Electronic Supplementary Material (ESI) for Dalton Transactions.

Alkyne-Alkenyl Coupling at a Diruthenium Complex

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Supporting Information

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Figure S1. ^{1}H NMR spectrum (401 MHz, $CDCl_3$) of **2**.

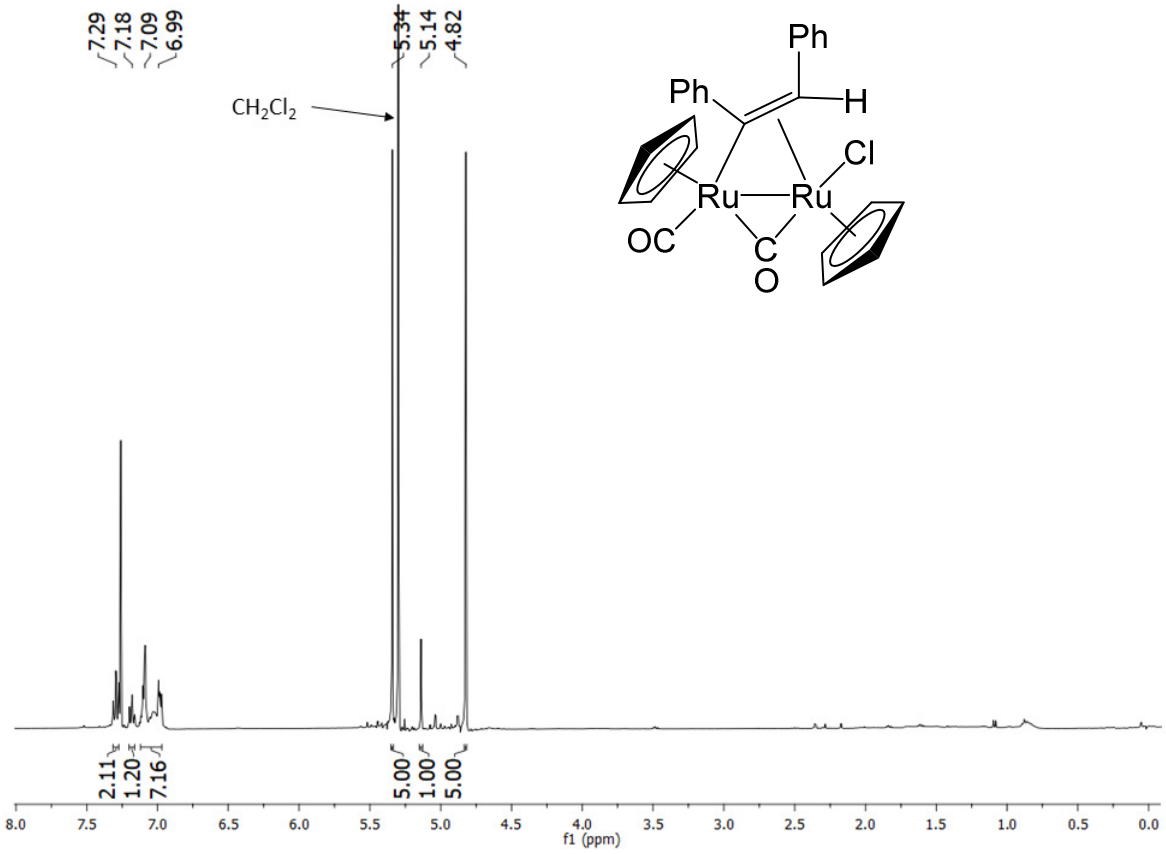


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, $CDCl_3$) of **2**.

