

η^6 -Coordinated Ruthenabenzenes from Three-Component Assembly on a Diruthenium μ -Allenyl Scaffold

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Supporting Information

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Figure S1. DFT optimized structure of $[2]^+$ and selected Hirshfeld charges (a.u.) in parenthesis. Hydrogen atoms, with the exception of the hydroxyl moiety, are omitted for clarity. Colour map: Ru, green; C, grey; O, red; H, white. Selected computed bond lengths (Å): Ru1-C6 2.046, C1-C7 1.428, C7-C1 1.432, C1-C2 1.425, C2-C5 1.438, C5-Ru1 2.005, Ru1---Ru2 2.754, Ru2-C6 2.151, Ru2-C1 2.195, Ru2-C2 2.219, Ru2-C5 2.186, C5-O 1.347.

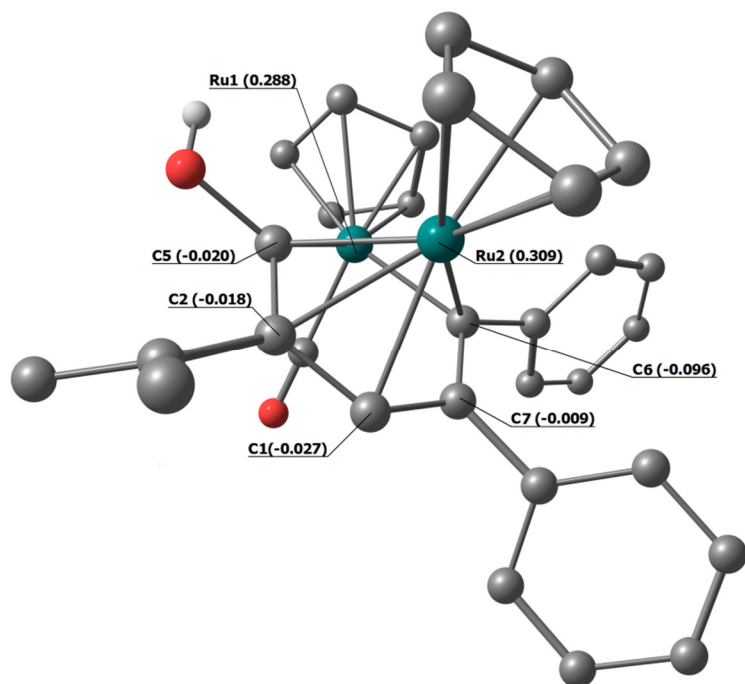


Table S1. Density (ρ) and potential energy density (V) values (a.u.) for selected b.c.p. in $[2]^+$.

Bond	ρ	V
Ru2-C1	0.094	-0.114
Ru2-C3	0.082	-0.103
Ru2-C4	0.080	-0.097
Ru2-C5	0.089	-0.102

Figure S2. DFT optimized structures of $[\text{Ru}_2\text{Cp}^*_2(\text{SiMe}_3)(\mu\text{-}\eta^2\text{:}\eta^5\text{-C}_5\text{H}_5)]$ (a) and $[\text{Ru}_3(\text{CO})_9\{\mu_3\text{-(FcCCH)}_2\text{CC=CPh}_2\}]$ (b). Hydrogen atoms are omitted for clarity. Colour map: Ru, green; Fe, violet; Si, dark yellow; C, grey; O, red. RDS with respect to X-ray data: 0.049 Å for (a), 0.593 Å for (b).

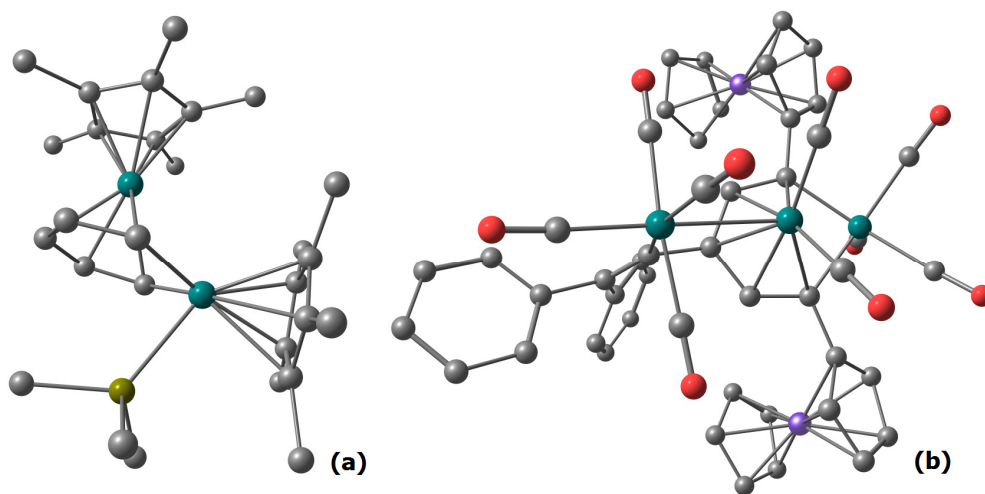


Figure S3. Comparison of DFT-optimized isomers of **5** (structures and relative Gibbs free energy). Hydrogen atoms, with the exception of the ruthenacene moiety, are omitted for clarity. Colour map: Ru, green; C, grey; O, red; H, white.

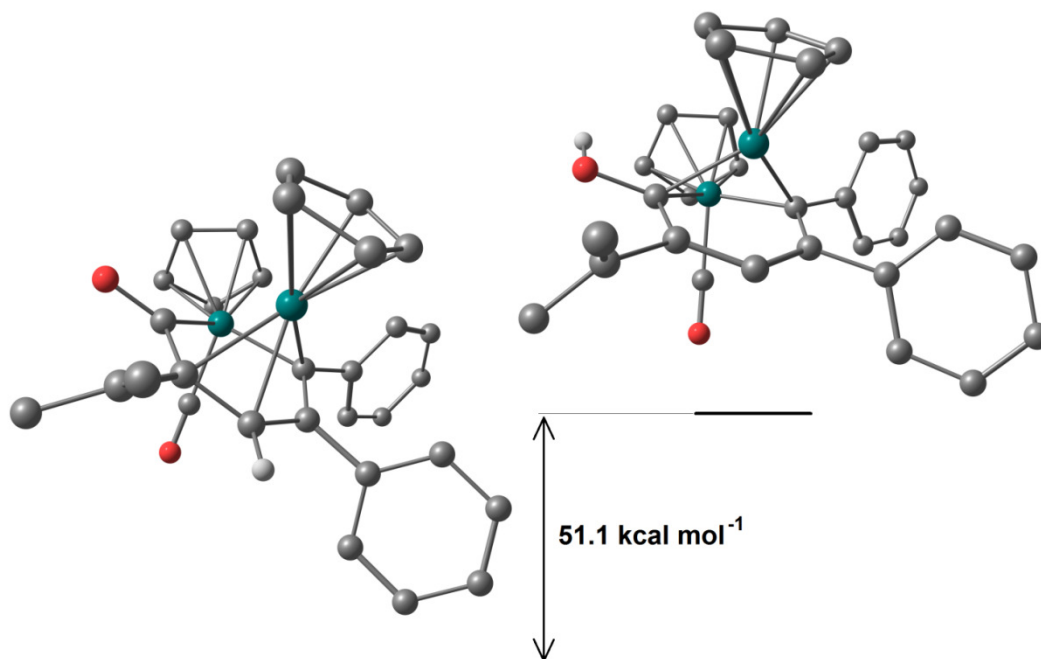


Figure S4. ^1H NMR spectrum (401 MHz, acetone- d_6) of **2**.

