Electronic Supplementary Material (ESI) for Dalton Transactions.
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Electronic Supportion Information (ESI) for:

Synthesis and Complexation of Superbulky Imidazolium-2-dithiocarboxylate Ligands

Tomás F. Beltrán,[†] Guillermo Zaragoza,[‡] and Lionel Delaude[*,†]

[†]*Laboratory of Organometallic Chemistry and Homogeneous Catalysis, Institut de chimie (B6a), Allée du six Août 13, Quartier Agora, Université de Liège, 4000 Liège, Belgium*

[‡]*Unidade de Difracción de Raios X, Edificio CACTUS, Universidade de Santiago de Compostela, Campus Vida, 15782 Santiago de Compostela, Spain*

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Part 1 – Additional Figures

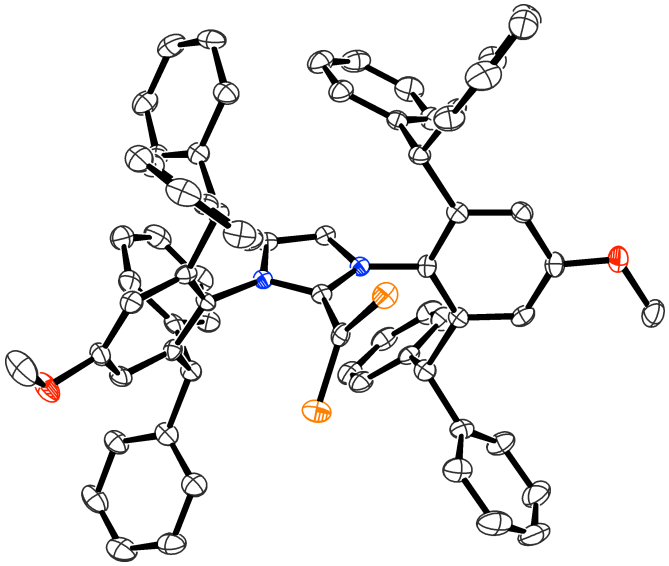

Figure S1. Molecular structure of IDip*OMe·CS_2 (**2**) with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms were omitted for clarity

