Supporting information

Double C-H Activation Results in Ru Complexes of a Neutral PCP Ligand With a Central Carbene Moiety

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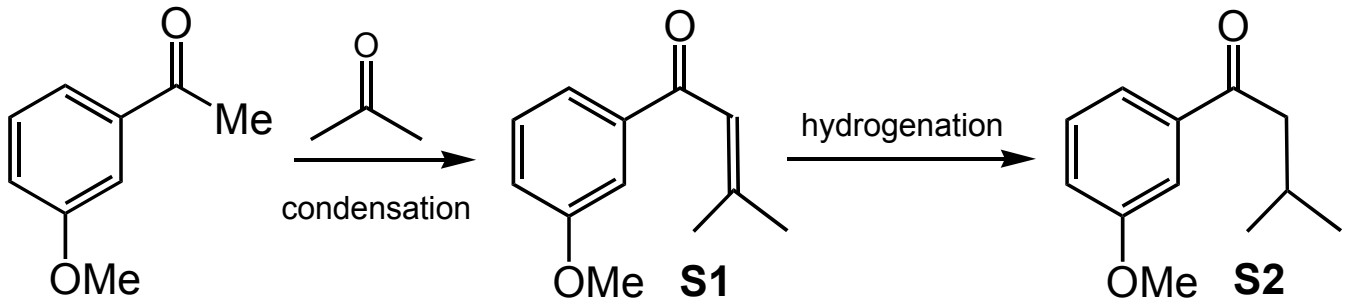
Formation of (3-methoxyphenyl)isobutylketone (S2). When 3-methoxyacetophenone (entry 4 in Table 1) was used as substrate in transfer hydrogenation, a small amount (4%) of compound **S2** was also isolated by chromatography. **S2** is likely the hydrogenation product of the α,β-unsaturated ketone **S1** (unobserved) which may be formed from the condensation of 3-methoxyacetophenone and the isopropanol-derived acetone (Scheme S1).