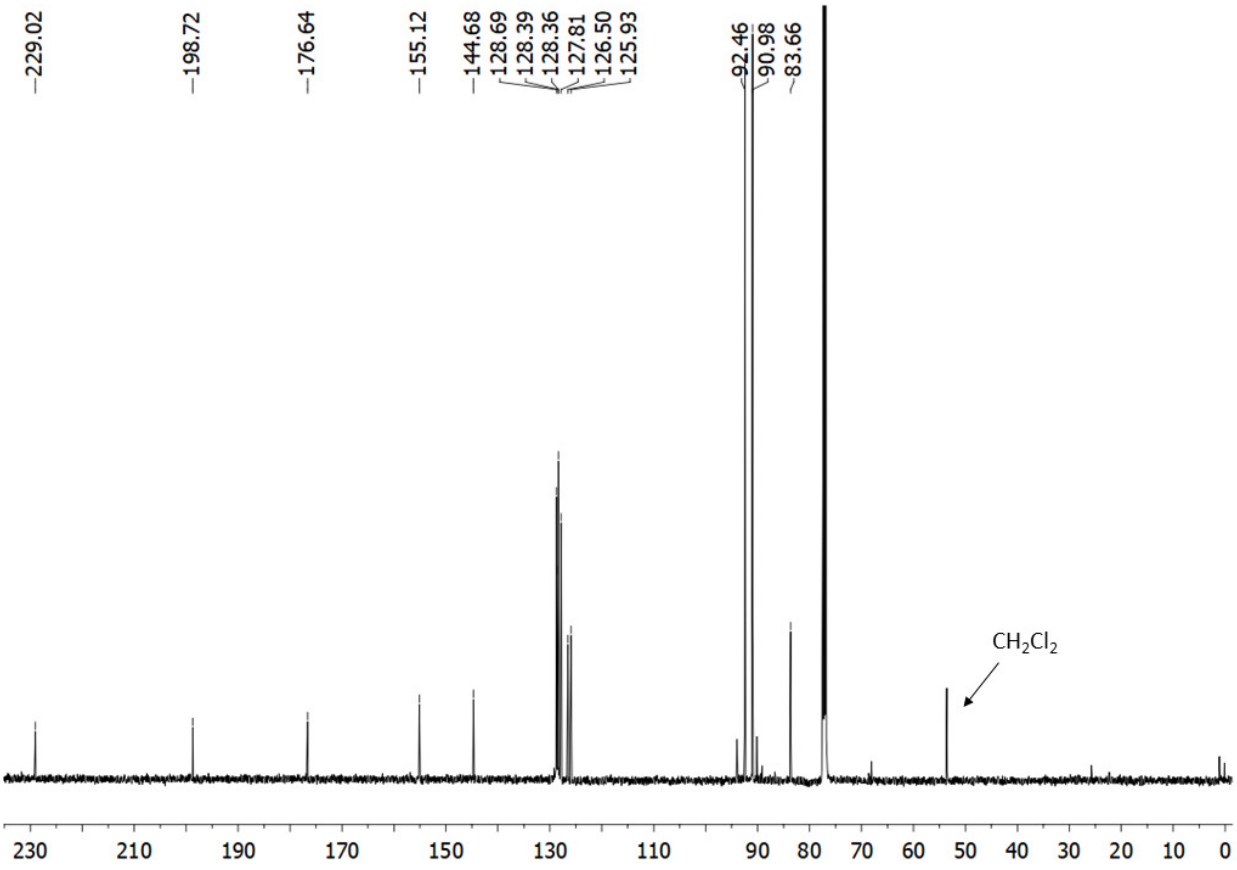


Figure S3. ^{1}H NMR spectrum (401 MHz, acetone-d_6) of **[3]CF_3SO_3**.

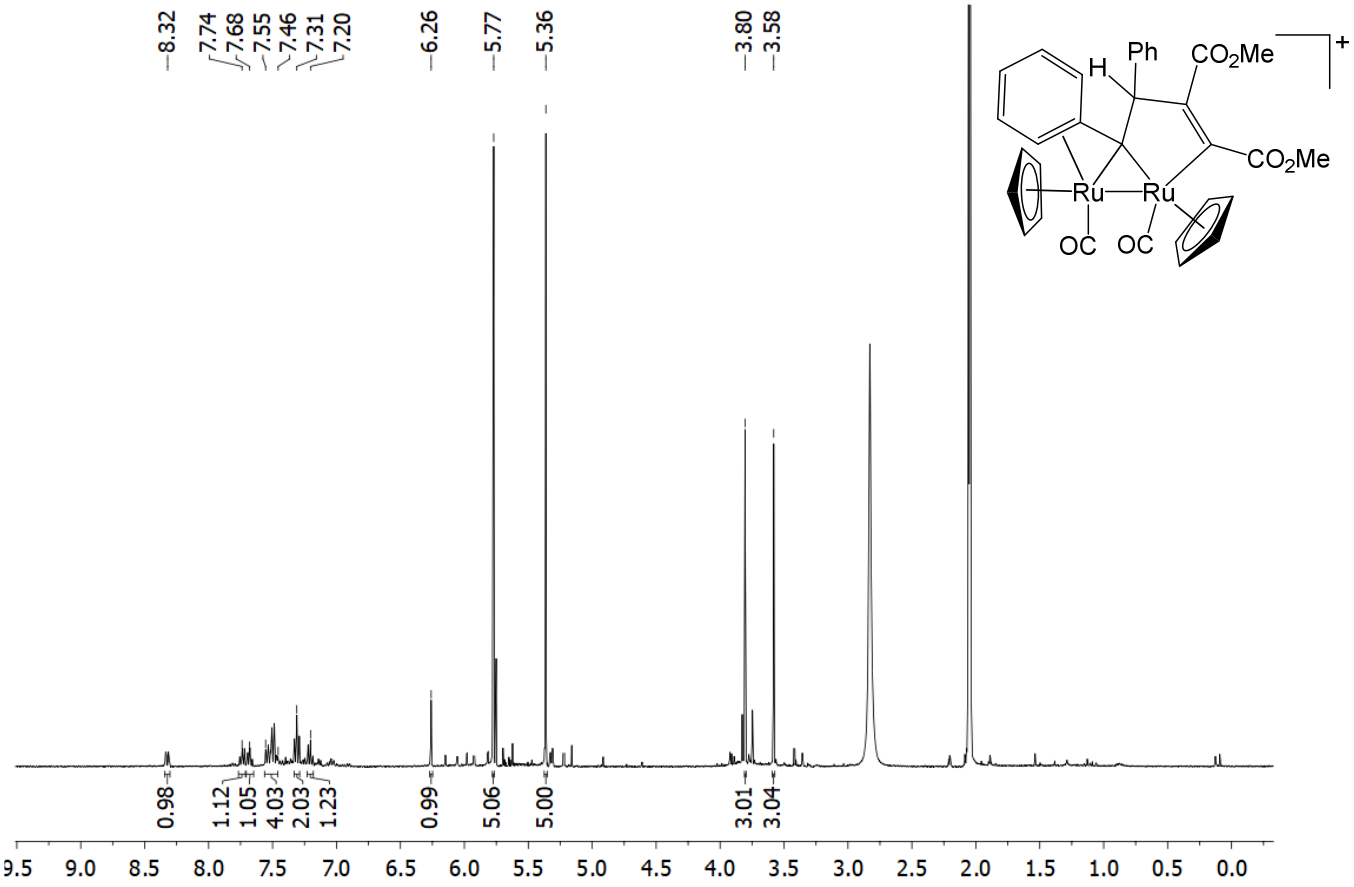


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, acetone-d_6) of **[3]CF_3SO_3**