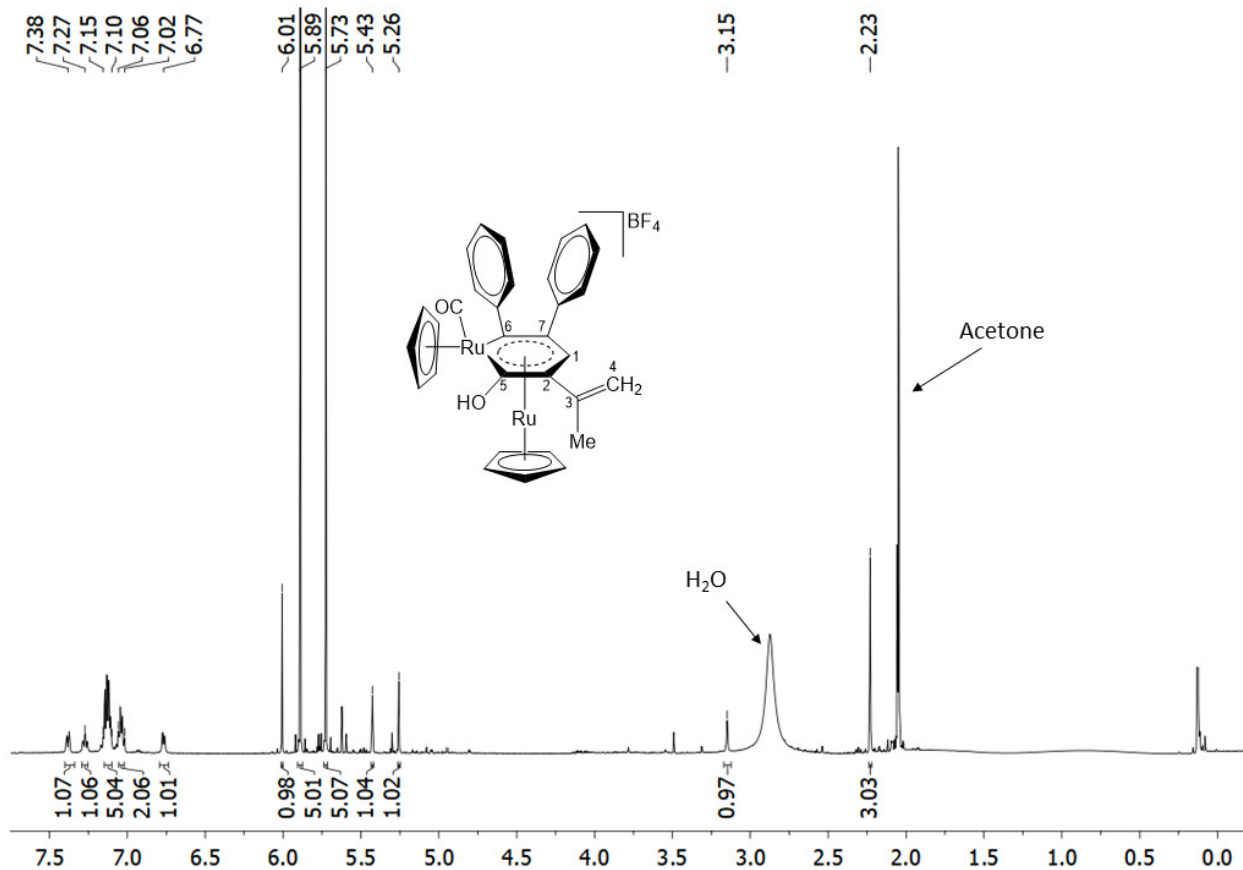


Figure S5. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, acetone- d_6) of **2**.

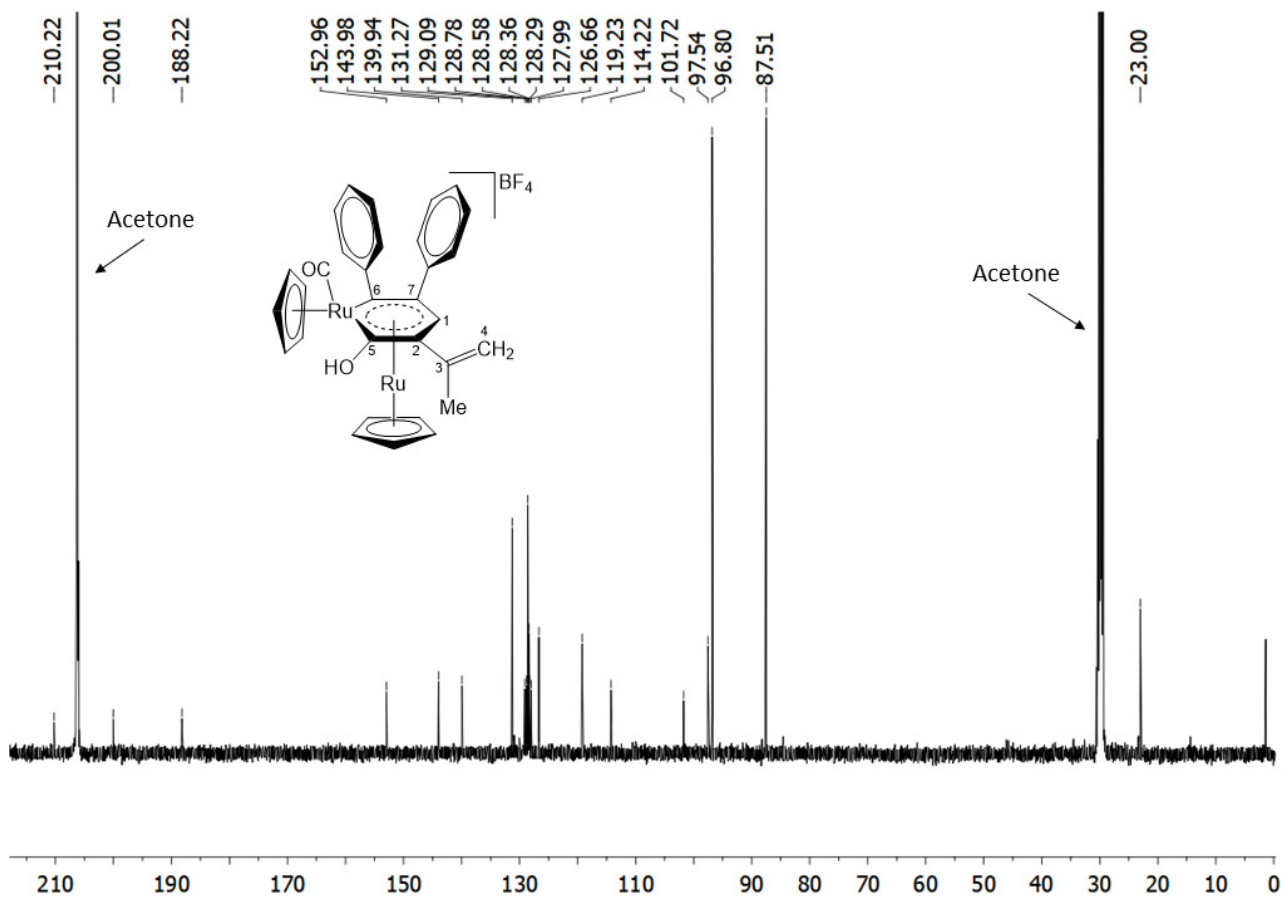


Figure S6. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum (376 MHz, acetone- d_6) of **2**.