Scheme S1



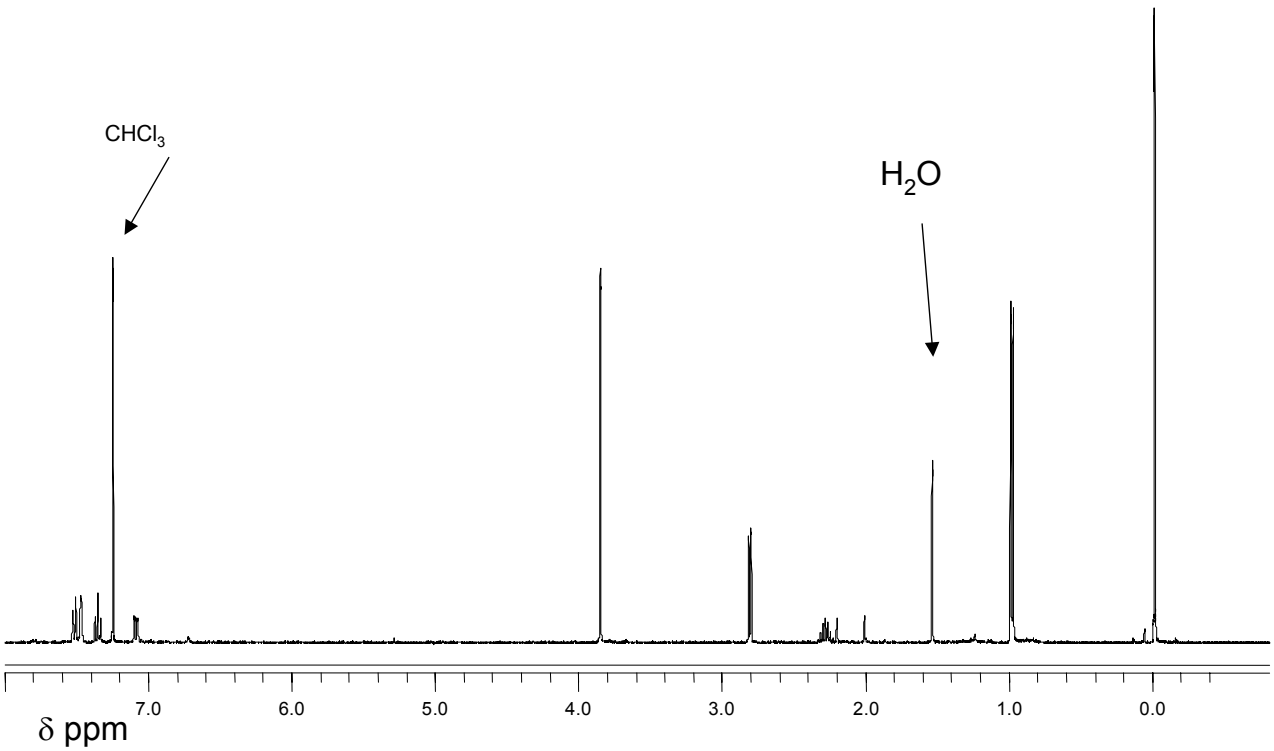


Figure S1. ^{1}H NMR spectrum of **S2** in $CDCl_3$ (silicon grease impurity at ca. δ 0 ppm).

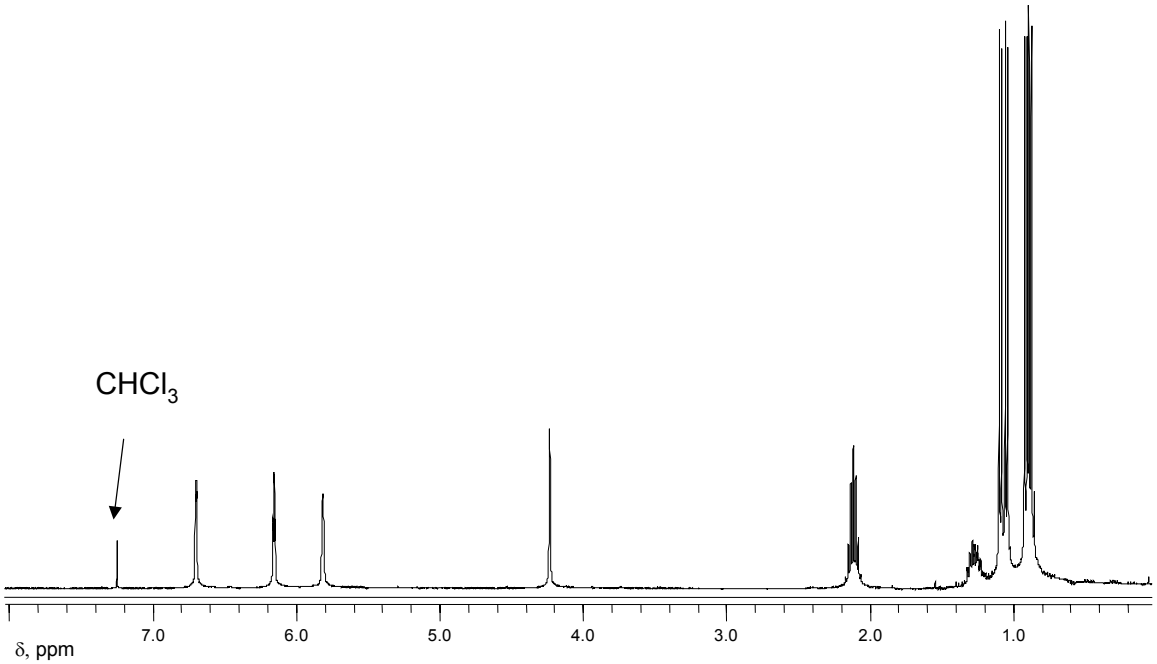


Figure S2. ^{1}H NMR spectrum of P_2CH_2 (**1**) in $CDCl_3$ (traces of pentane present).

