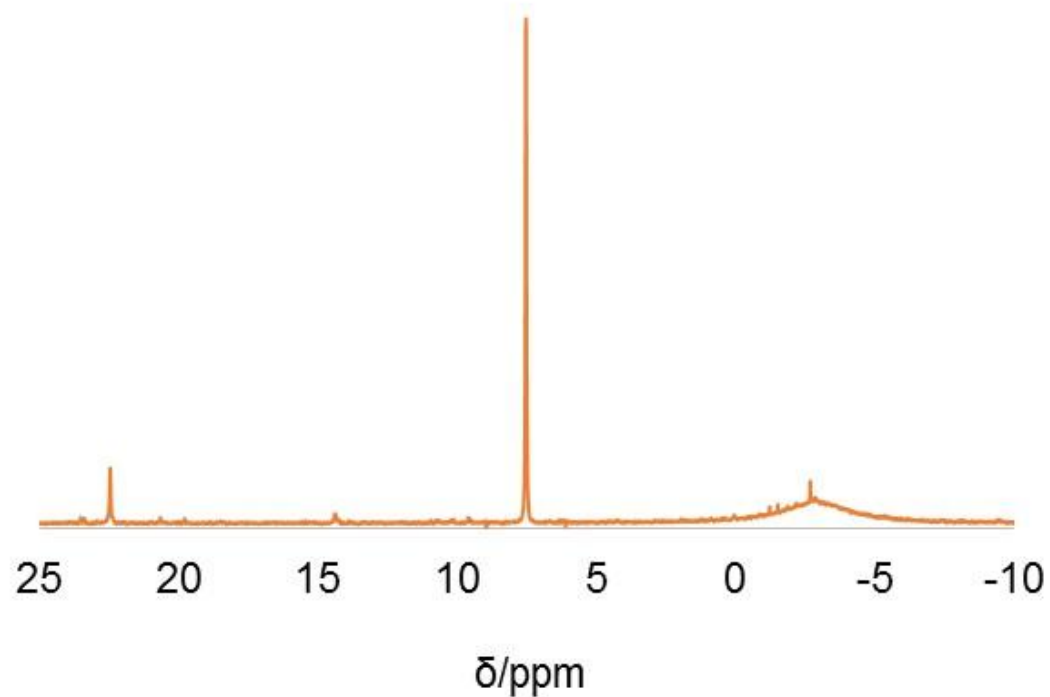
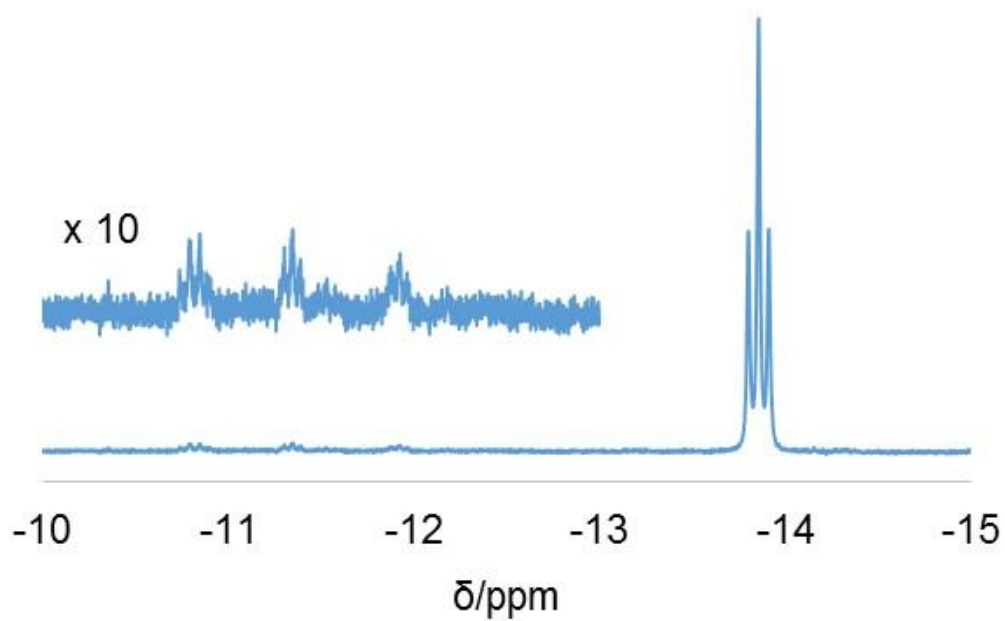


Figure 2S. ^1H (above) and $^{31}\text{P}\{^1\text{H}\}$ (below) NMR spectra of the solution obtained from $[\text{IrCl}(\text{COD})]_2$, PPh_3 (10 equiv.) and $\text{KO}t\text{Bu}$ (10 equiv.) in $i\text{PrOH}$. The solution was evaporated to dryness and redissolved in CDCl_3 .