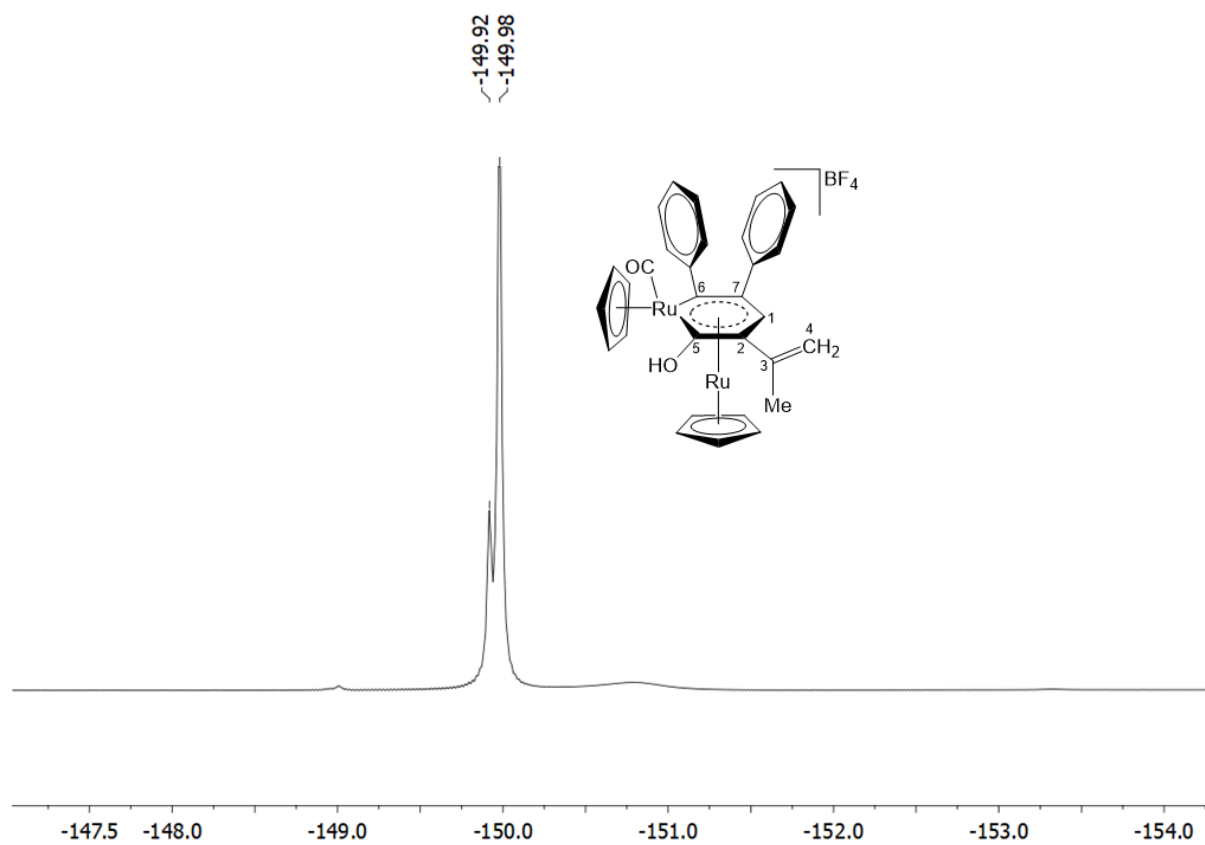


Figure S7. ^1H NMR spectrum (401 MHz, acetone- d_6) of **3**.

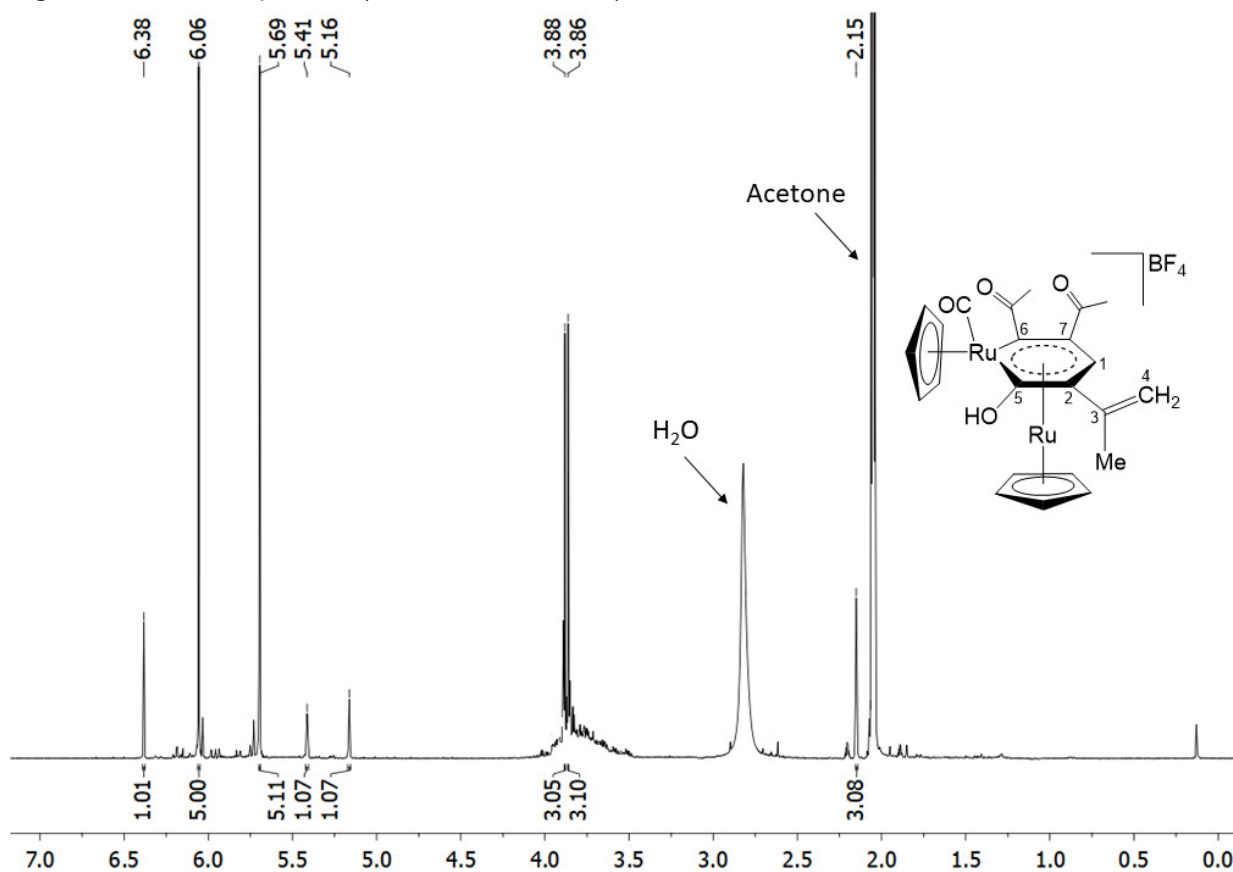


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, acetone- d_6) of **3**.