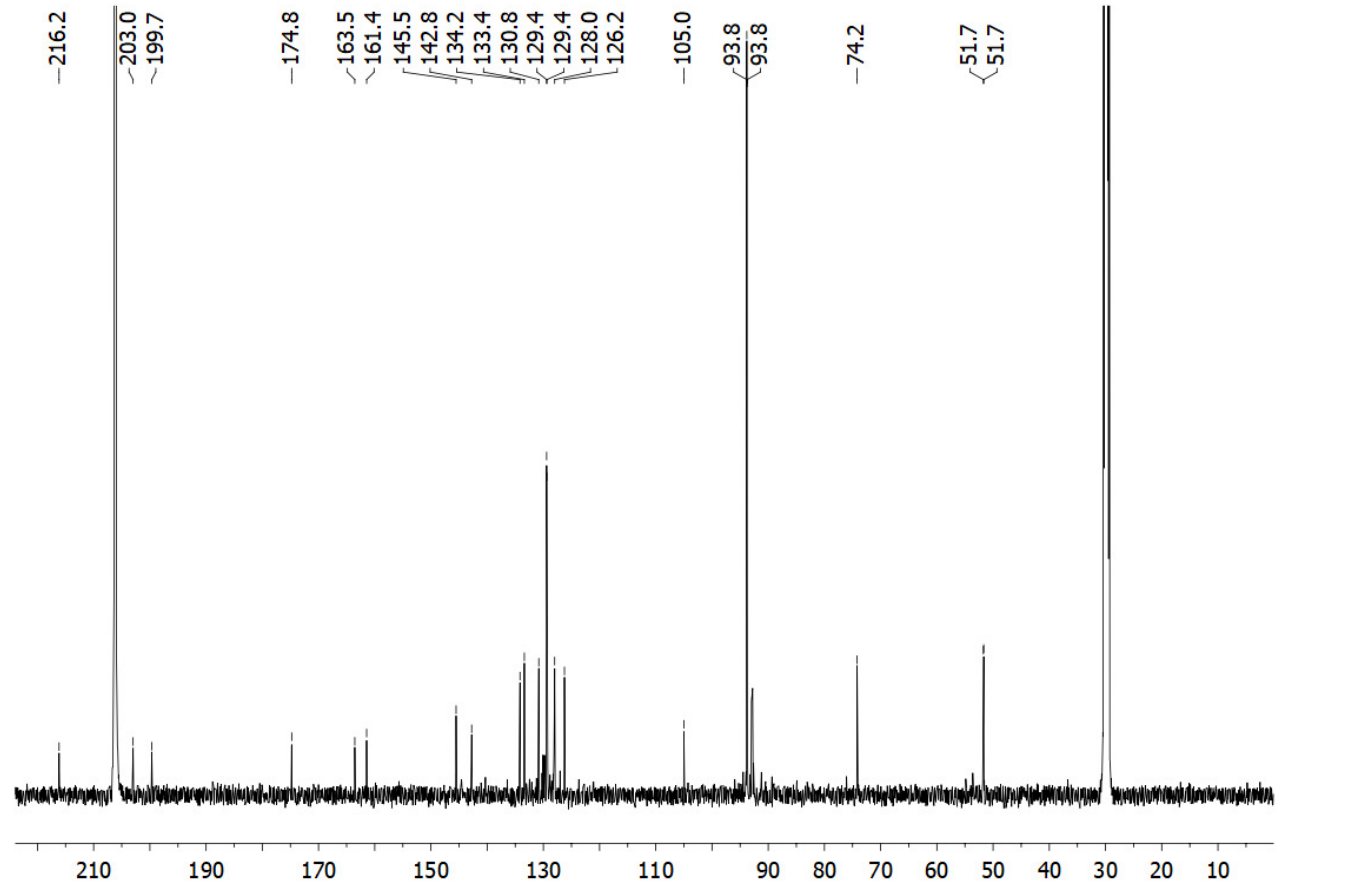


Figure S5. ^{1}H NMR spectrum (401 MHz, acetone-d_6) of **[4]BF$_4$**.

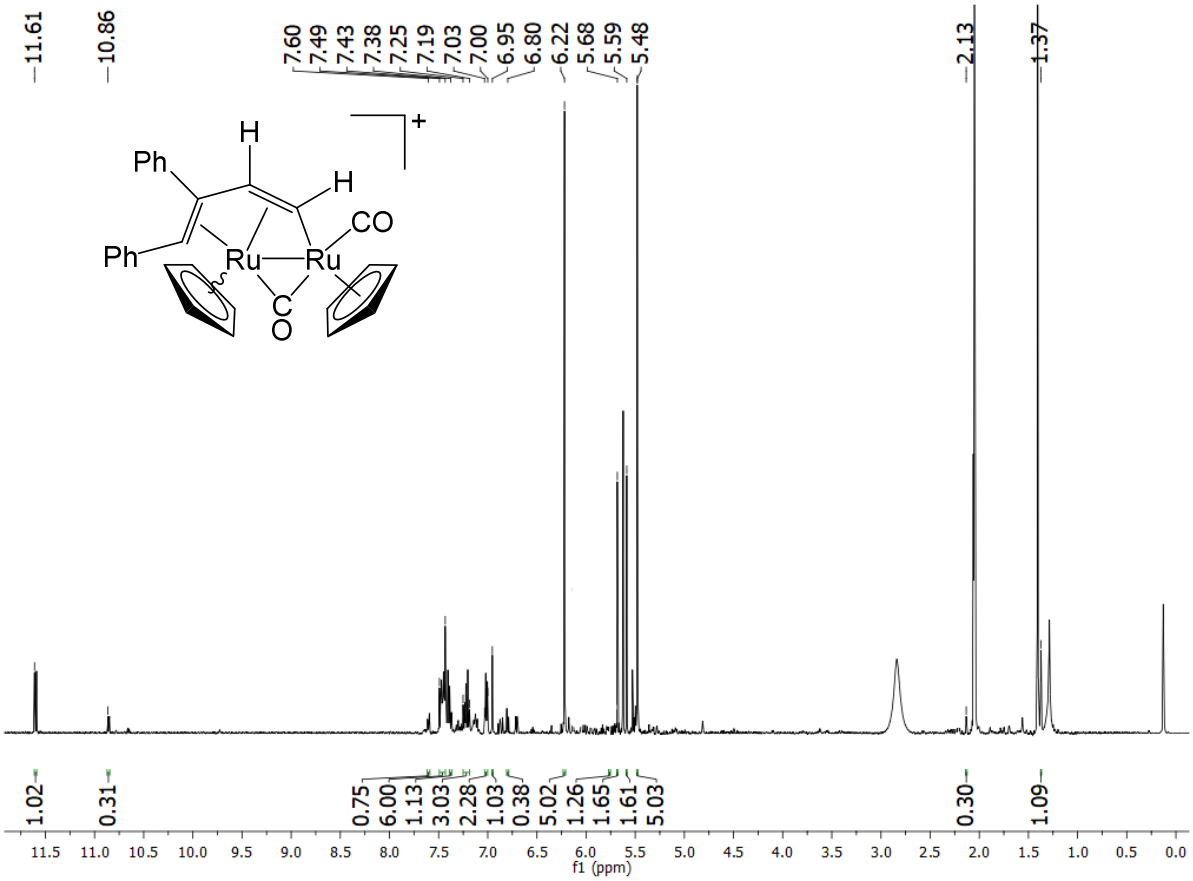


Figure S6. ^{13}C{^{1}H} NMR spectrum (101 MHz, acetone-d_6) of **[4]BF$_4$**.