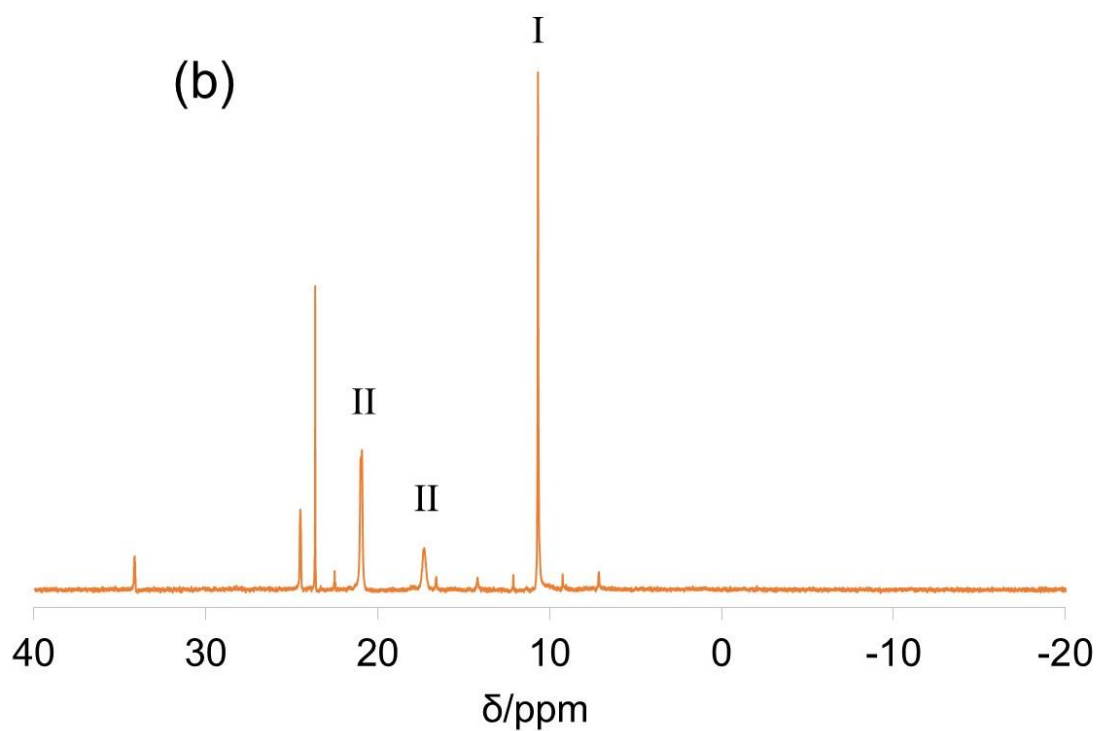
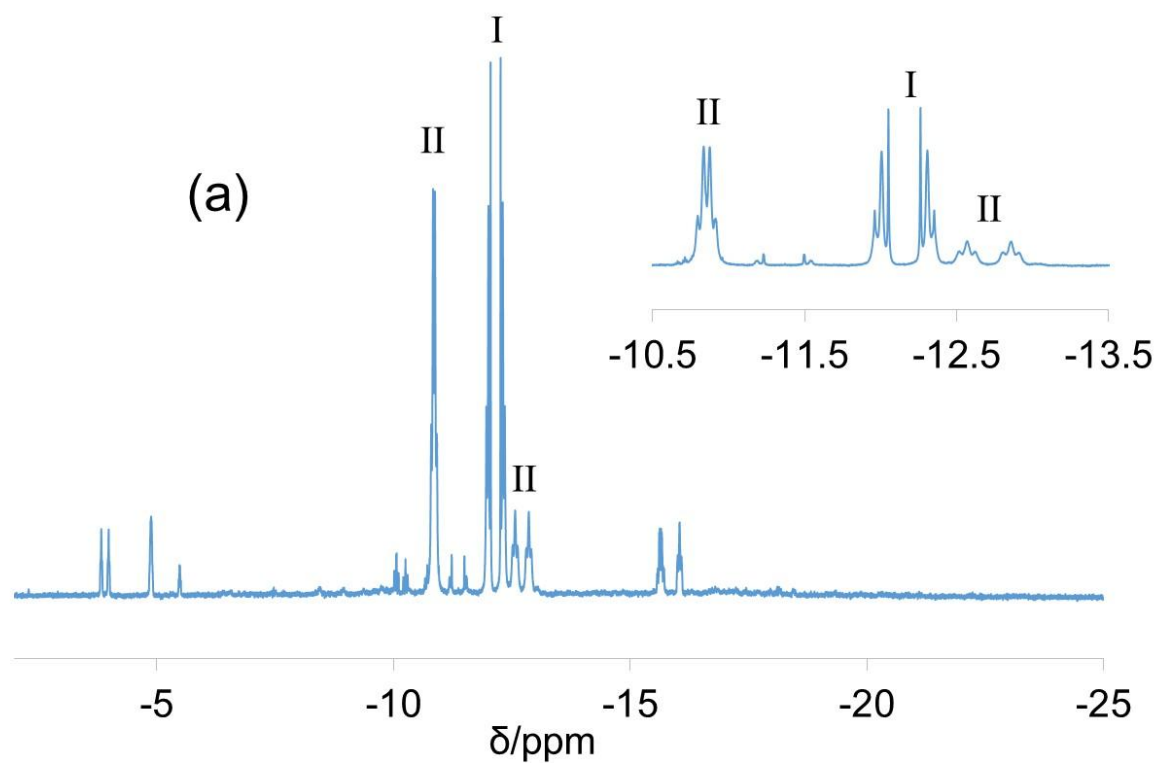


Figure 3S. ^1H NMR in the hydride region (above) and $^{31}\text{P}\{^1\text{H}\}$ (below) spectra of the product mixture from the reaction between $[\text{IrCl}(\text{COD})]_2$, PPh_3 (4 equiv) and excess NaOMe in boiling *i*PrOH for 3 h. The spectra were taken on the dried residue redissolved in $\text{THF-}d_8$.

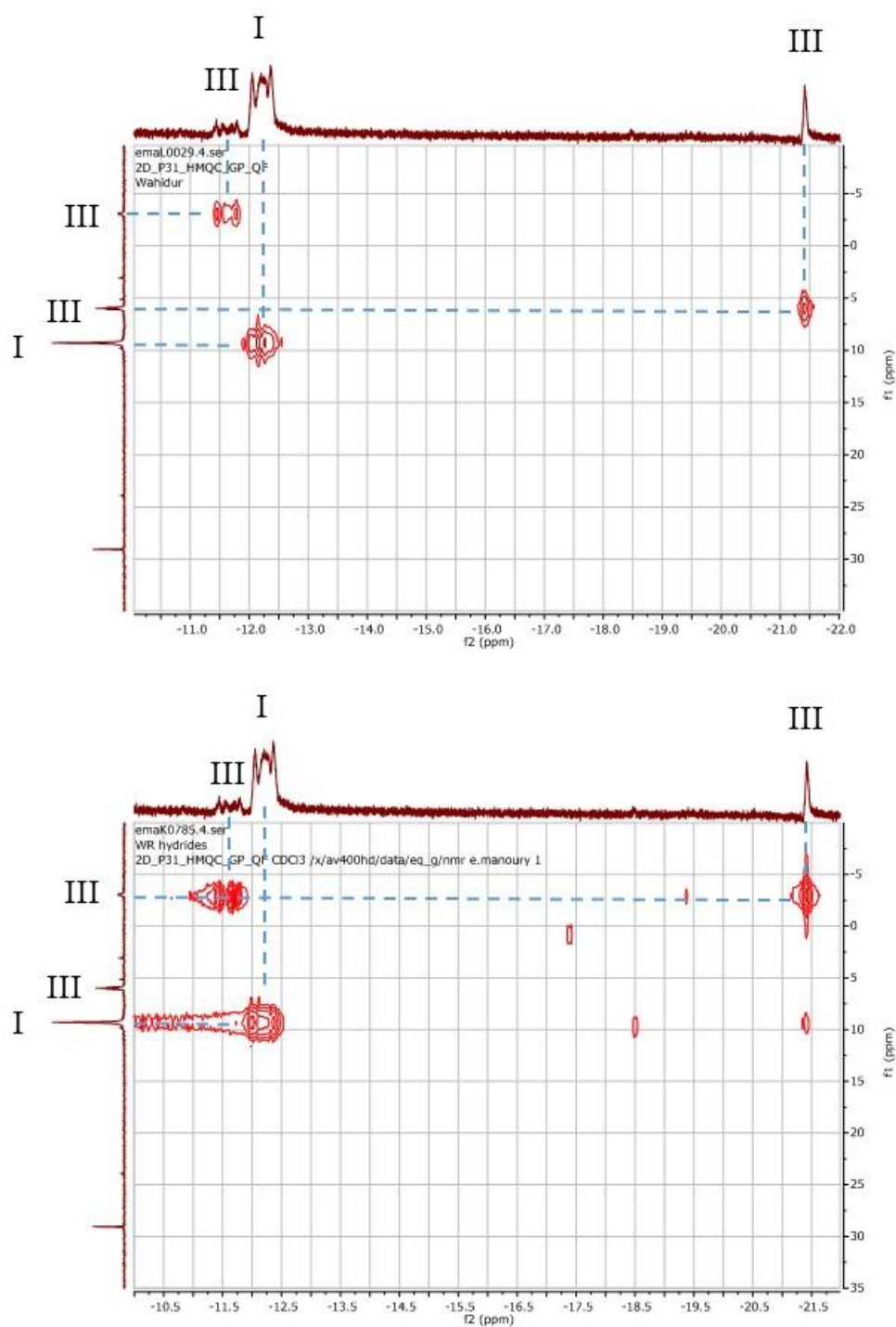


Figure 4S. ^1H - ^{31}P HMQC spectra (expansion of the ^1H hydride region) for the isolated product of the $[\text{IrCl}(\text{COD})]_2/4\text{PPh}_3/\text{KO}t\text{Bu}$ reaction in boiling isopropanol (solvent = CDCl_3). The delay was optimized for a J coupling of 5 Hz (above) or 10 Hz (below).