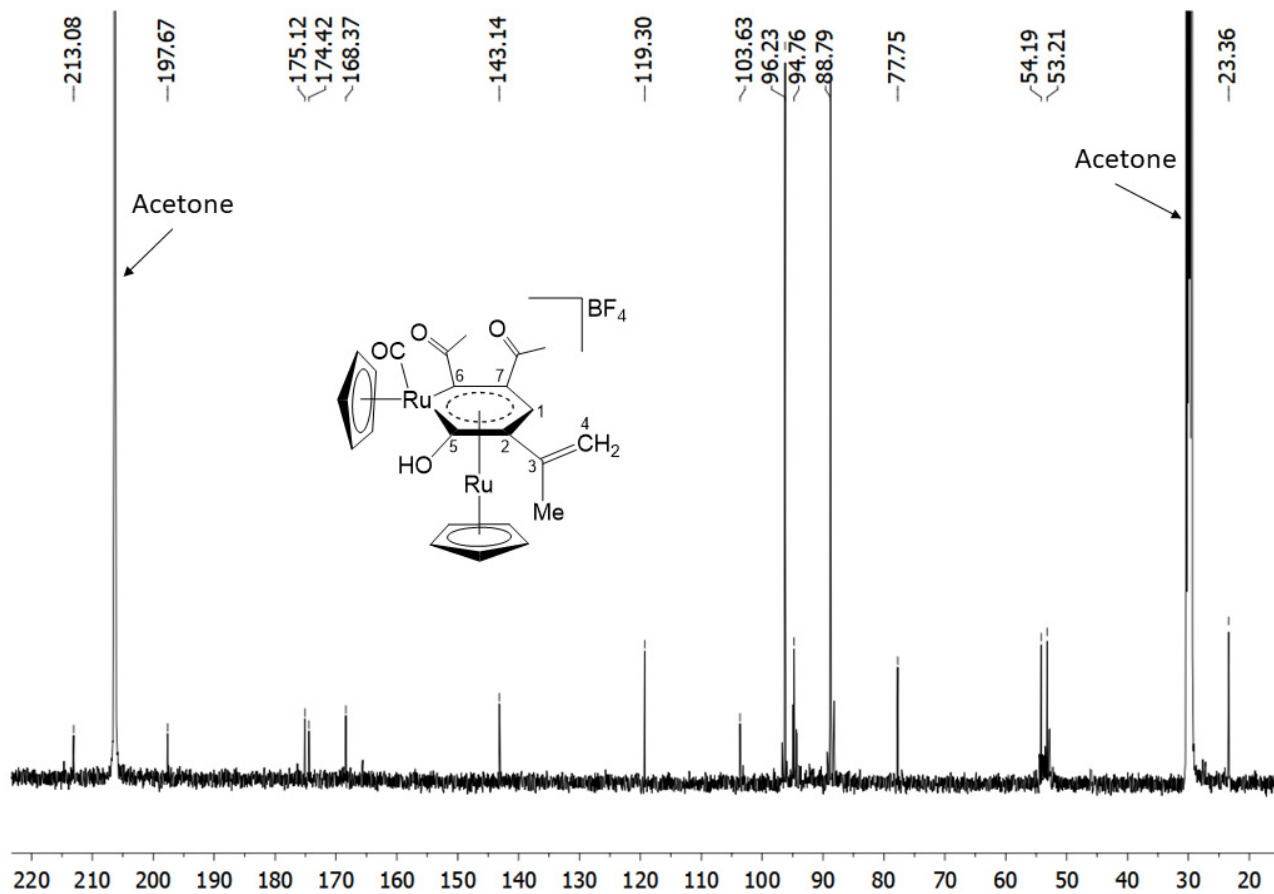


Figure S9. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum (376 MHz, acetone- d_6) of **3**.

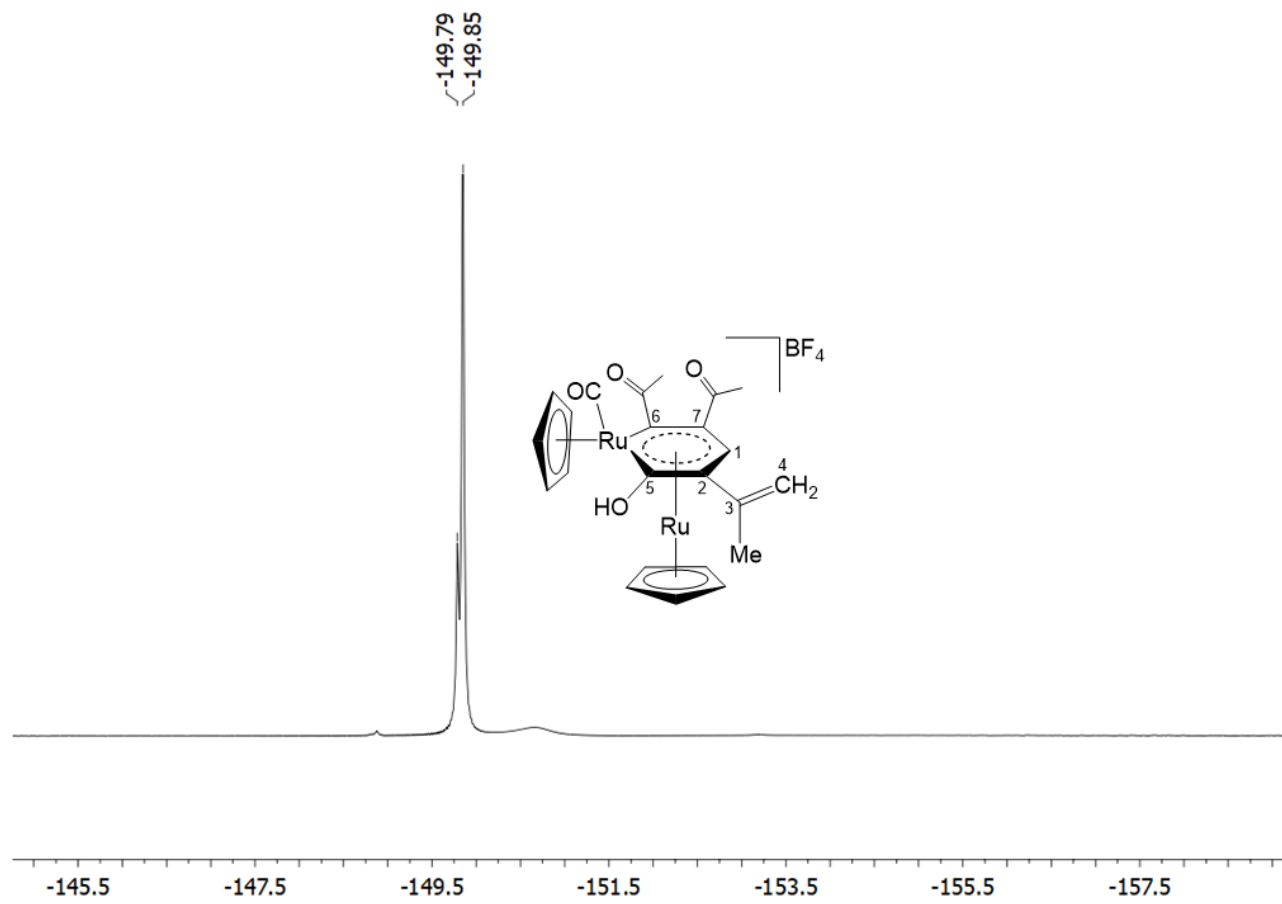


Figure S10. ^1H NMR spectrum (401 MHz, acetone- d_6) of **4**.