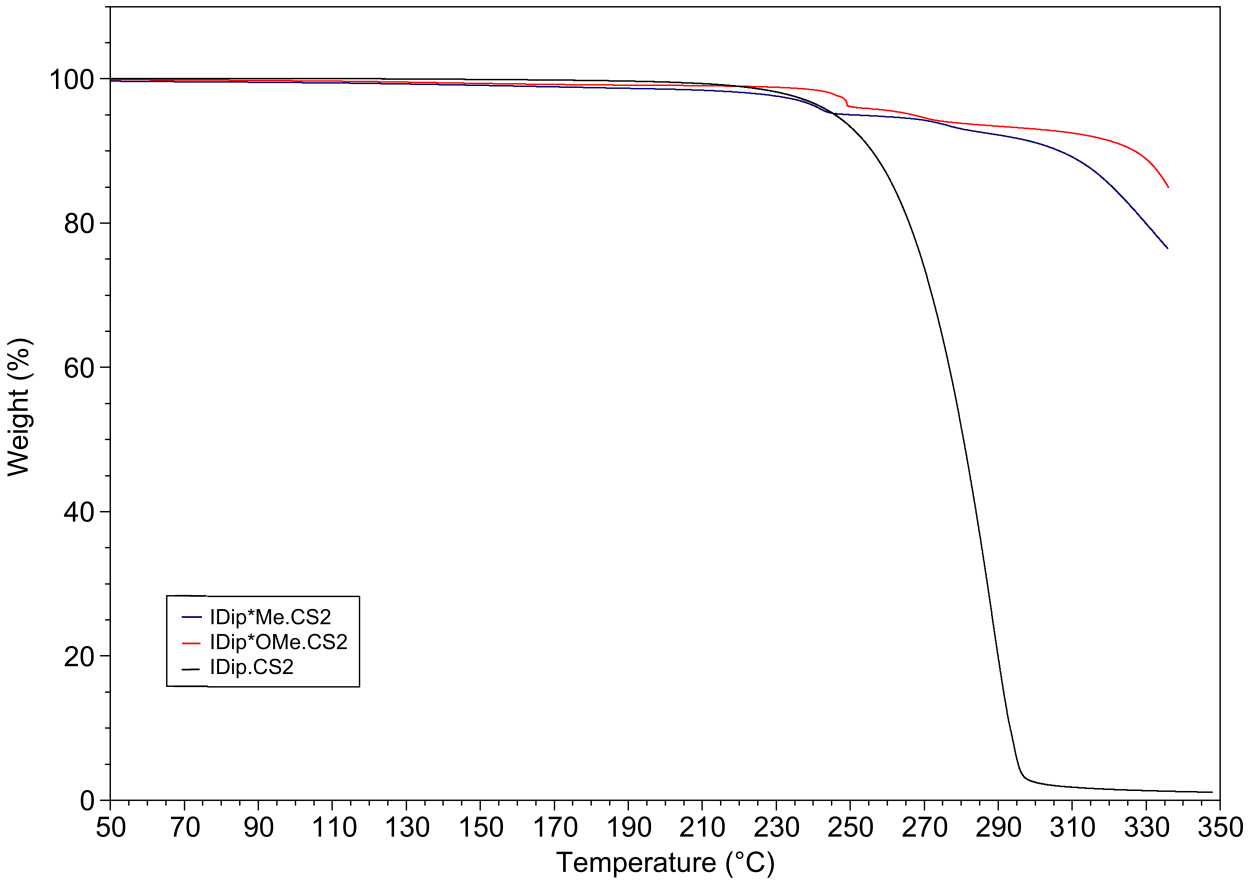

Figure S2. TGA curves of IDip·CS_2, IDip*Me·CS_2 (**1**), and IDip*OMe·CS_2 (**2**)

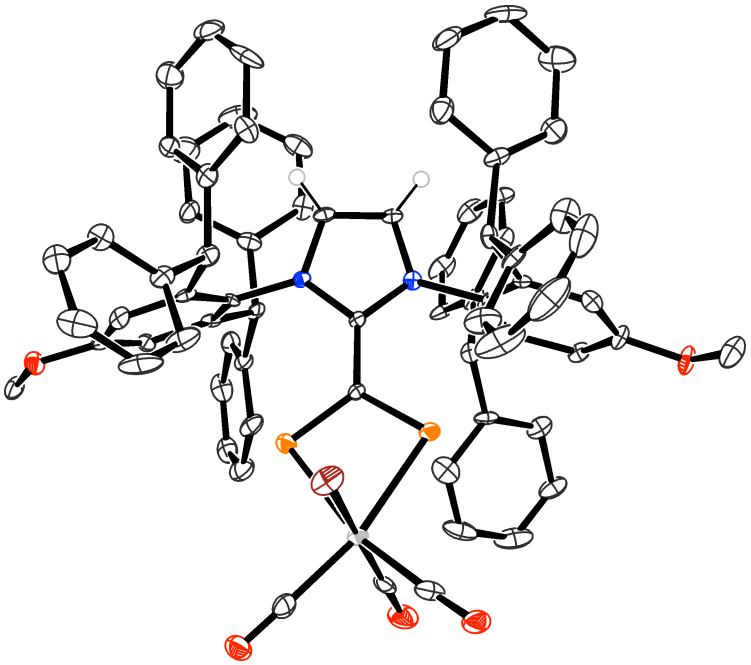

Figure S3. Molecular structure of [ReBr(CO)$_3$(S$_2$C·IDip*OMe)] (**4**) with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms were omitted for clarity

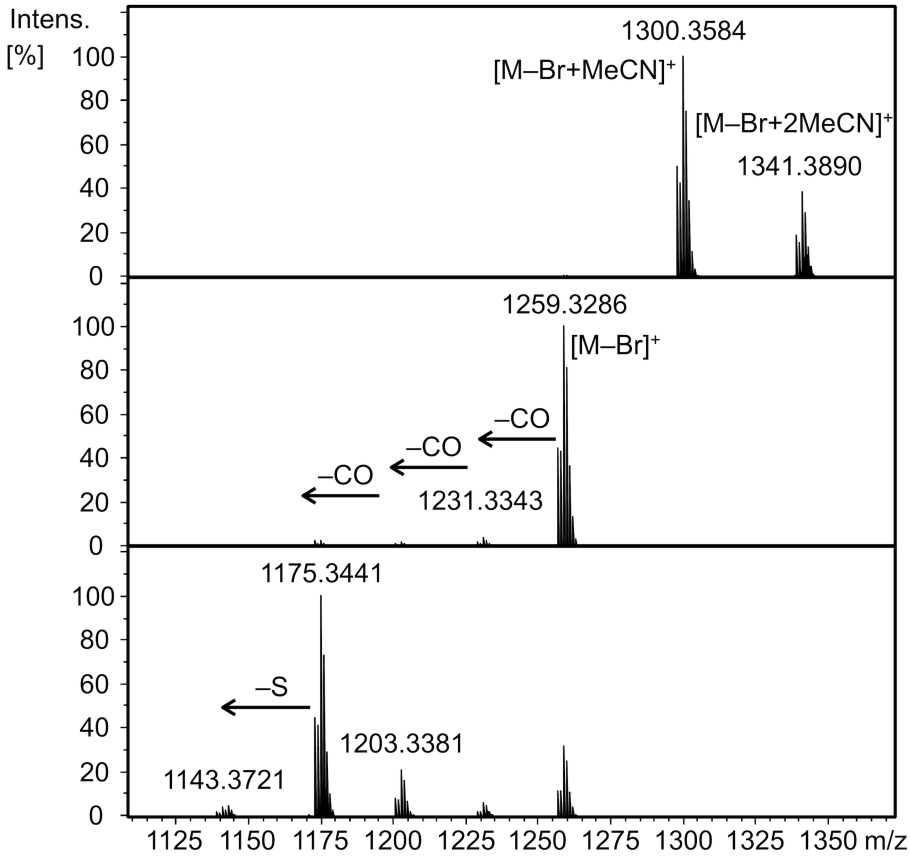

Figure S4. ESI-MS spectrum of [ReBr(CO)$_3$(S$_2$C·IDip*Me)] (**3**) (top) and MS/MS spectra of the [Re(CO)$_3$(S$_2$C·IDip*Me)]$^+$ ion ([M–Br]$^+$) at a collision energy of 20 V (middle) and 30 V (bottom)