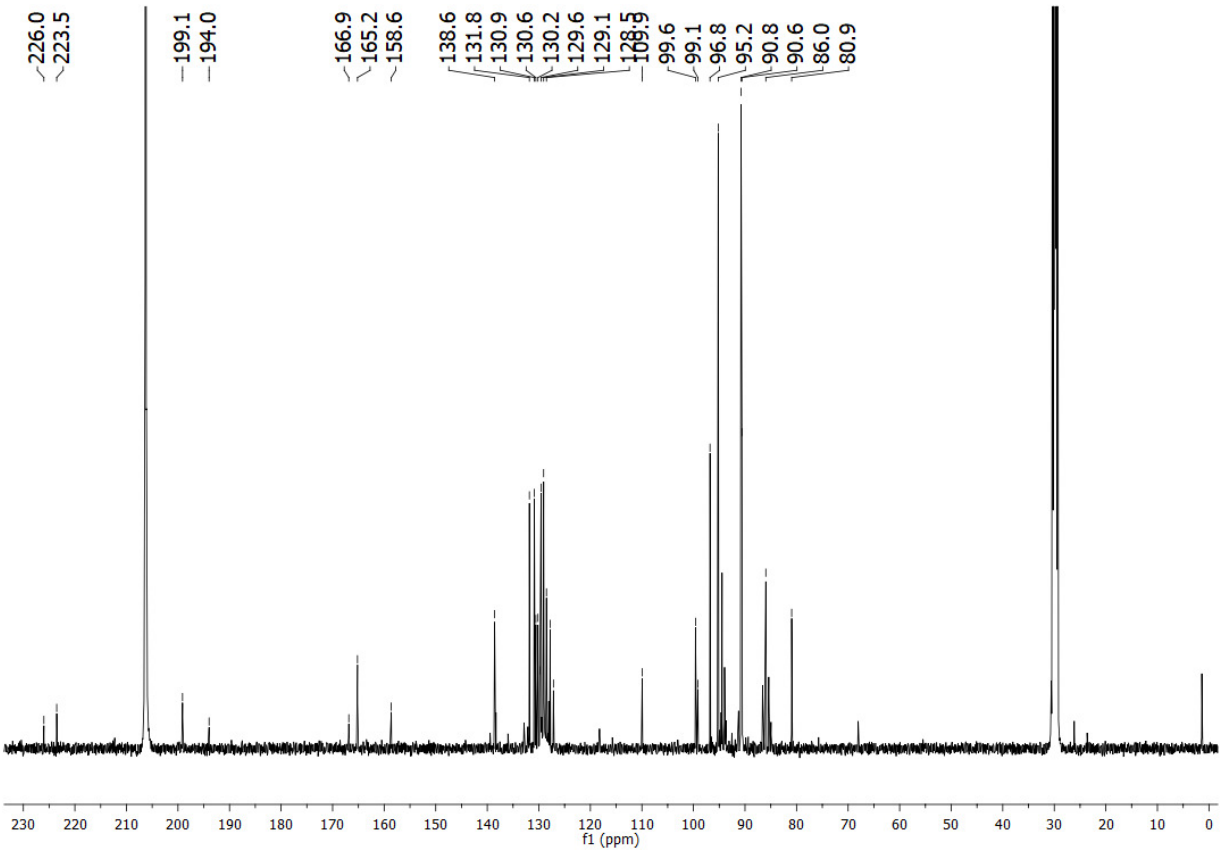


Figure S7. ^{1}H NMR spectrum (401 MHz, acetone-d_6) of **[5]CF_3SO_3**.