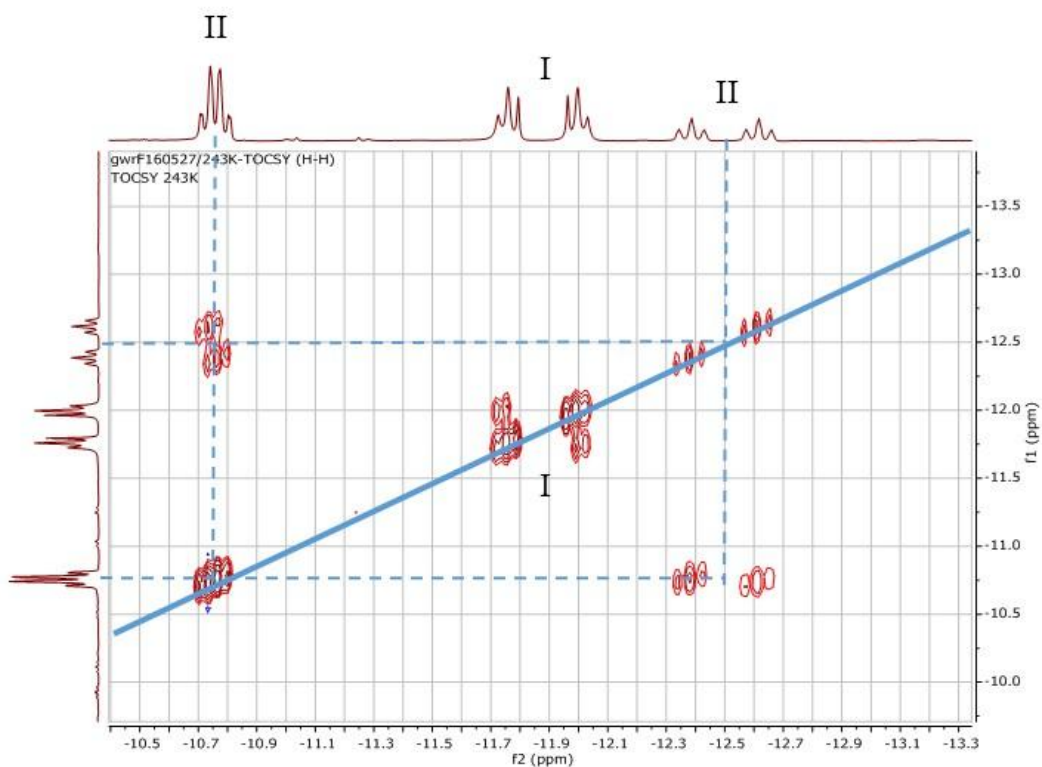
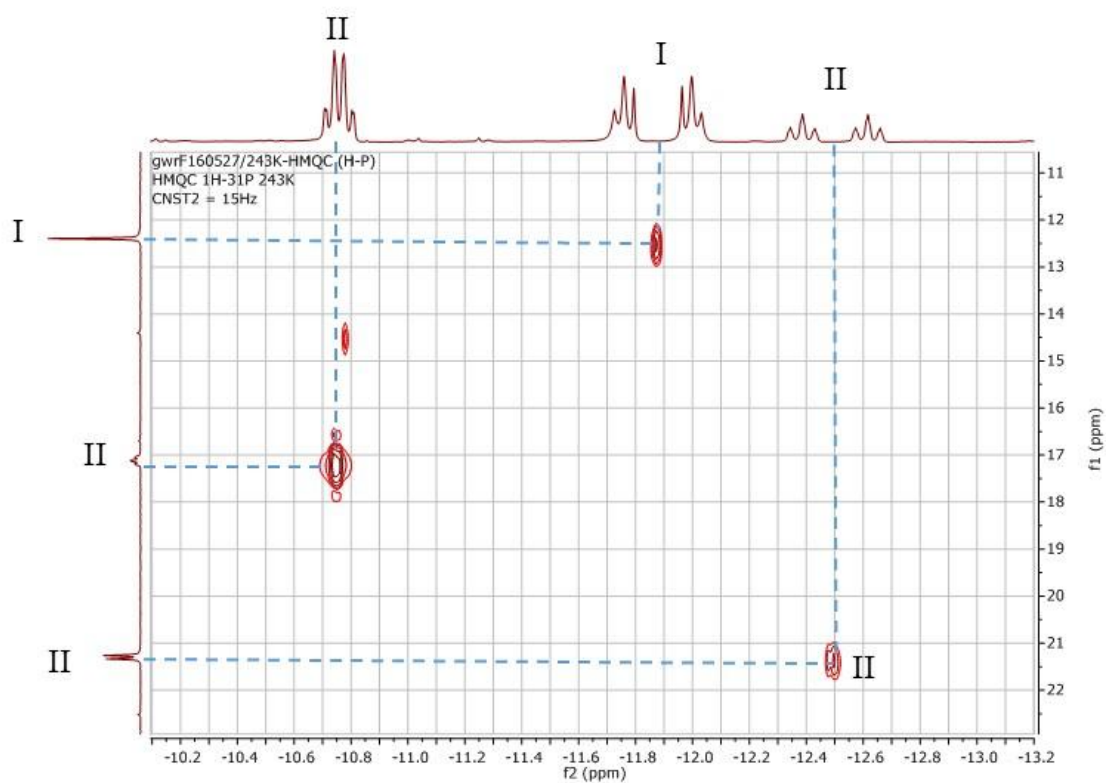


Figure 5S. ^1H - ^{31}P HMQC (above) and ^1H COSY (below) spectra (expansion of the ^1H hydride region) for the product mixture from the reaction between $[\text{IrCl}(\text{COD})]_2$, PPh_3 (4 equiv) and excess NaOMe in boiling *i*PrOH for 3 h. The spectra were taken on the dried residue redissolved in $\text{THF-}d_8$.