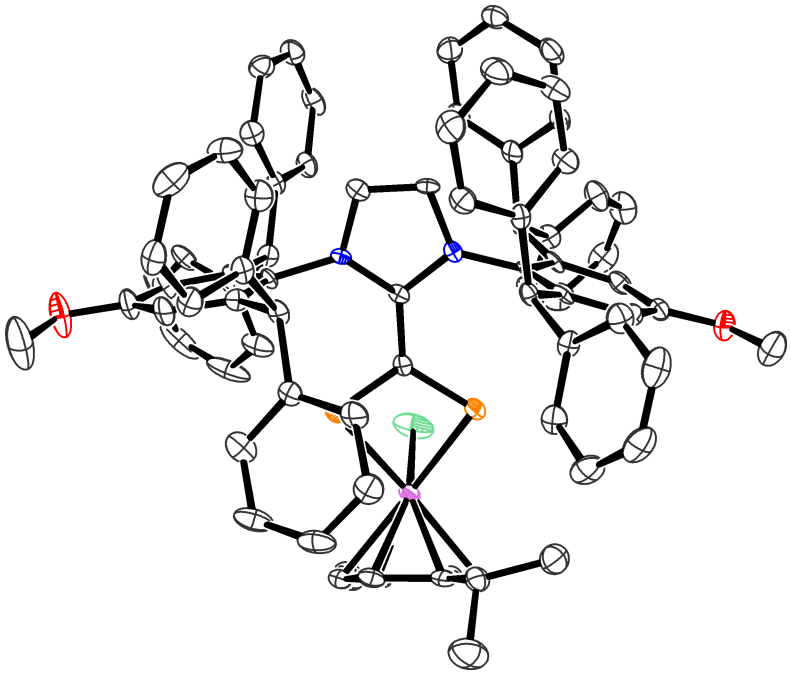

Figure S5. Molecular structure of [RuCl(*p*-cymene)(S_2C·IDip*OMe)]PF_6 (**6**) with thermal ellipsoids drawn at the 50% probability level. Hydrogen atoms, co-crystallized solvents, and the PF_6^- counterion were omitted for clarity

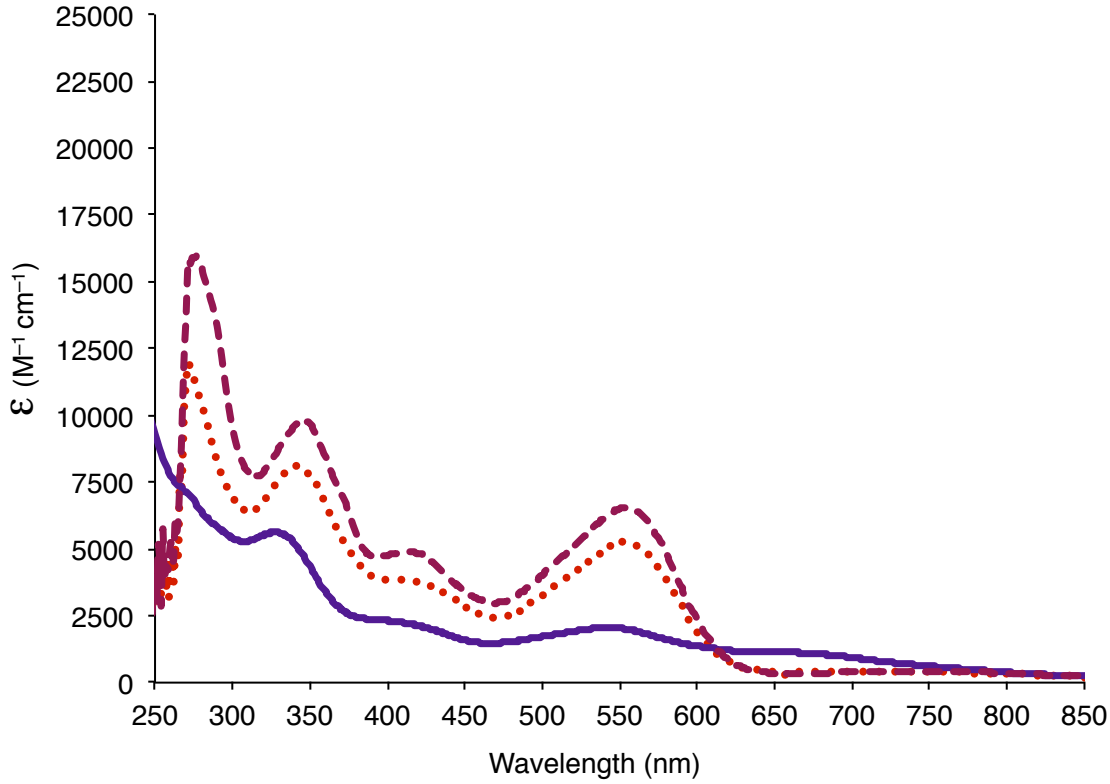

Figure S6. Electronic absorption spectra of [RuCl(*p*-cymene)(S_2C·IDip)]PF_6 (dark purple solid line), [RuCl(*p*-cymene)(S_2C·IDip*Me)]PF_6 (**5**, red dotted line), and [RuCl(*p*-cymene)(S_2C·IDip*OMe)]PF_6 (**6**, purple broken line)