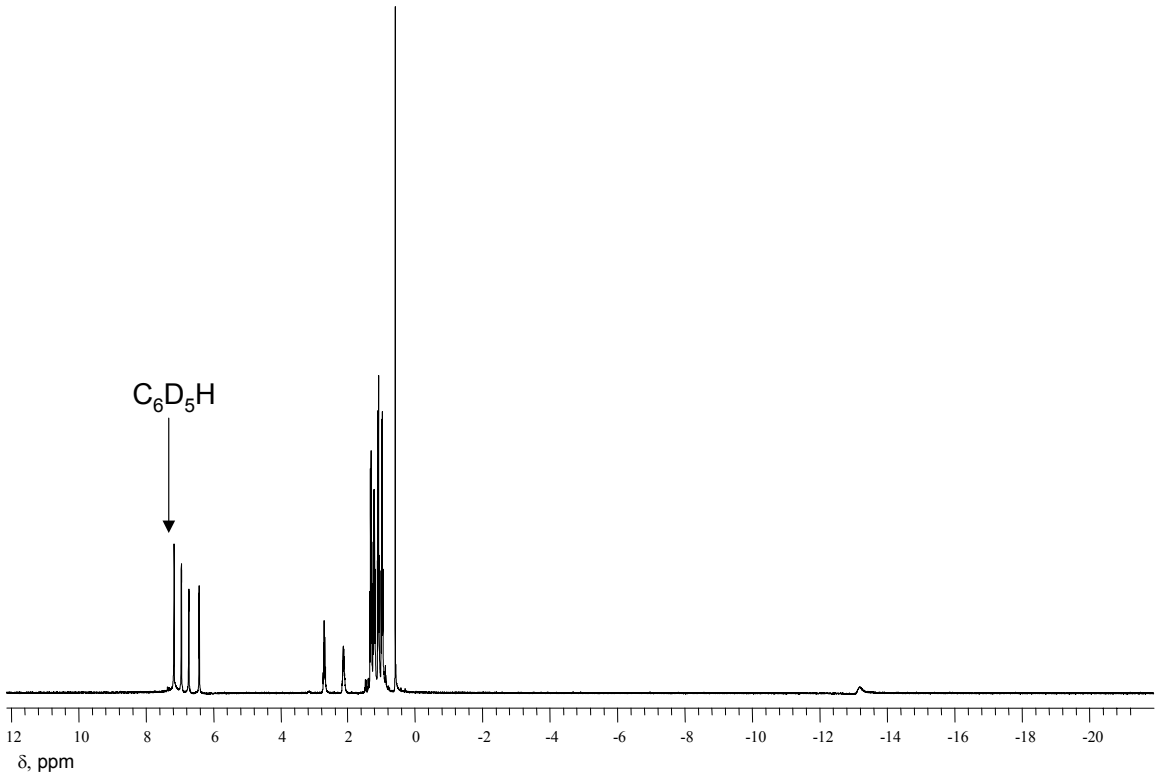


Figure S3. ^{1}H NMR spectrum of (P_2C=)RuHCl(NCMe) (**3**) in C_6D_6.

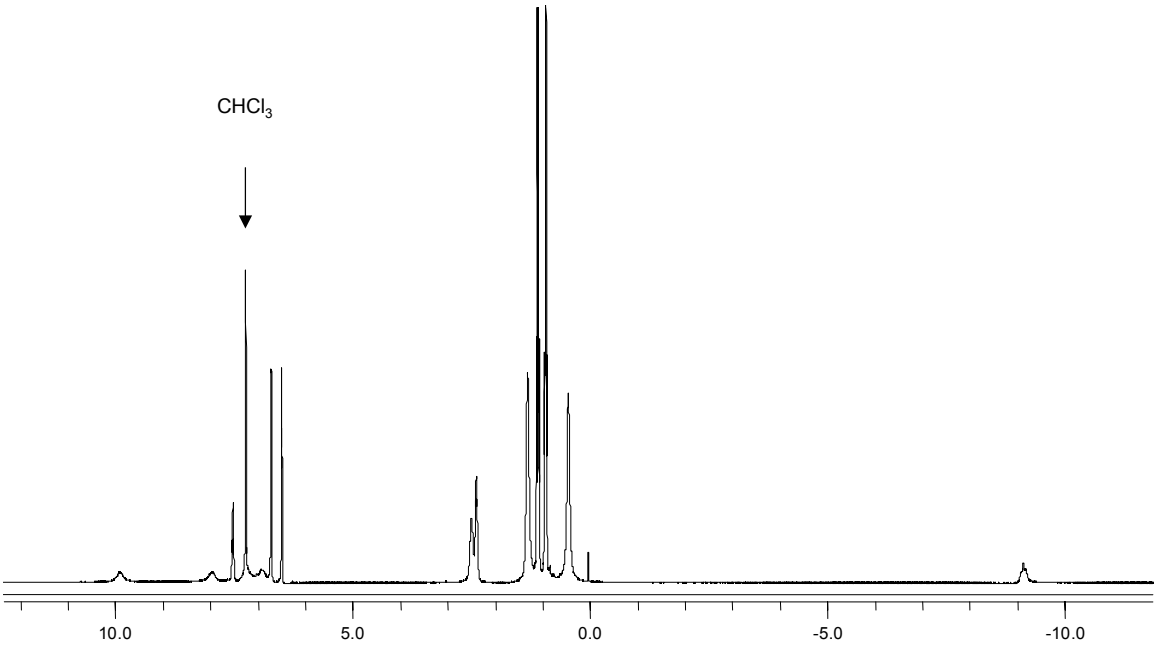


Figure S4. ^{1}H NMR spectrum of (P_2C=)RuHCl(py) (**4**) in C_6D_6.