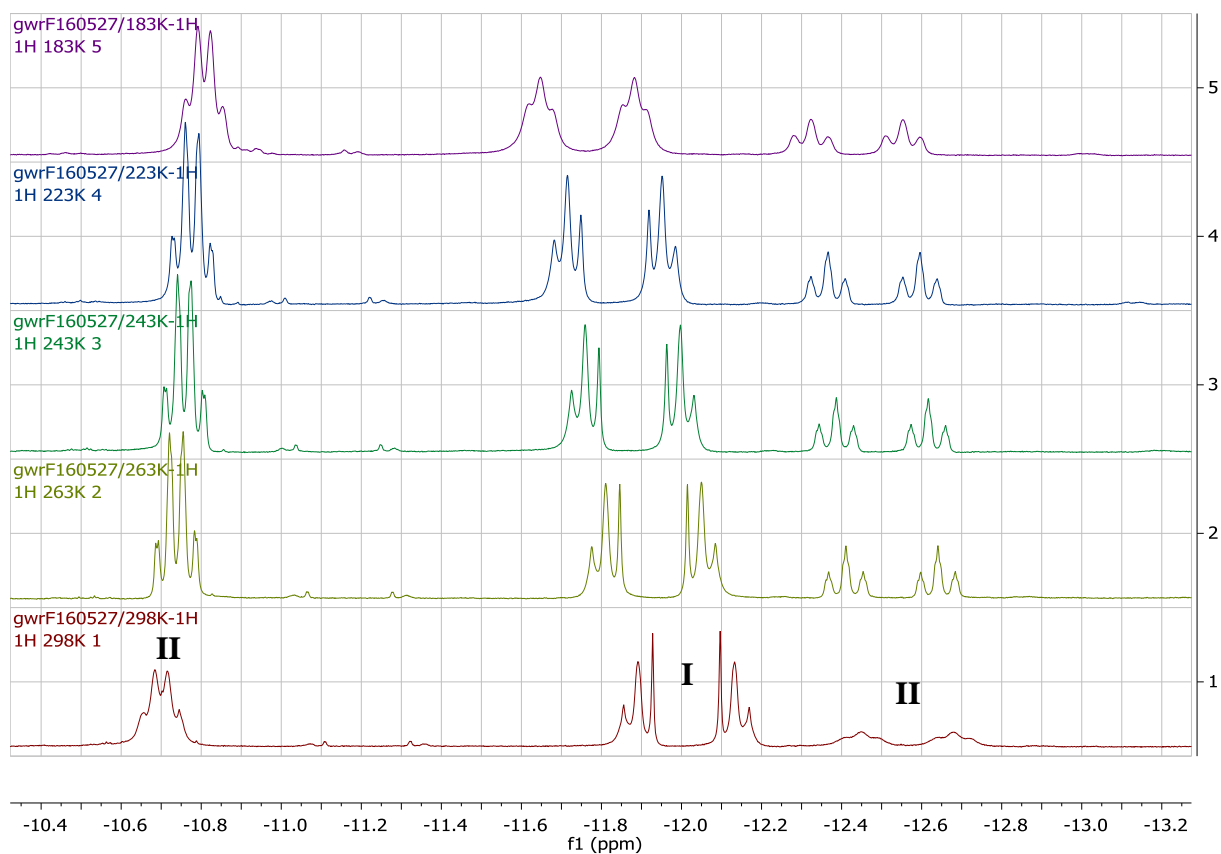


Figure 6S. Detail of the hydride region showing compounds **I** and **II** in THF- d_8 solution at different temperatures. The sample is the same one giving the spectra shown in Figures 3S and 5S.