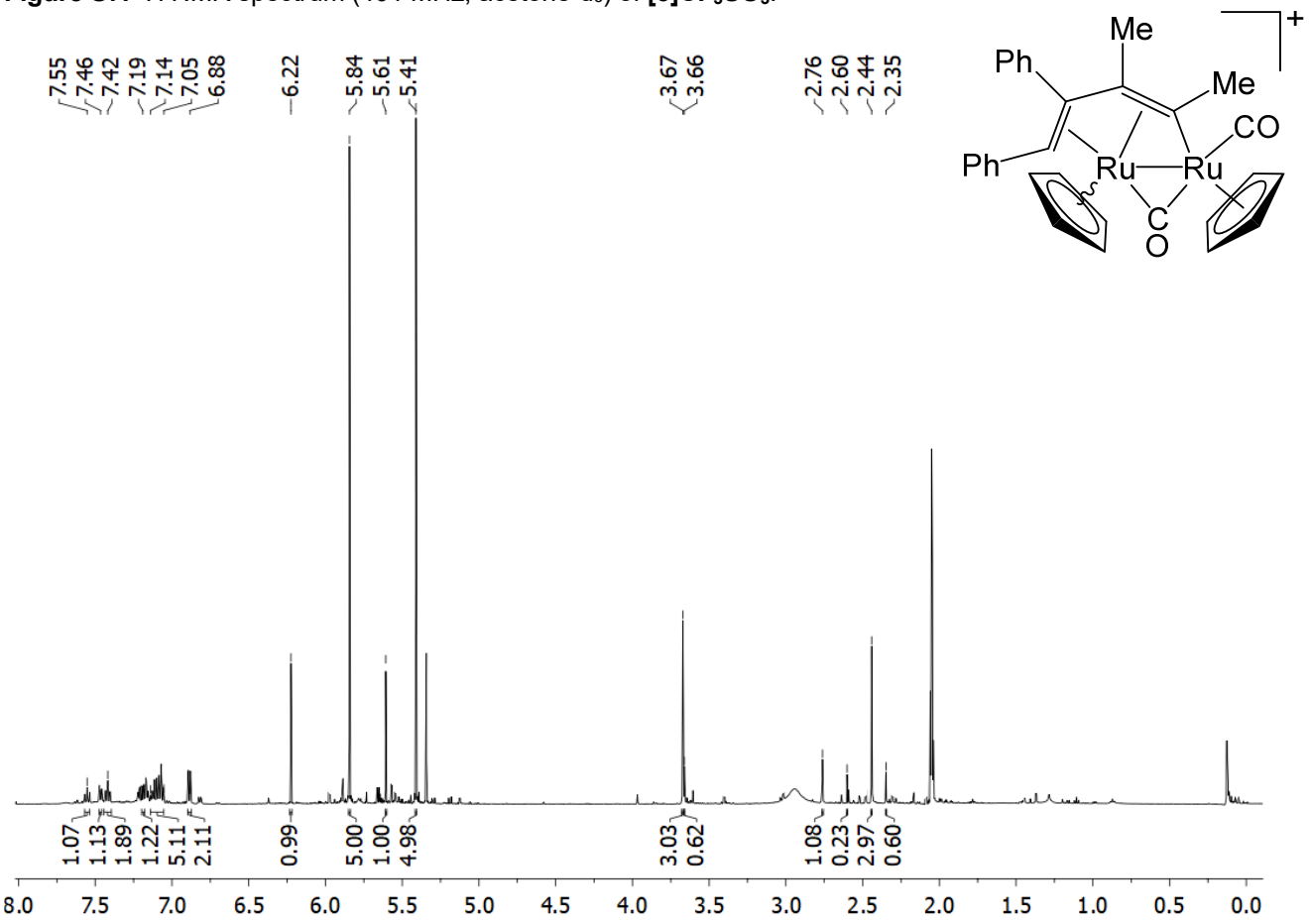


Figure S8. ^{13}C{^{1}H} NMR spectrum (101 MHz, acetone-d_6) of **[5]CF_3SO_3**.

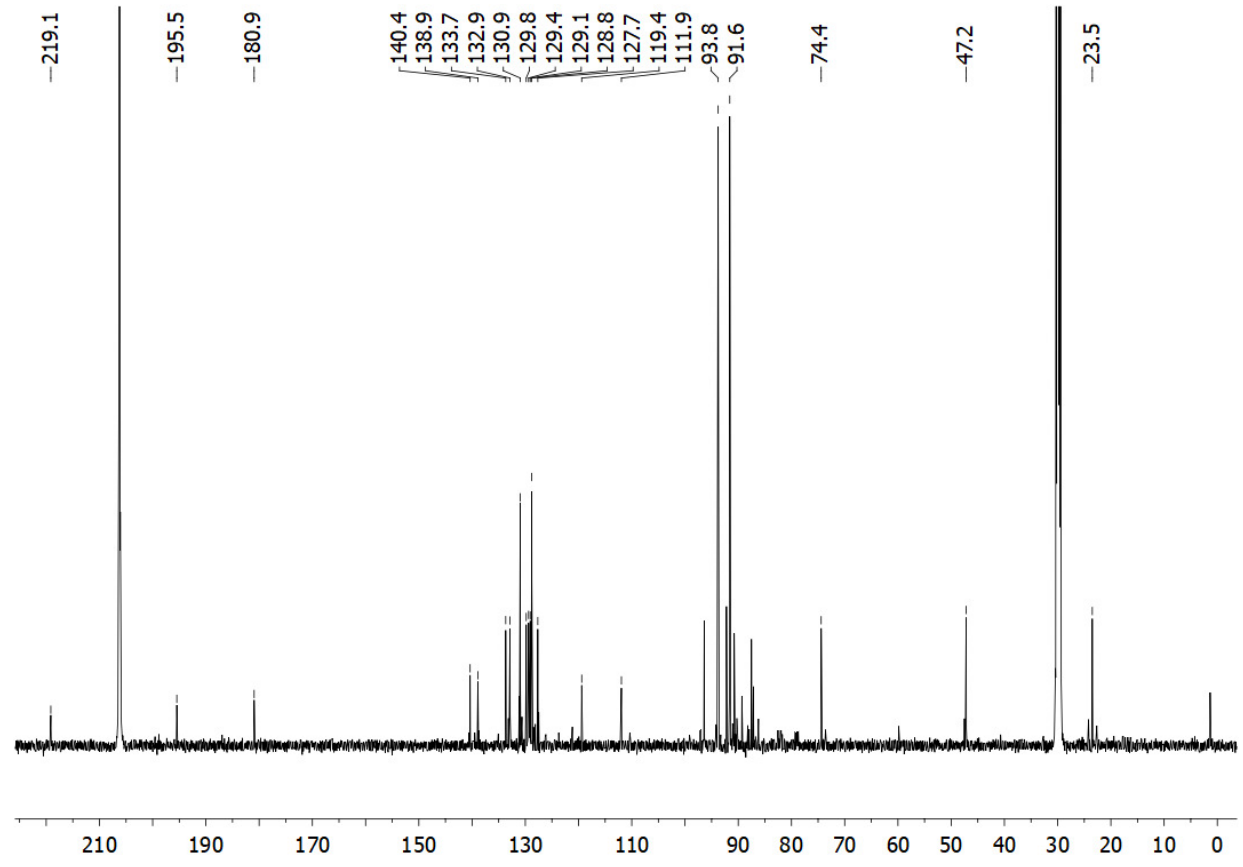


Figure S9. ^{1}H NMR spectrum (401 MHz, acetone-d_6) of **[6]CF_3SO_4**.