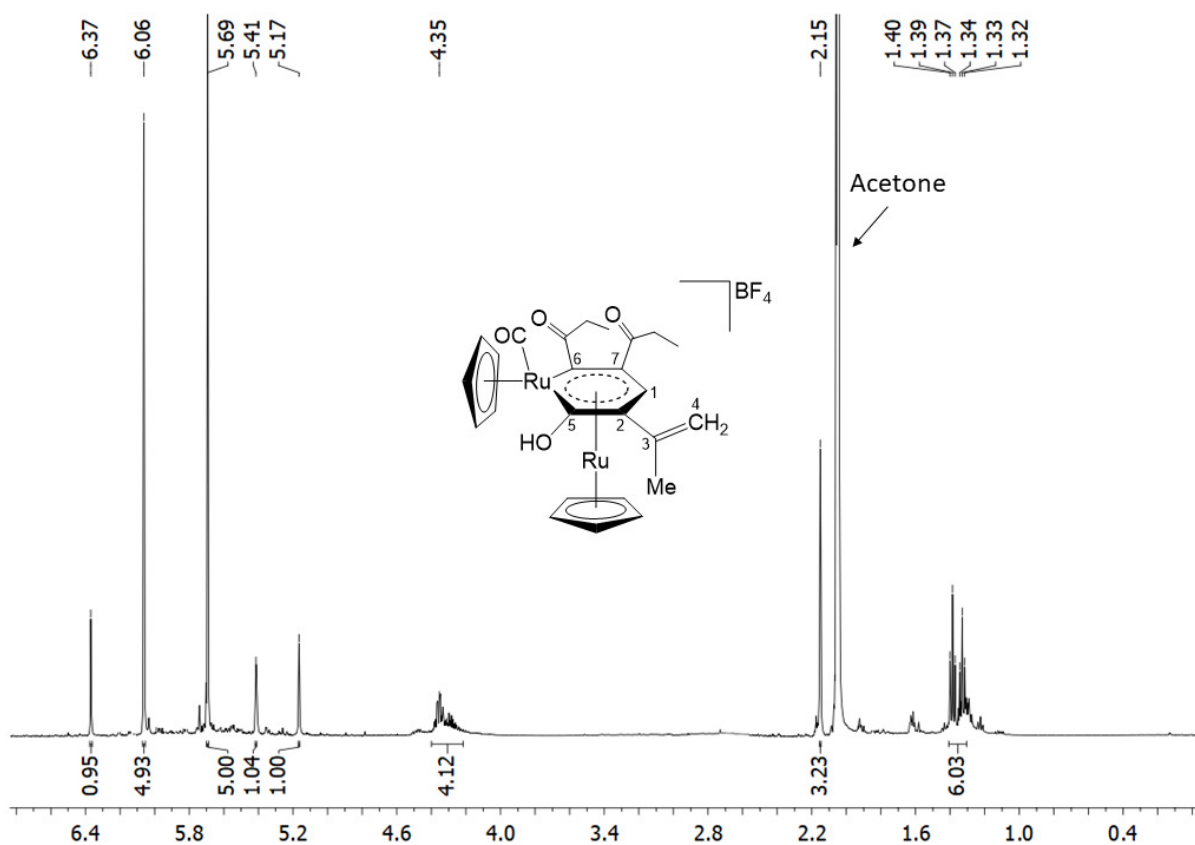


Figure S11. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, acetone- d_6) of **4**.

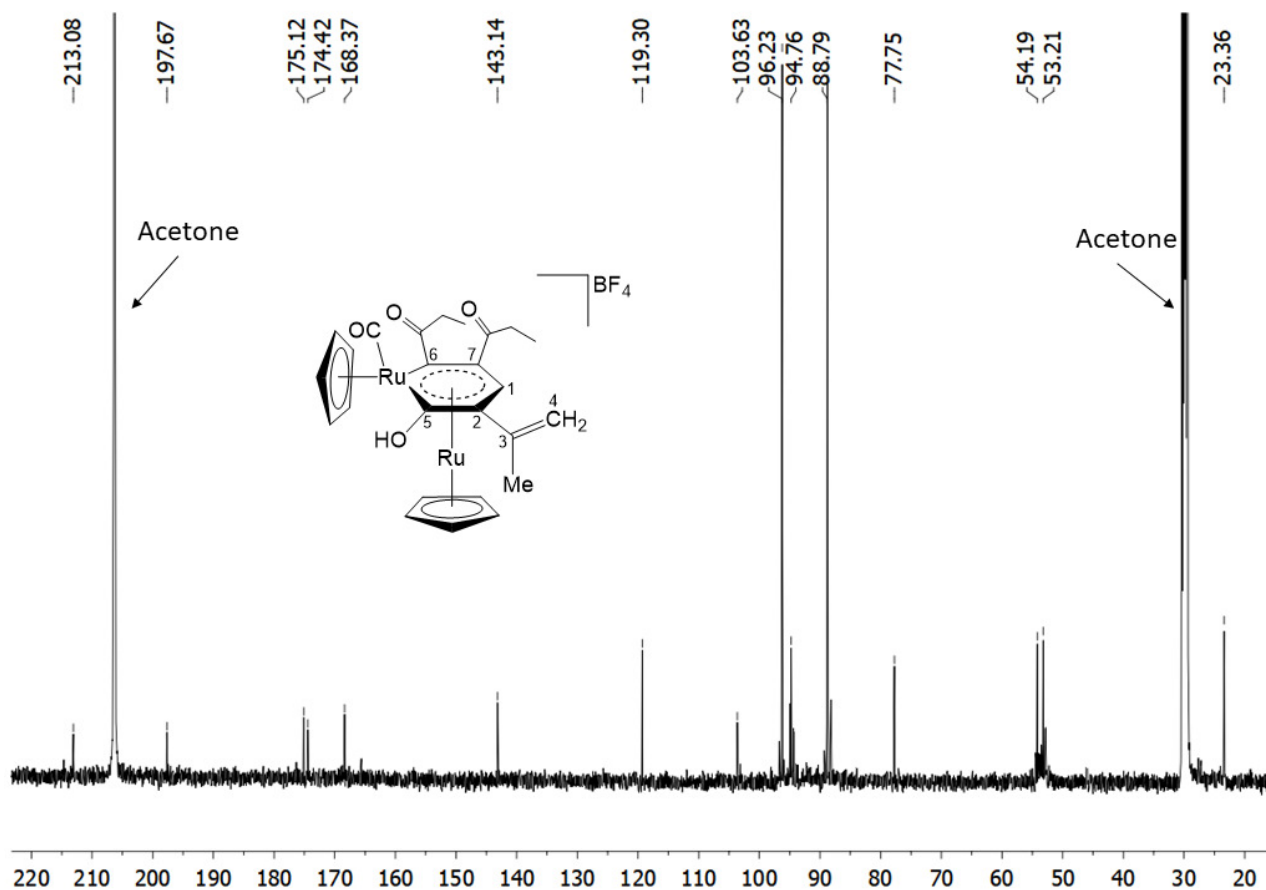


Figure S12. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum (376 MHz, acetone- d_6) of **4**.