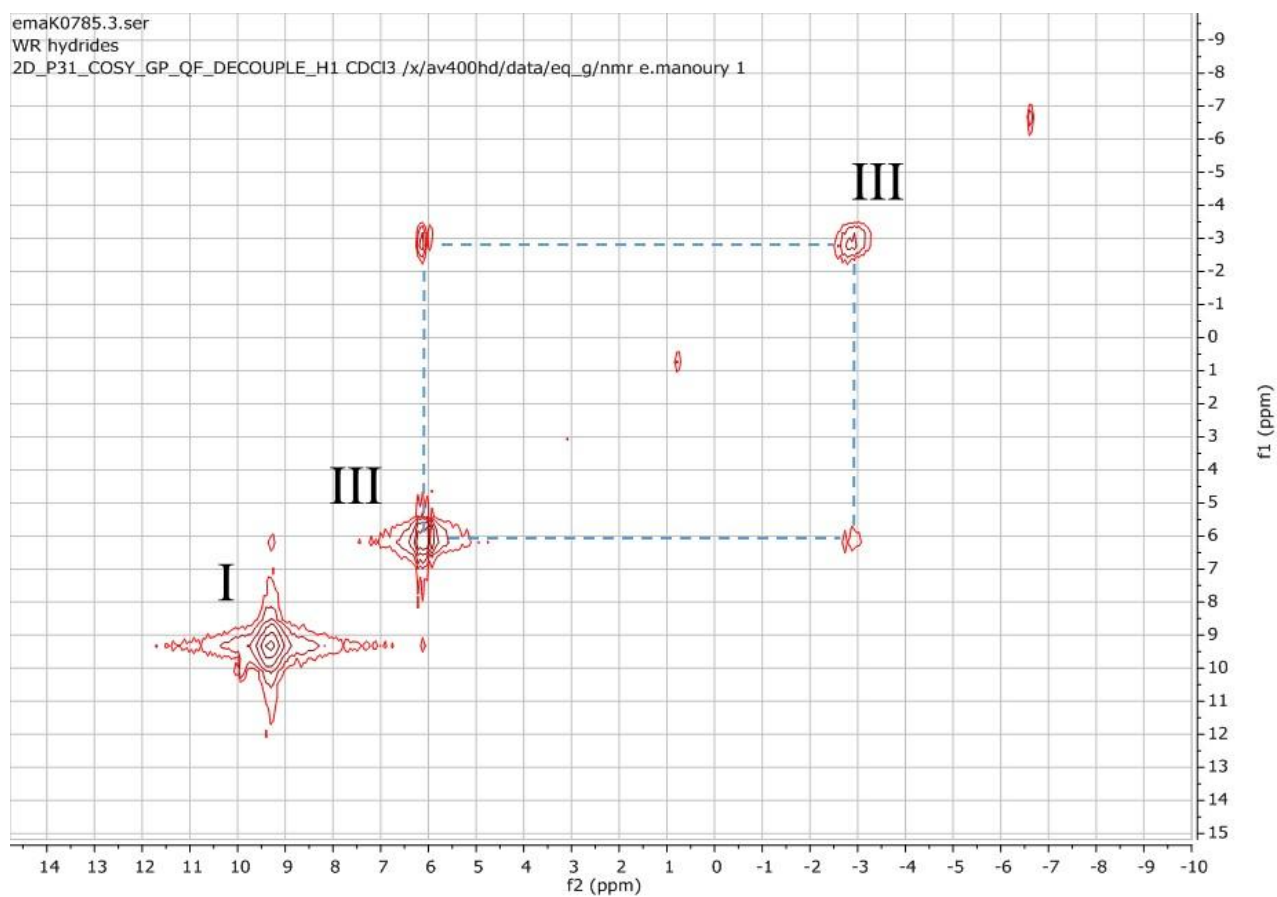


Figure 7S. ^{31}P COSY NMR properties of the minor product **III**. The sample is the same one giving the spectra shown in Figure 4 of the main article.