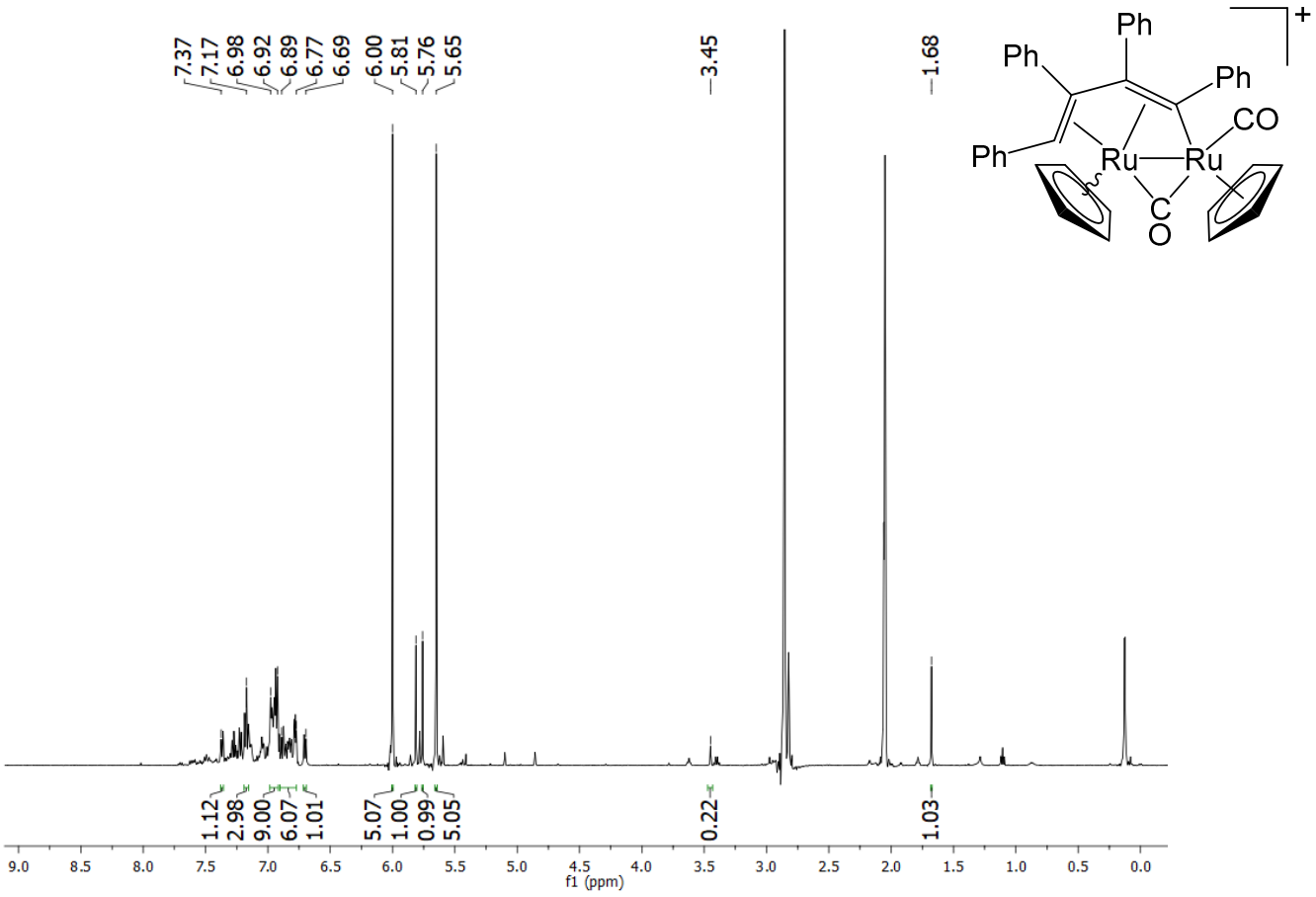


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, acetone-d_6) of **[6]CF_3SO_4**.

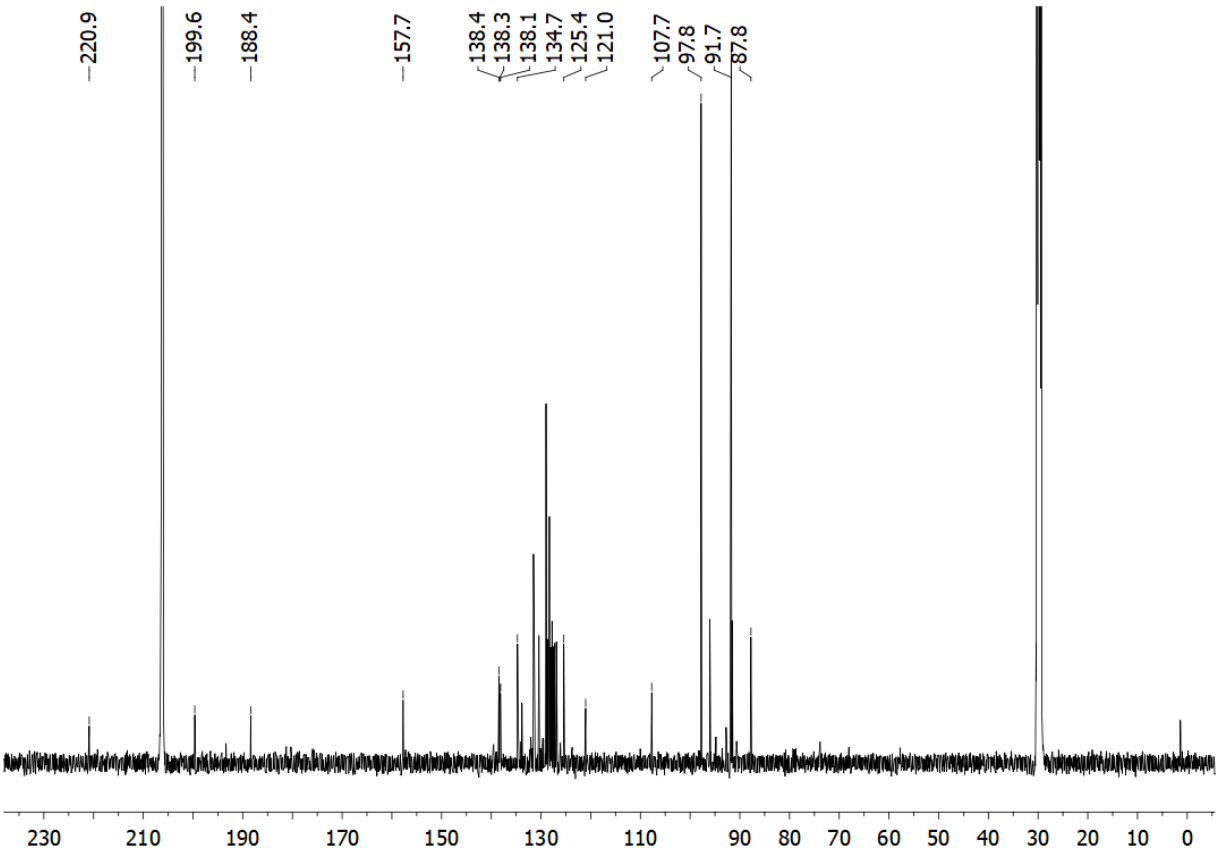


Figure S11. ^{1}H NMR spectrum (401 MHz, acetone-d_6) of **[7]CF_3SO_3**.