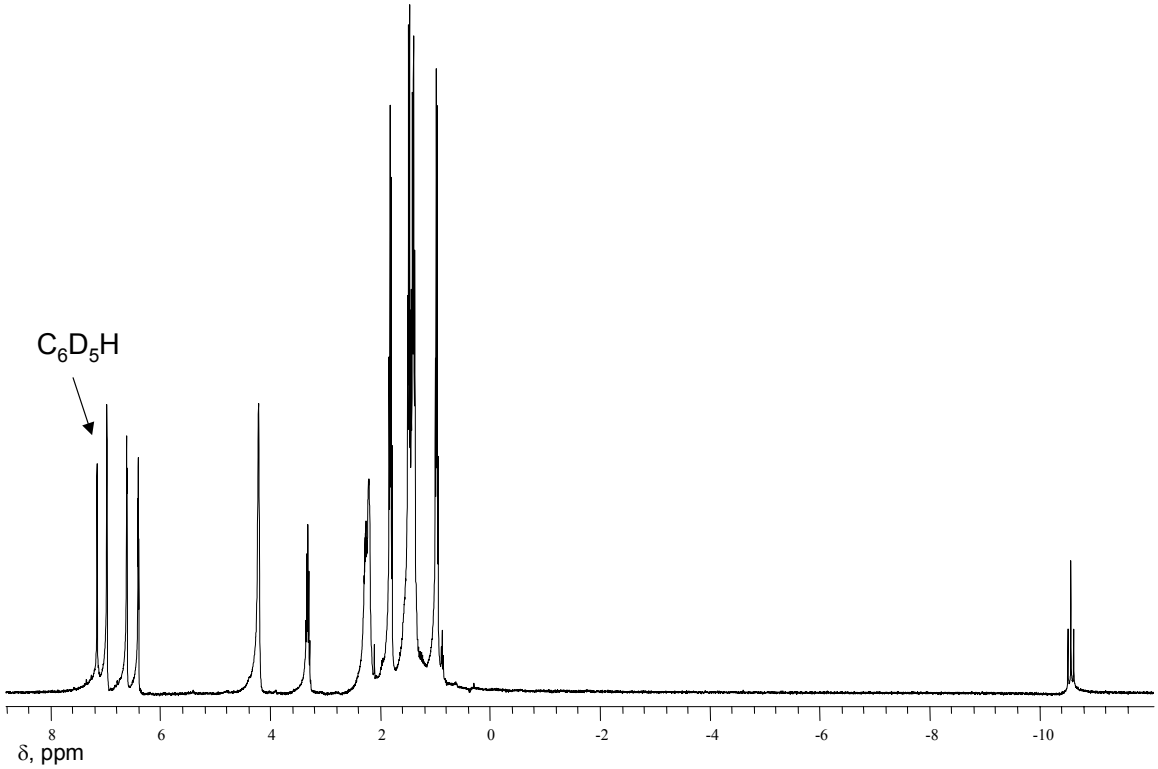


Figure S5. ^{1}H NMR spectrum of (P_2C=)RuH(μ-Cl)$_2$Rh(COD) (**6**) in C_6D_6.