Part 2 – NMR spectra

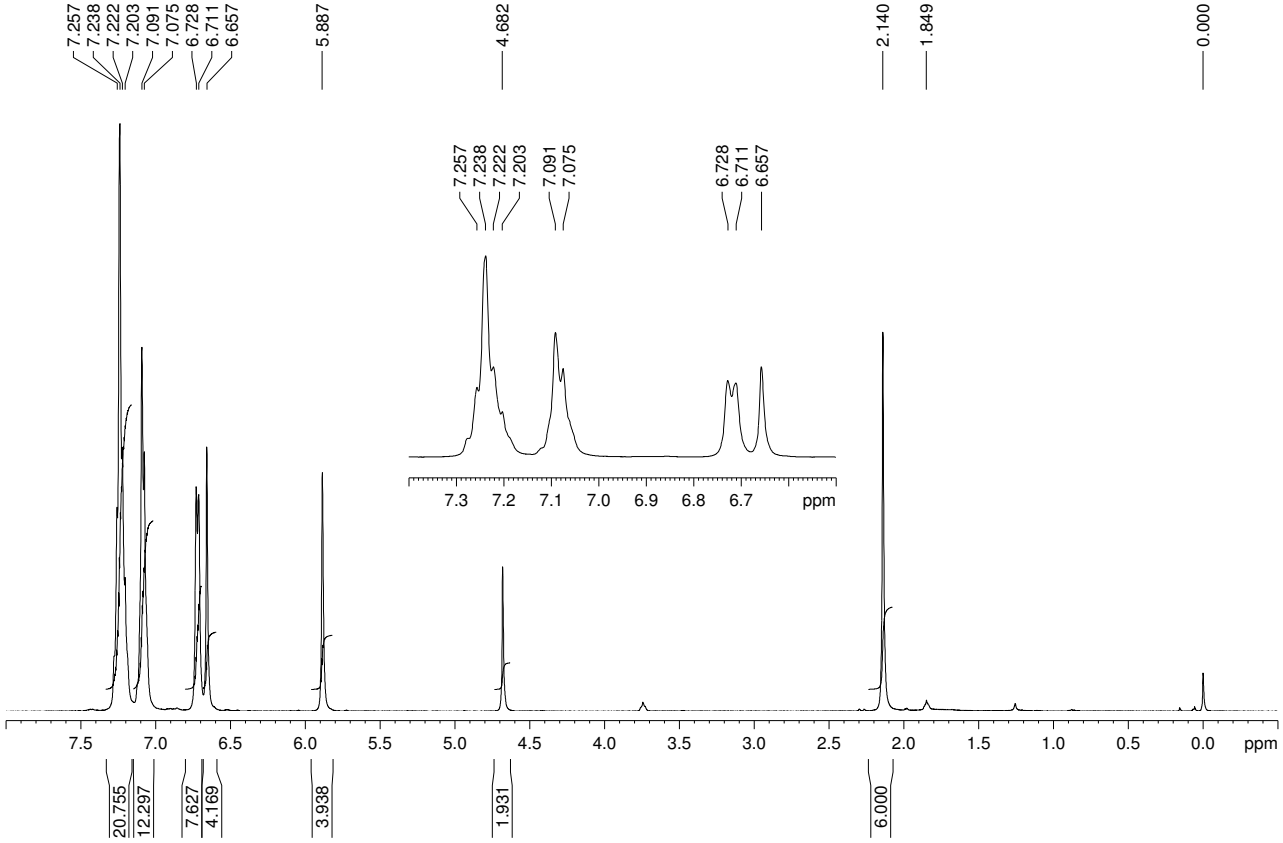

Figure S7. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of IDip*Me·CS_2 (**1**)