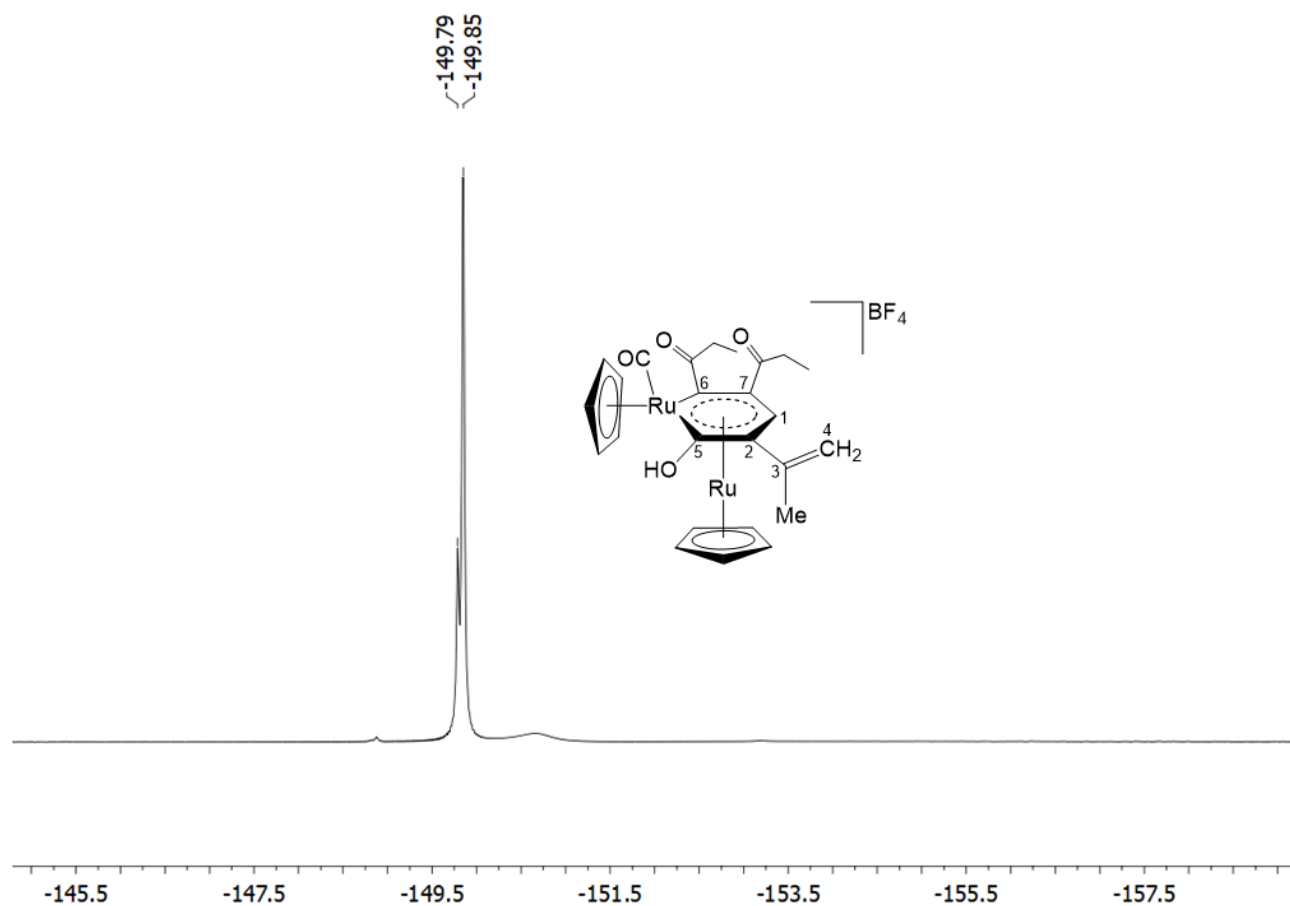


Figure S13. ^1H NMR spectrum (401 MHz, CDCl_3) of **5**.

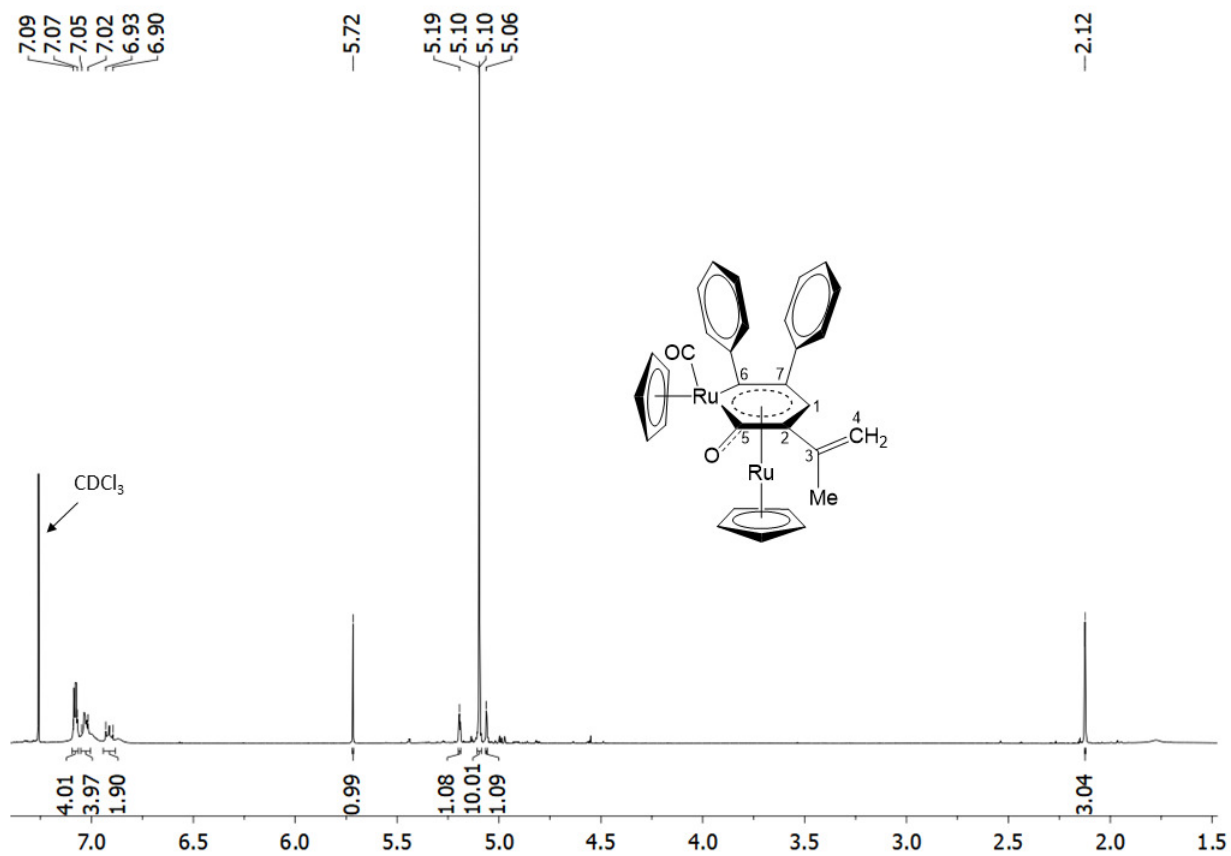


Figure S14. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **5**.