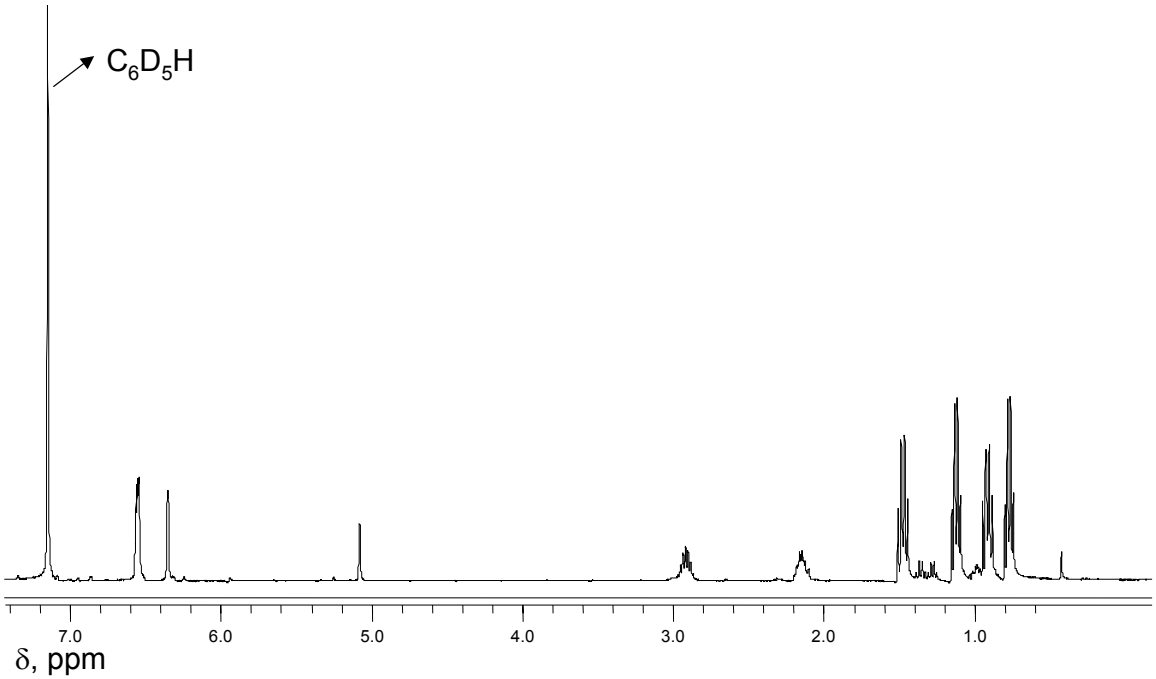


Figure S6. ^{1}H NMR spectrum of $(P_2CH)RuCl(CO)_2$ (**7a/b**) in C_6D_6.

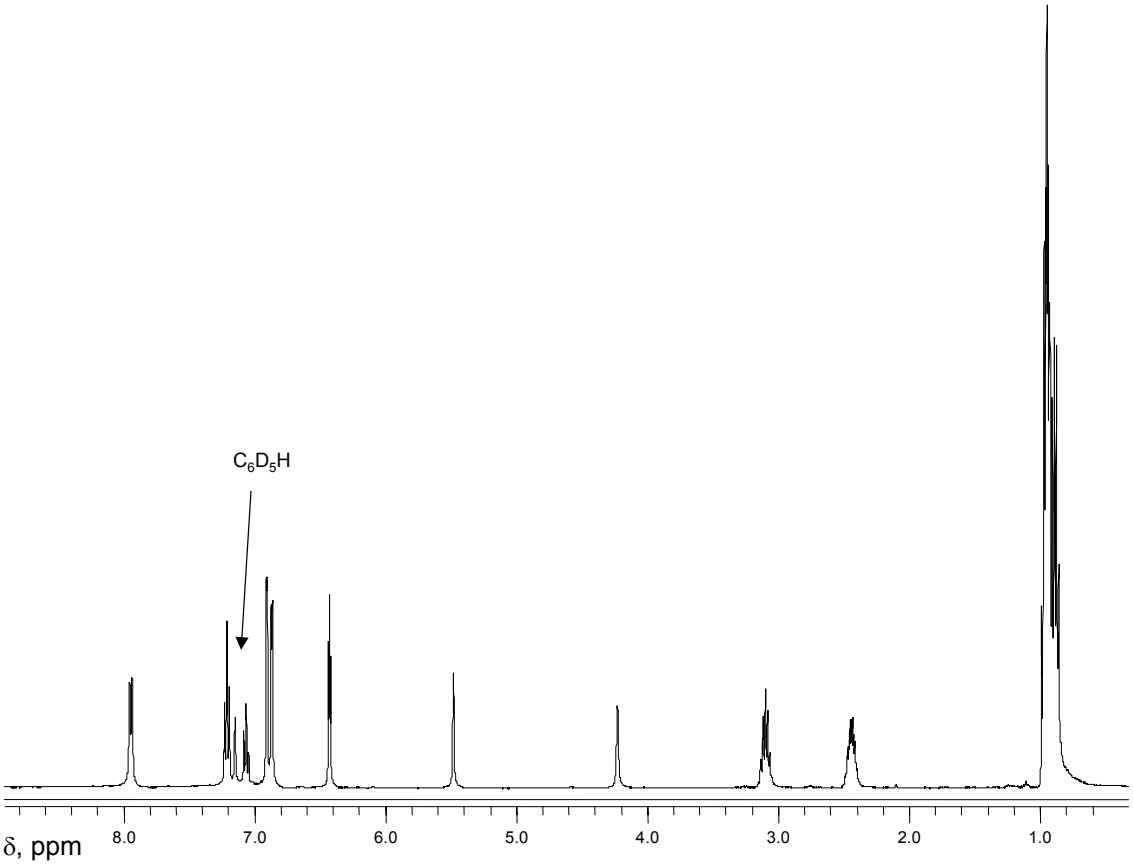


Figure S7. ^{1}H NMR spectrum of (P_2C=)RuCl(-CPh=CH_2) (**10**) in C_6D_6.