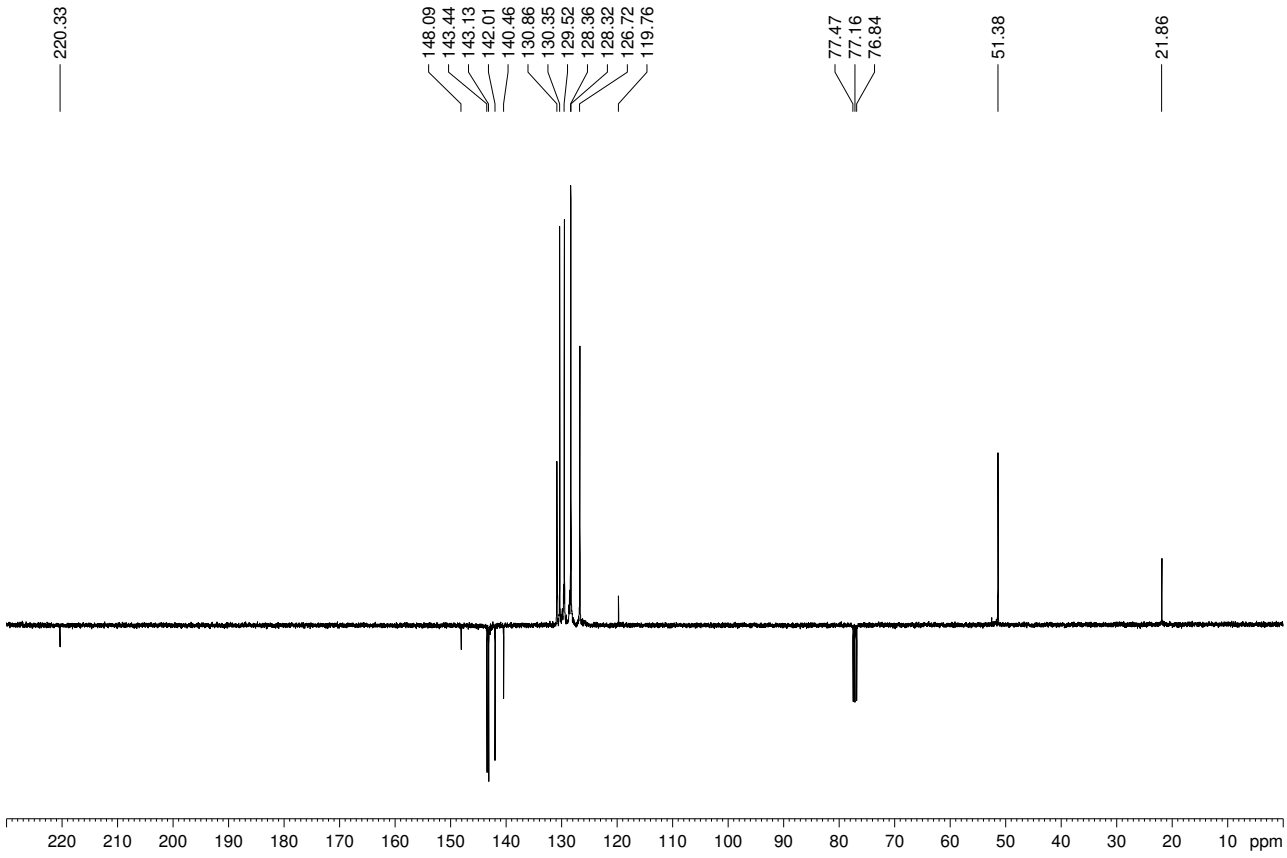

Figure S8. ^{13}C APT NMR spectrum (100 MHz, $CDCl_3$, 298 K) of IDip*Me·CS_2 (**1**)