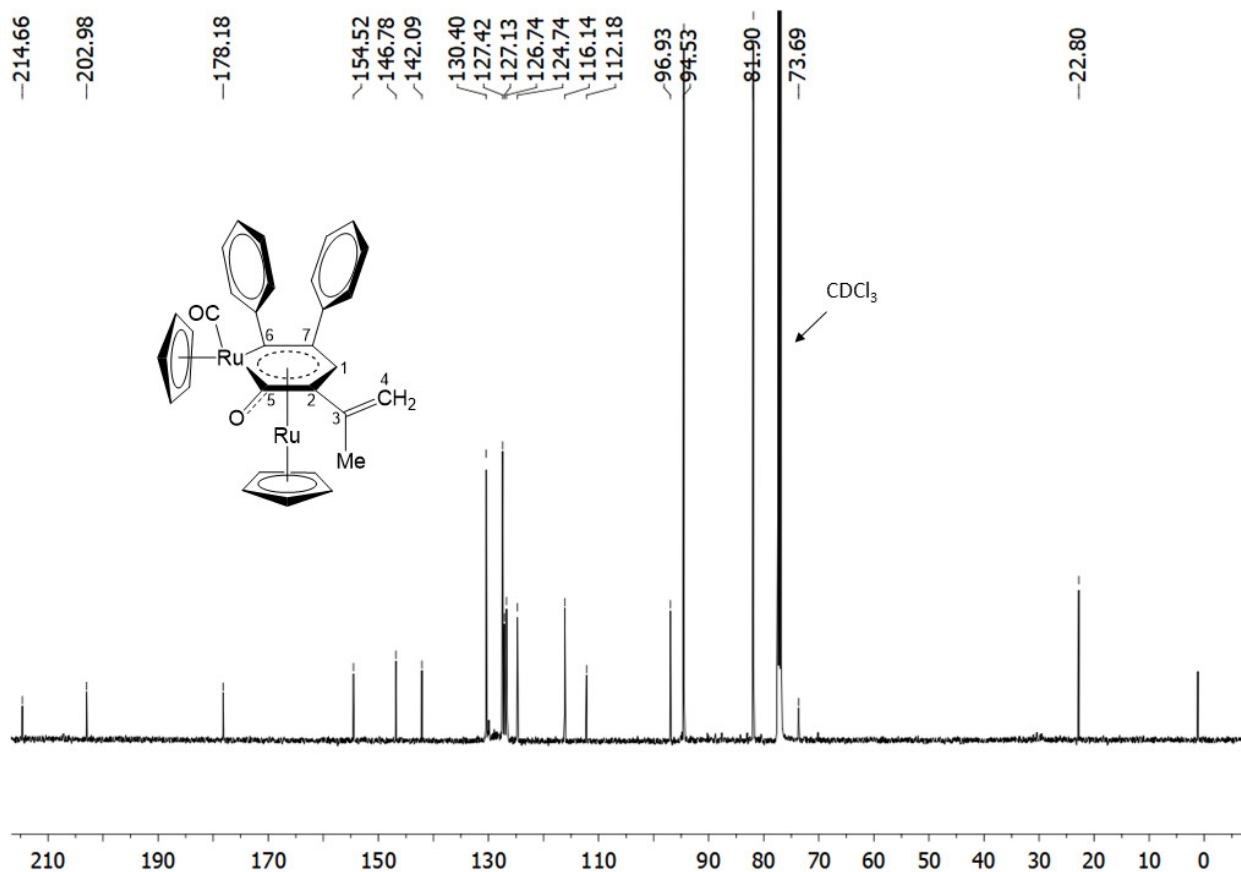


Figure S15. ^1H NMR spectrum (401 MHz, CDCl_3) of **6**.

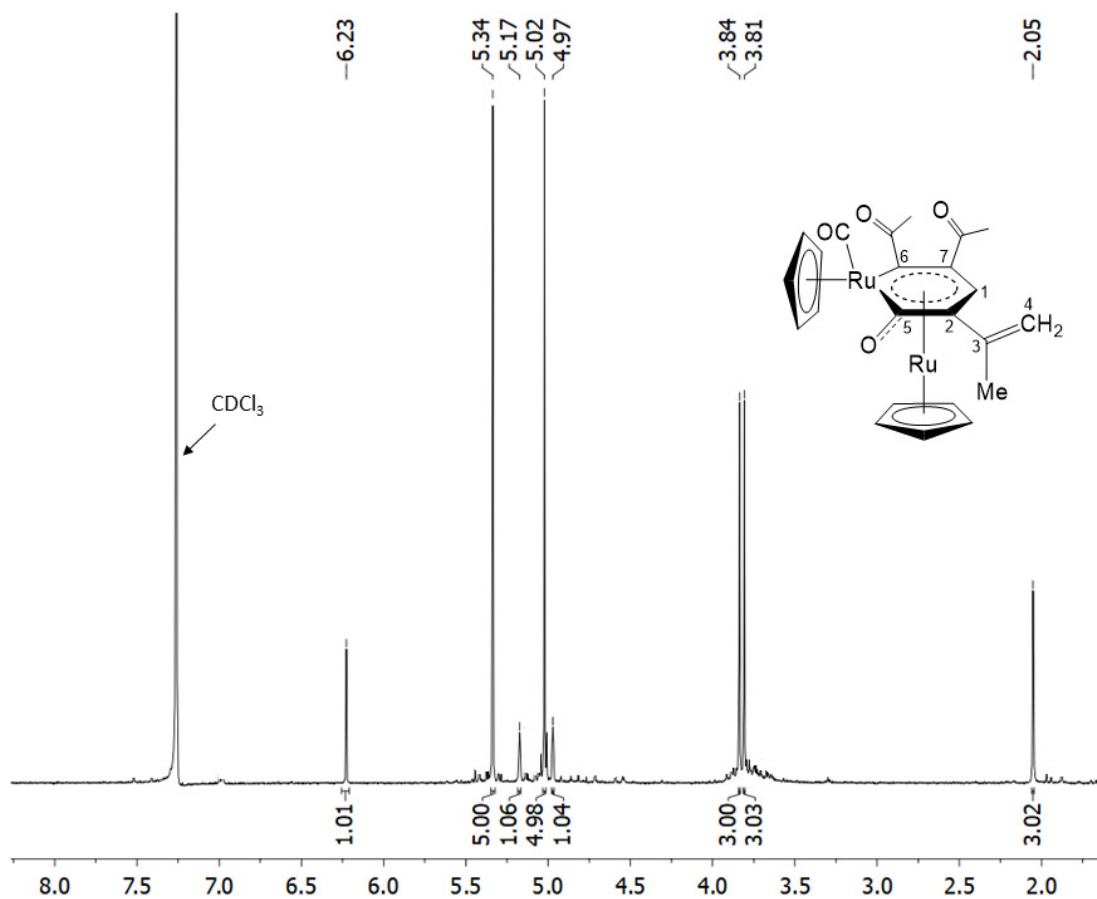


Figure S16. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of **6**.