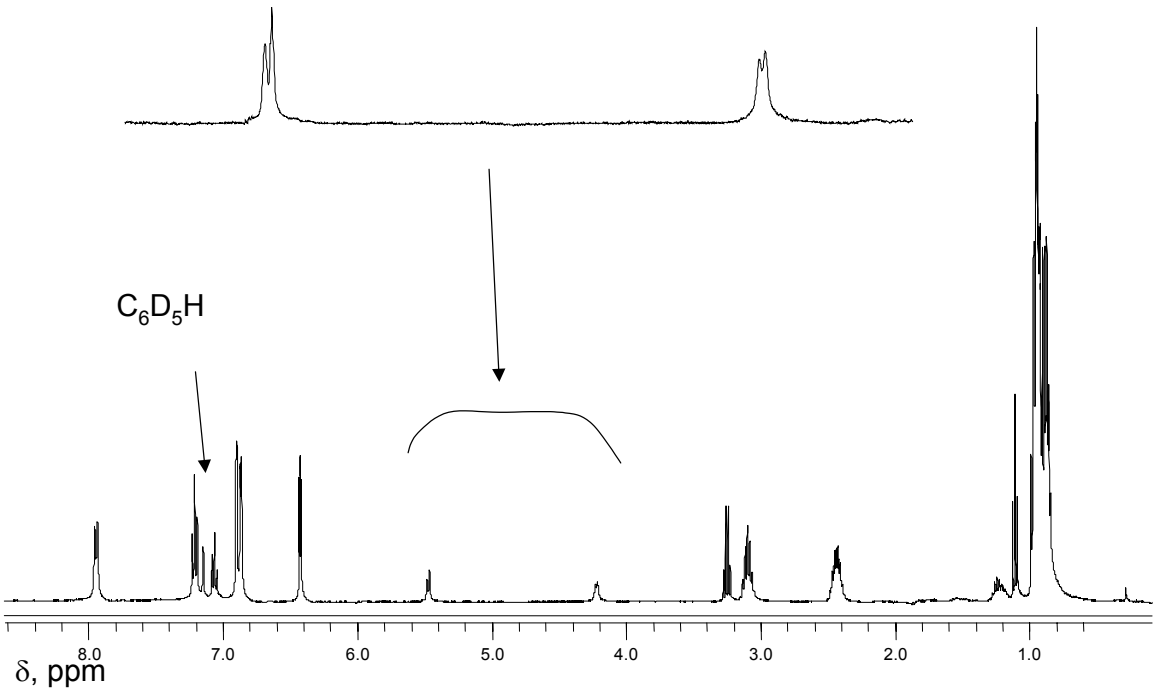


Figure S8. ^{1}H NMR spectrum of 4 isotopomers of $(P_2C=)RuCl(\text{-}CPh=C(H,D)_2)$ (**10**) in C_6D_6.