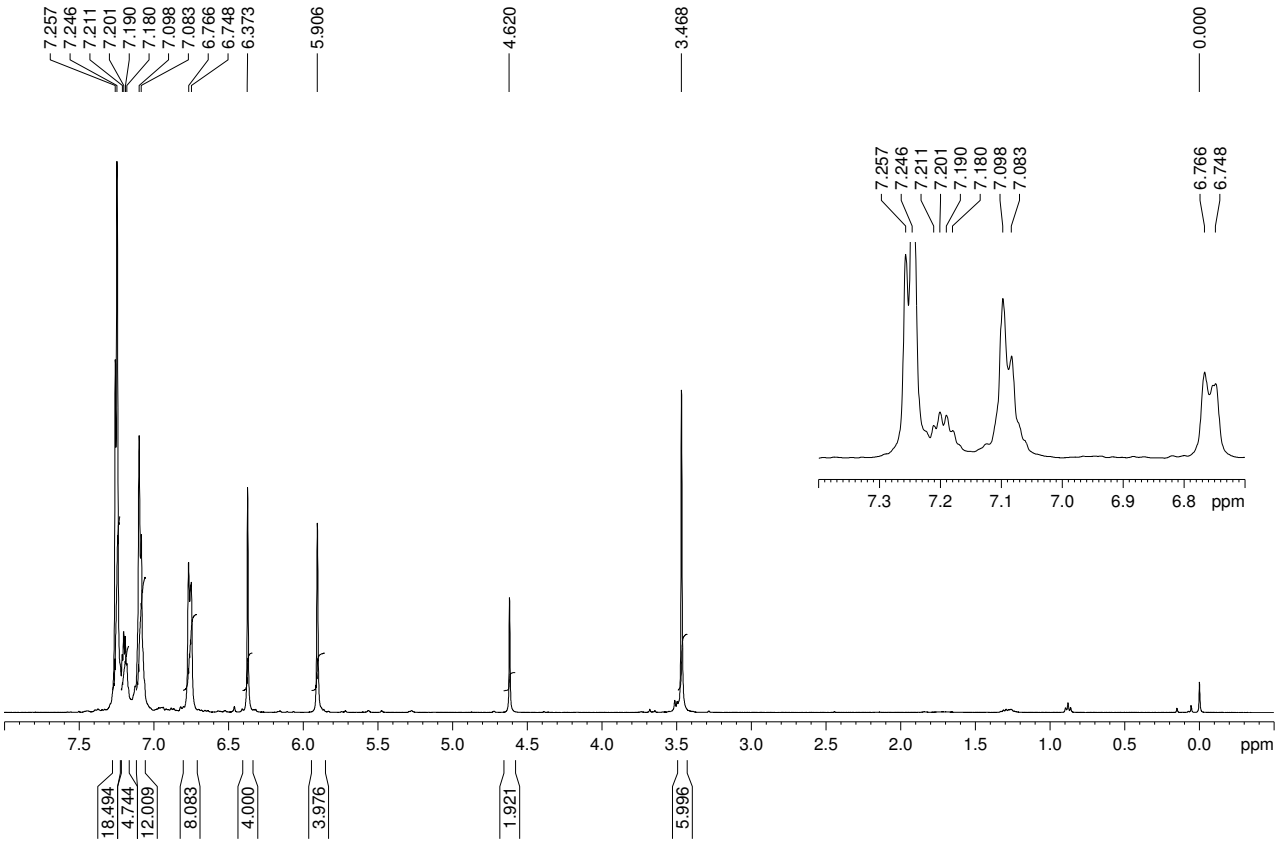

Figure S9. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 298 K) of IDip*OMe·CS_2 (**2**)

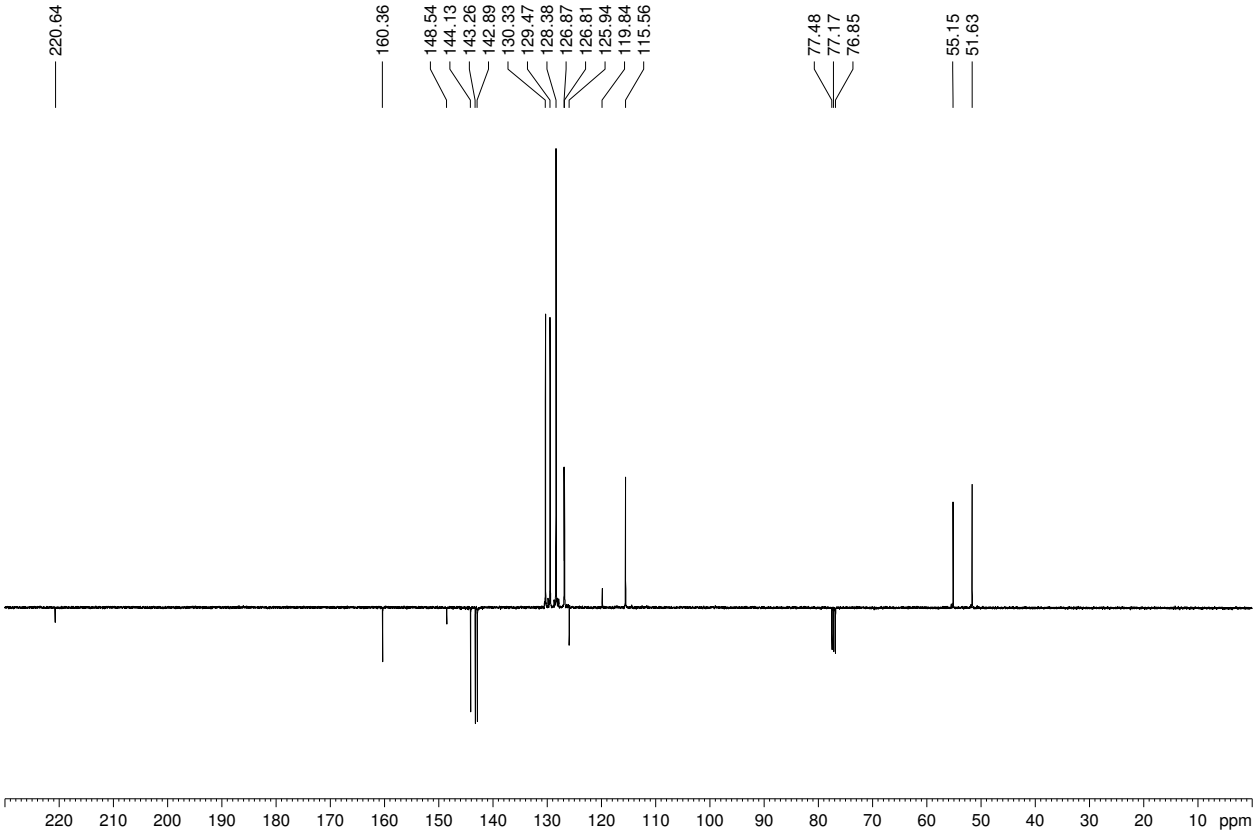

Figure S10. ^{13}C APT NMR spectrum (100 MHz, $CDCl_3$, 298 K) of IDip*OMe·CS_2 (**2**)