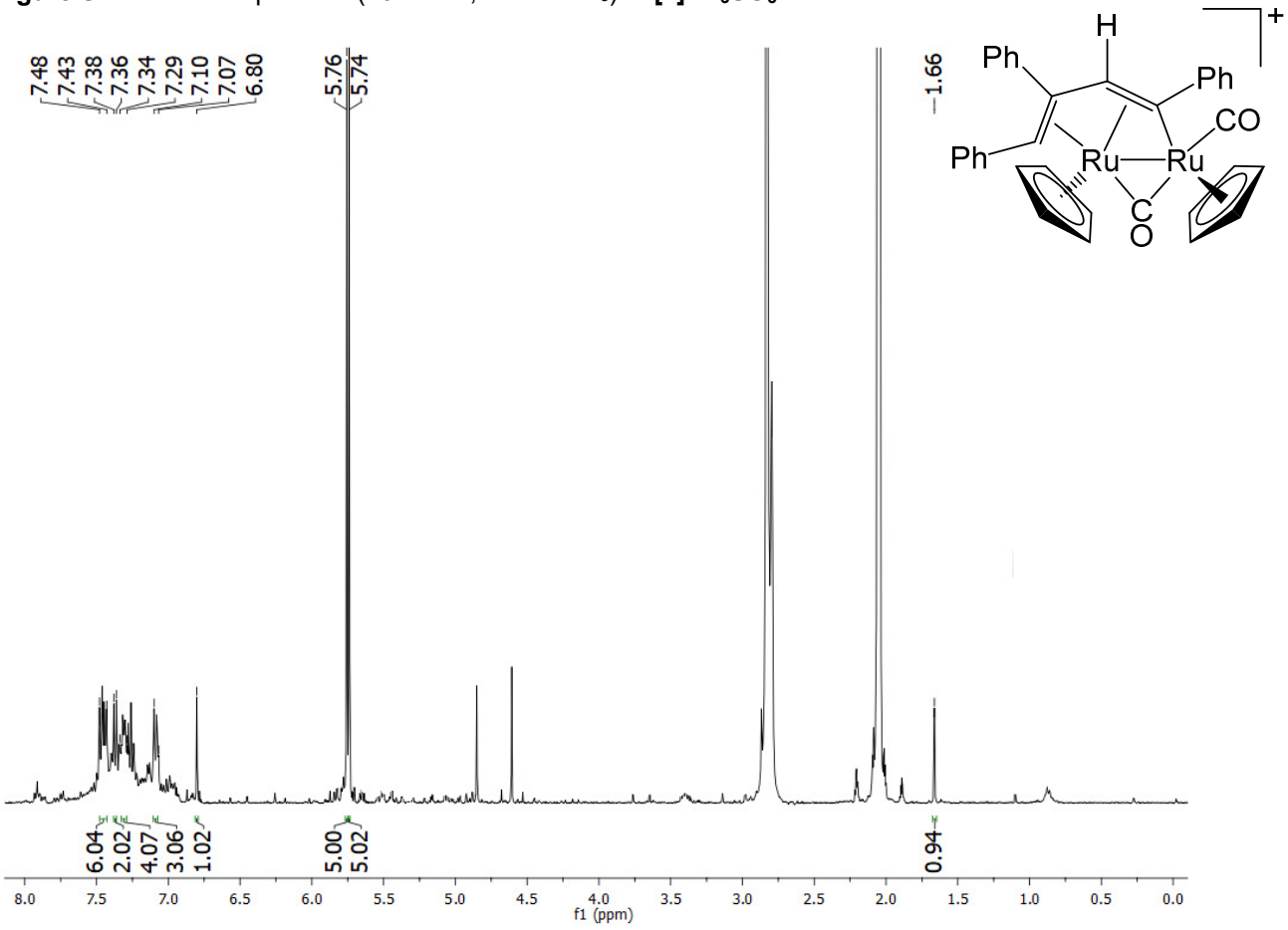
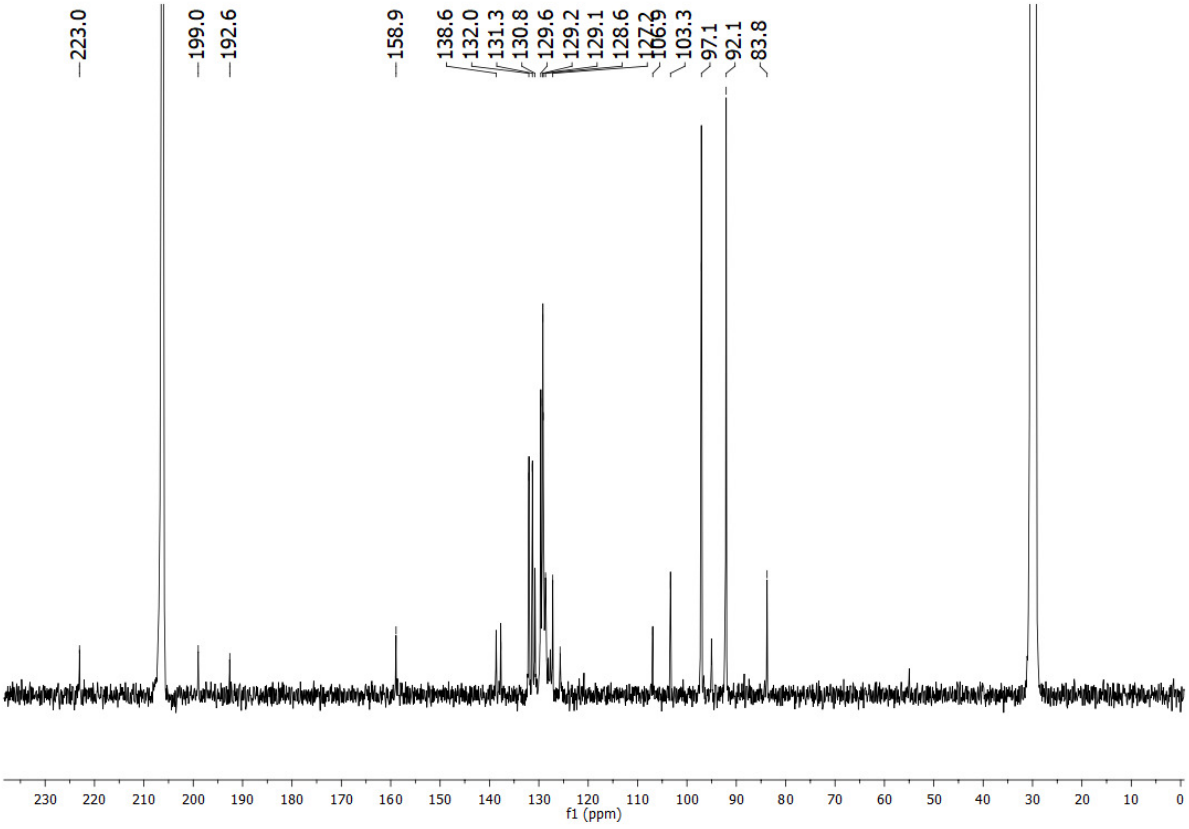