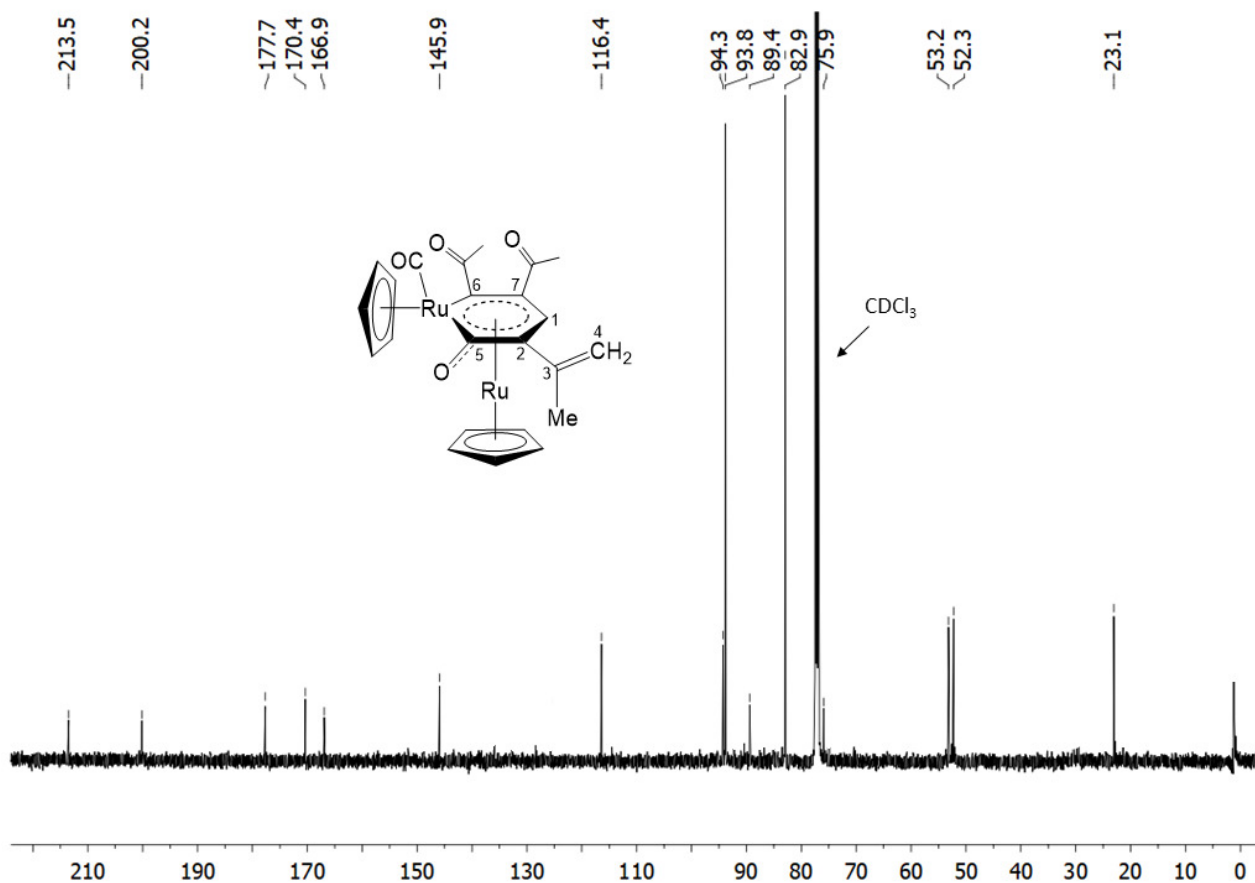


Figure S17. ^1H NMR spectrum (401 MHz, CDCl_3) of 7.

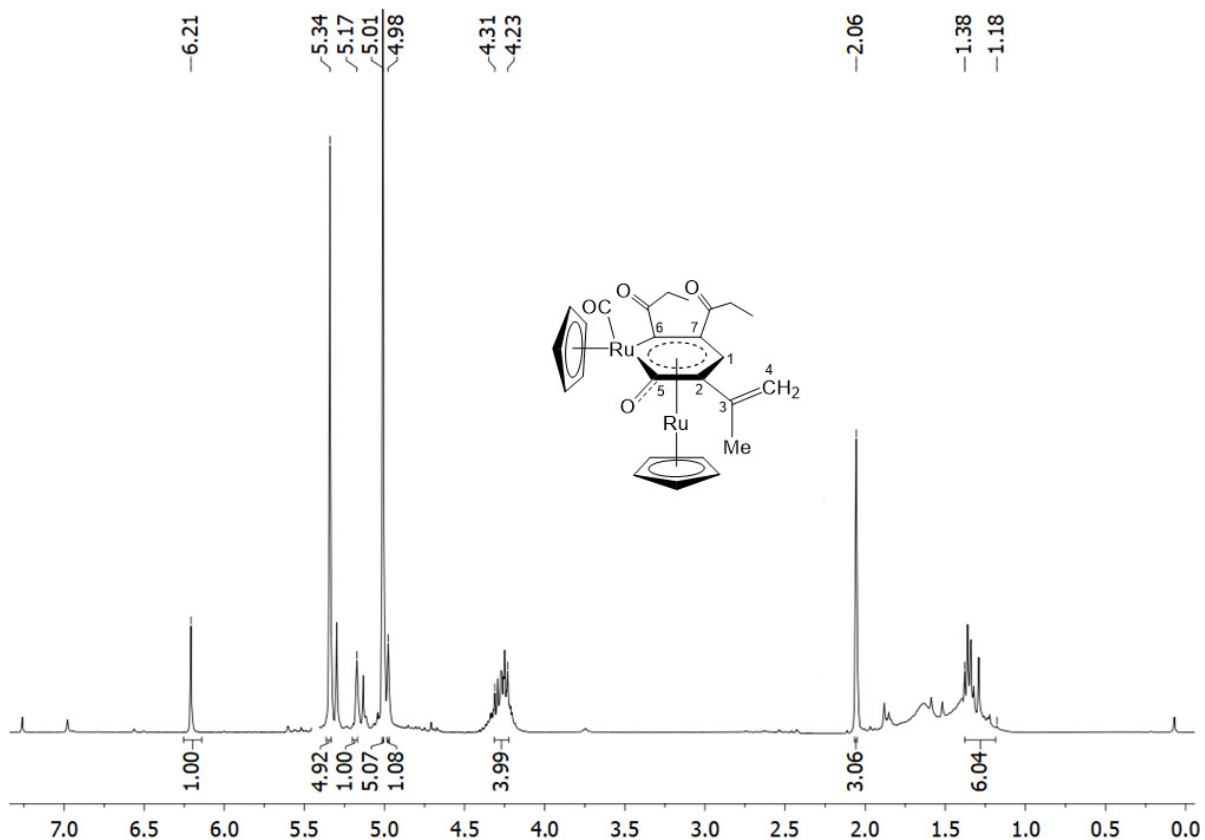


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, CDCl_3) of 7.