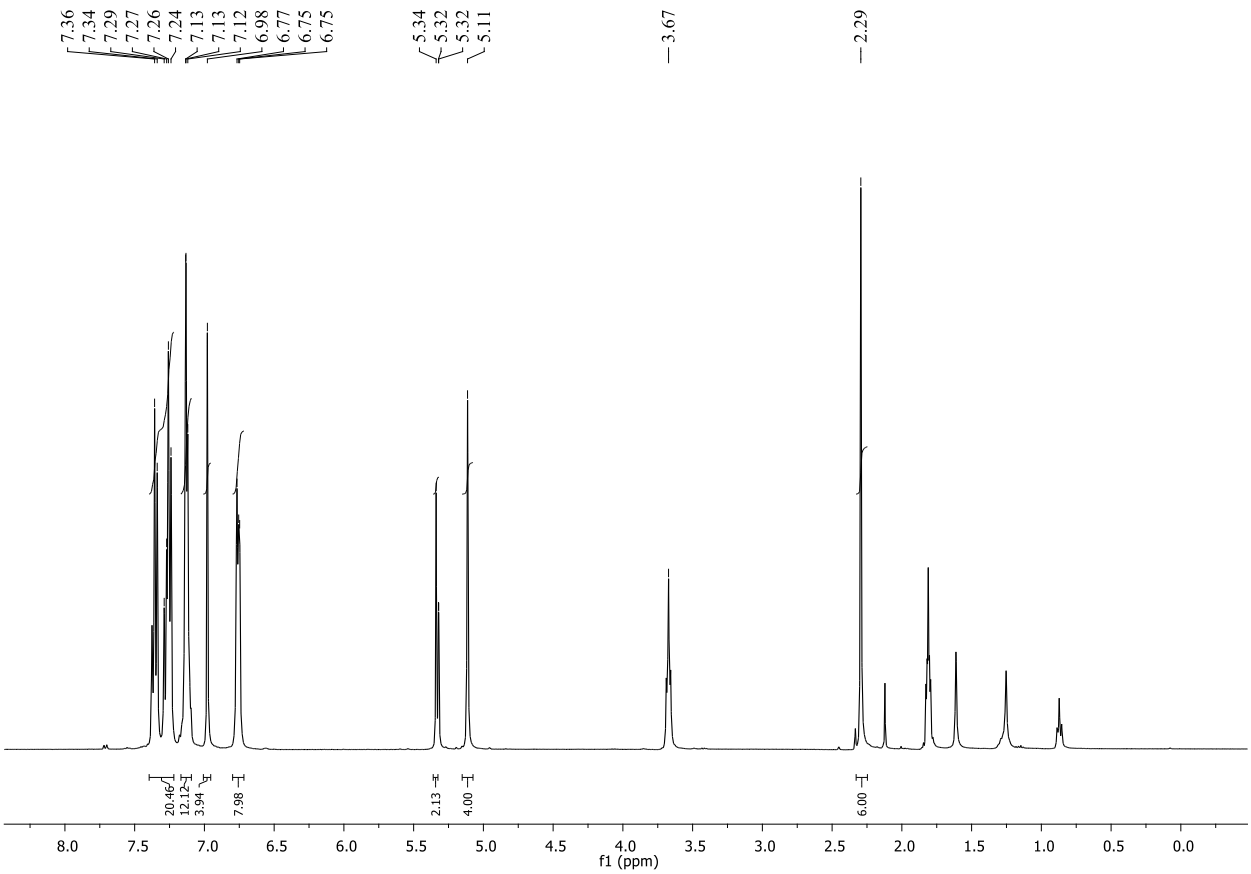

Figure S11. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2, 273 K) of [$ReBr(CO)_3(S_2C{\cdot}IDip^*Me)$] (**3**)