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, acetone-d_6) of **[7]CF_3SO_3**.



Spectroscopic characterization of [6b]CF_3SO_3.

Dark-yellow solid. IR (CH_2Cl_2): ϋ/cm^{-1} = 2006vs (CO), 1868s (μ-CO). ^{1}H NMR (acetone-d_6): δ/ppm = 7.37, 7.17, 6.98-6.92, 6.89-6.77, 6.69 (m, 20 H, Ph); 6.00, *5.81*, *5.76*, 5.65 (s, 10 H, Cp); *3.45*, 1.68 (s, 1 H, CH). Isomeric ratio (cis/trans) = 5.

Figure S13. DFT-optimized structures of diruthenium complexes and relative Gibbs free energies (kcal mol^{-1}, C-PCM/PBEh-3C calculations). Ru, green; O, red; C, white. Hydrogen atoms are omitted for clarity.

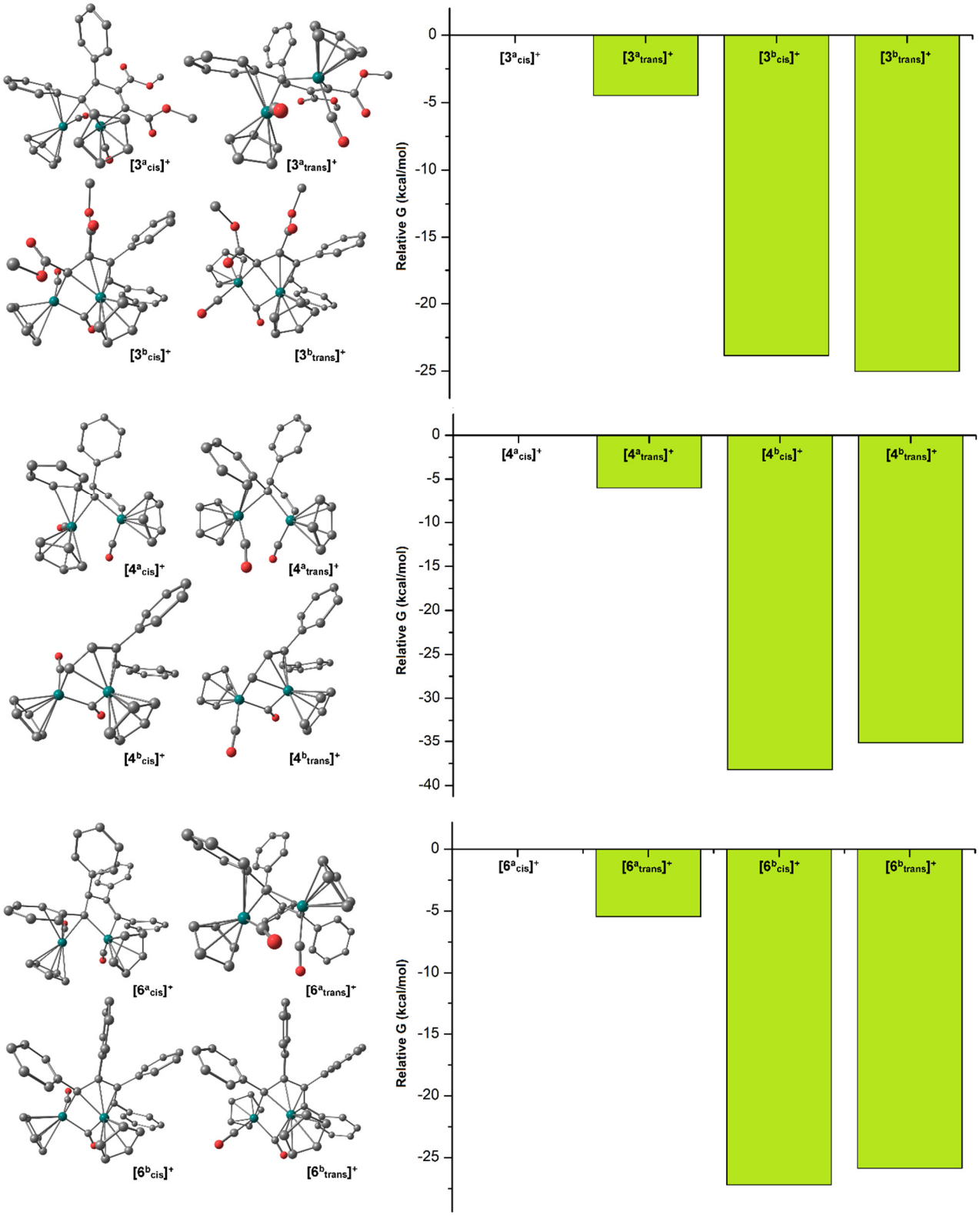


Figure S14. DFT-optimized structures of stereoisomers of **[6$^{b}_{cis}$]$^{+}$** differing in the orientation of H and Ph bound to one carbon atom, and Gibbs free energy difference (kcal mol^{-1}, C-PCM/PBEh-3C calculations). Ru, green; O, red; C, white. Hydrogen atoms are omitted for clarity.