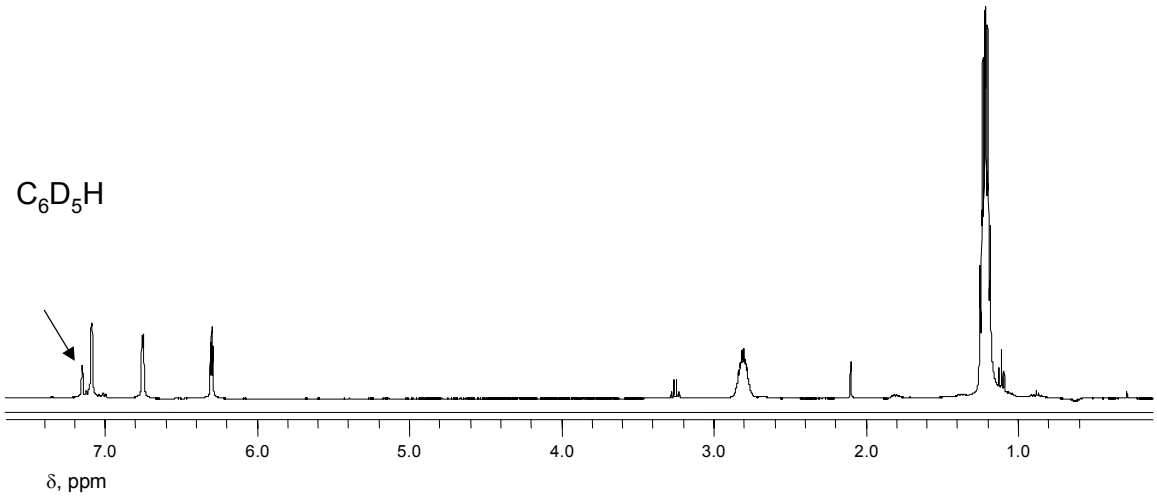


Figure S9. ^{1}H NMR spectrum of $(P_2C=)RuCl_2$ (**12**) in C_6D_6 (traces of toluene, ether present).

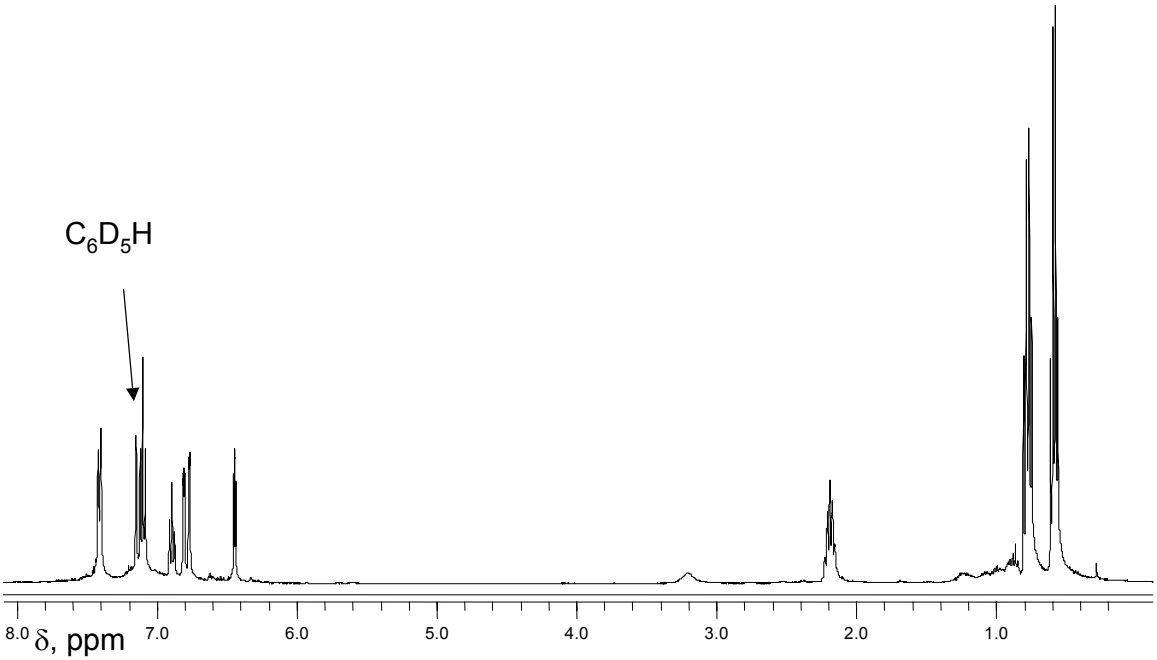


Figure S10. ^{1}H NMR spectrum of (P_2C=)$RuPh_2$ (**13**) in C_6D_6 (traces of toluene, ether present).

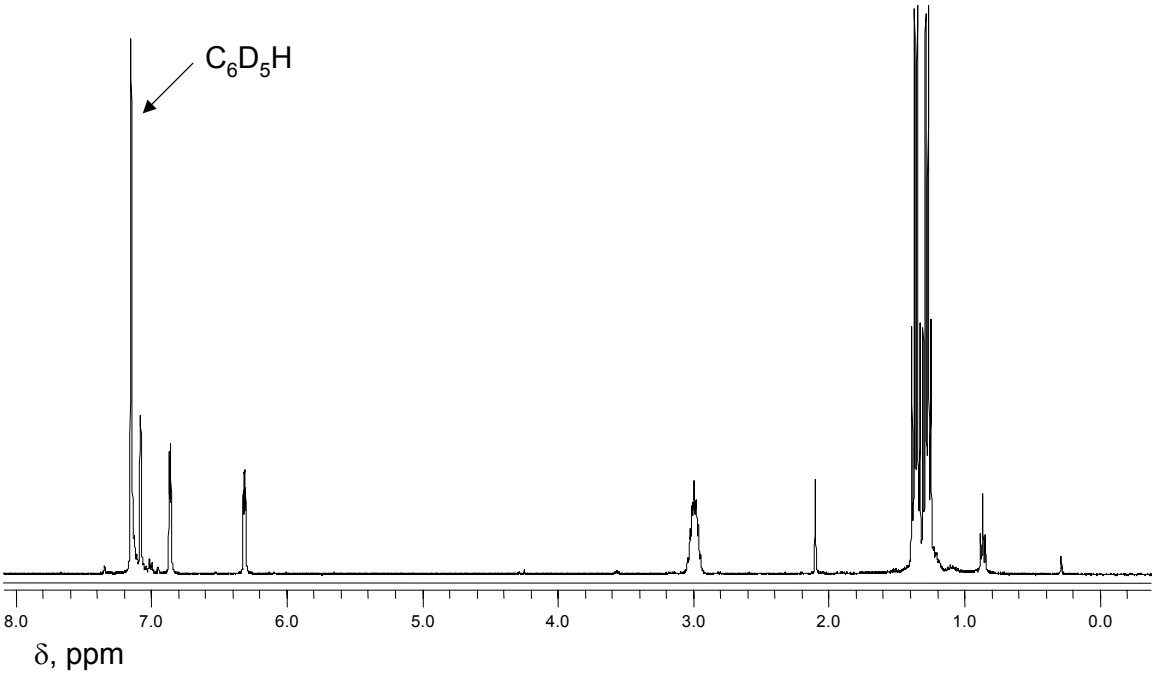


Figure S11. ^{1}H NMR spectrum of *trans*-(P_2C=)$RuCl_2$(CO) (**14a**) in C_6D_6 (traces of toluene, pentane, grease present).

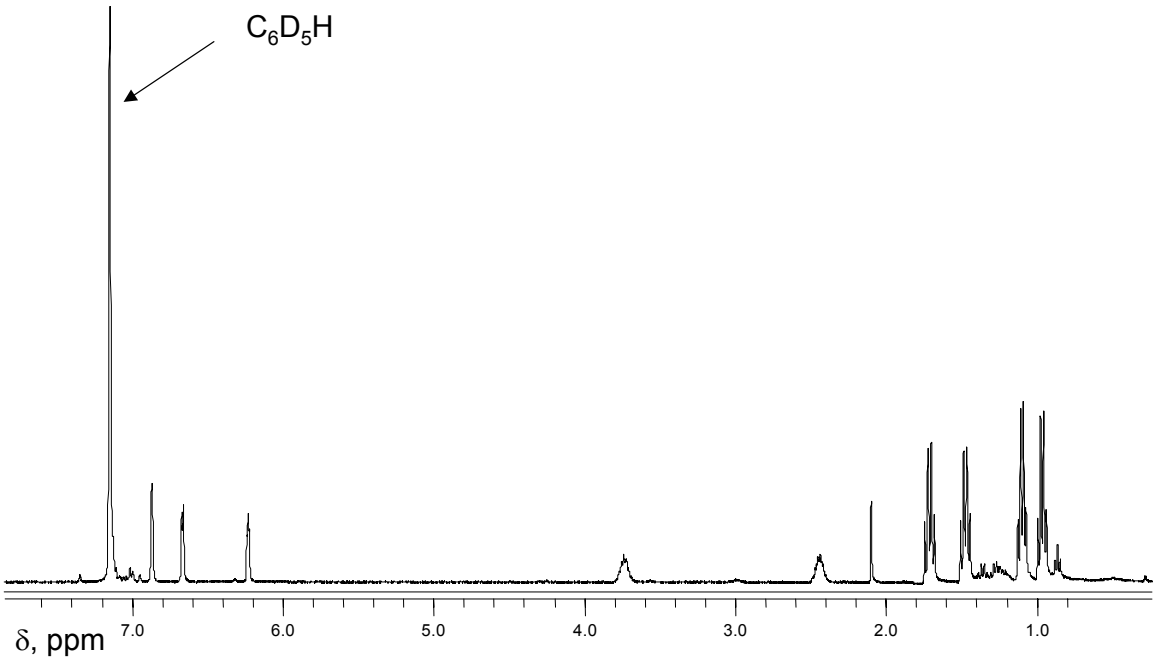


Figure S12. ^{1}H NMR spectrum of *cis*-(P_2C=)$RuCl_2$(CO) (**14b**) in C_6D_6 (8% of **14a** and traces of toluene, ether present).