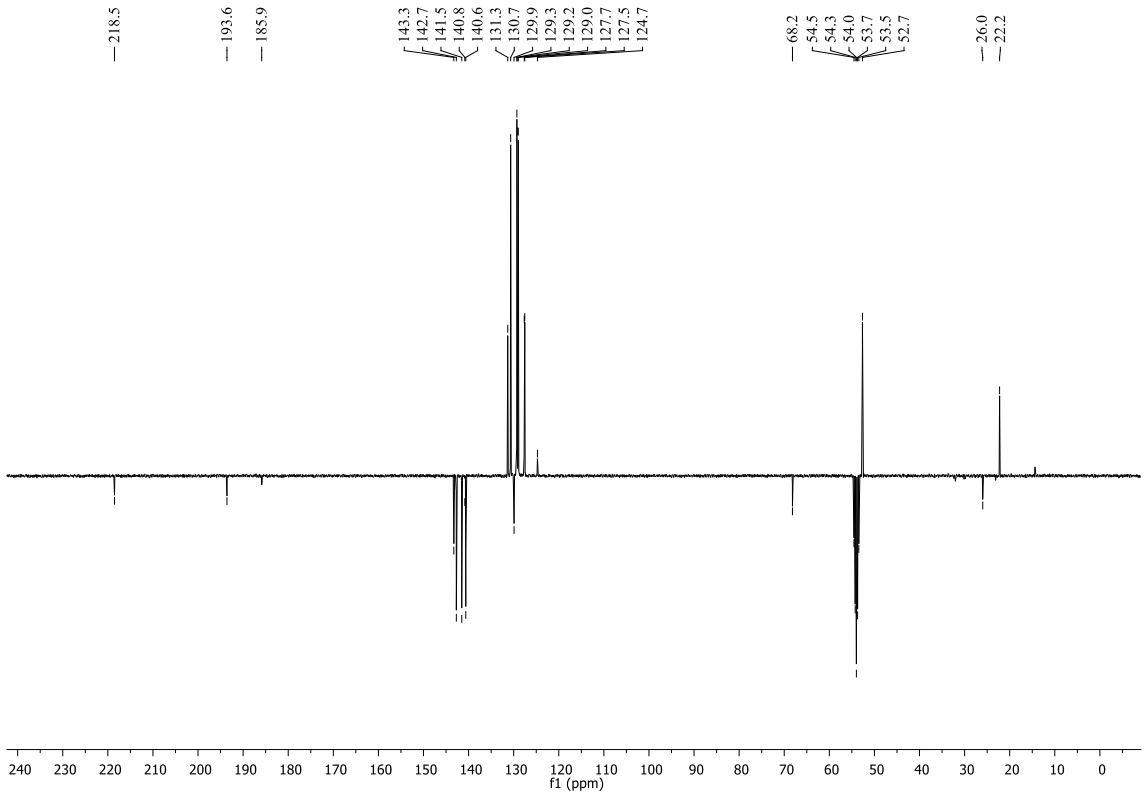

Figure S12. ^{13}C NMR spectrum (100 MHz, CD_2Cl_2, 273 K) of [$ReBr(CO)_3(S_2C{\cdot}IDip^*Me)$] (**3**)

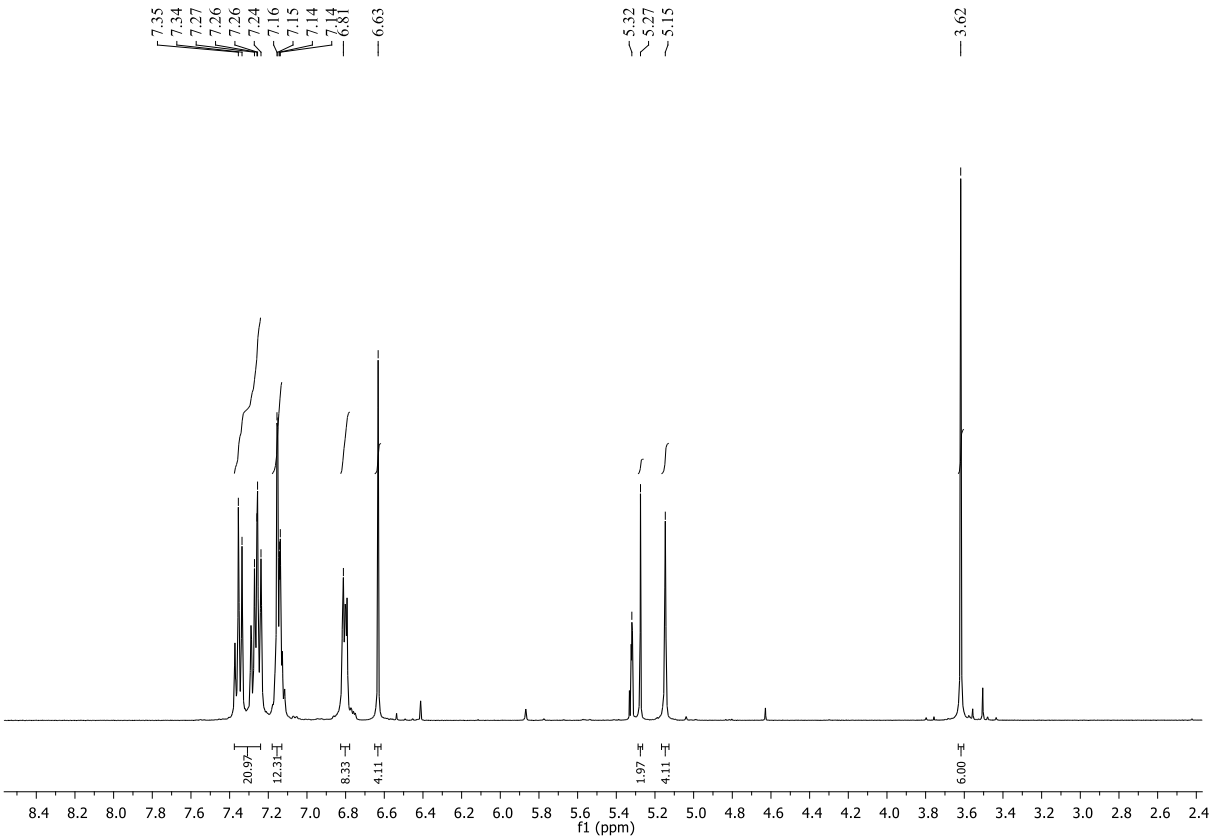

Figure S13. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2, 298 K) of [$ReBr(CO)_3(S_2C{\cdot}IDip^*OMe)$] (**4**)

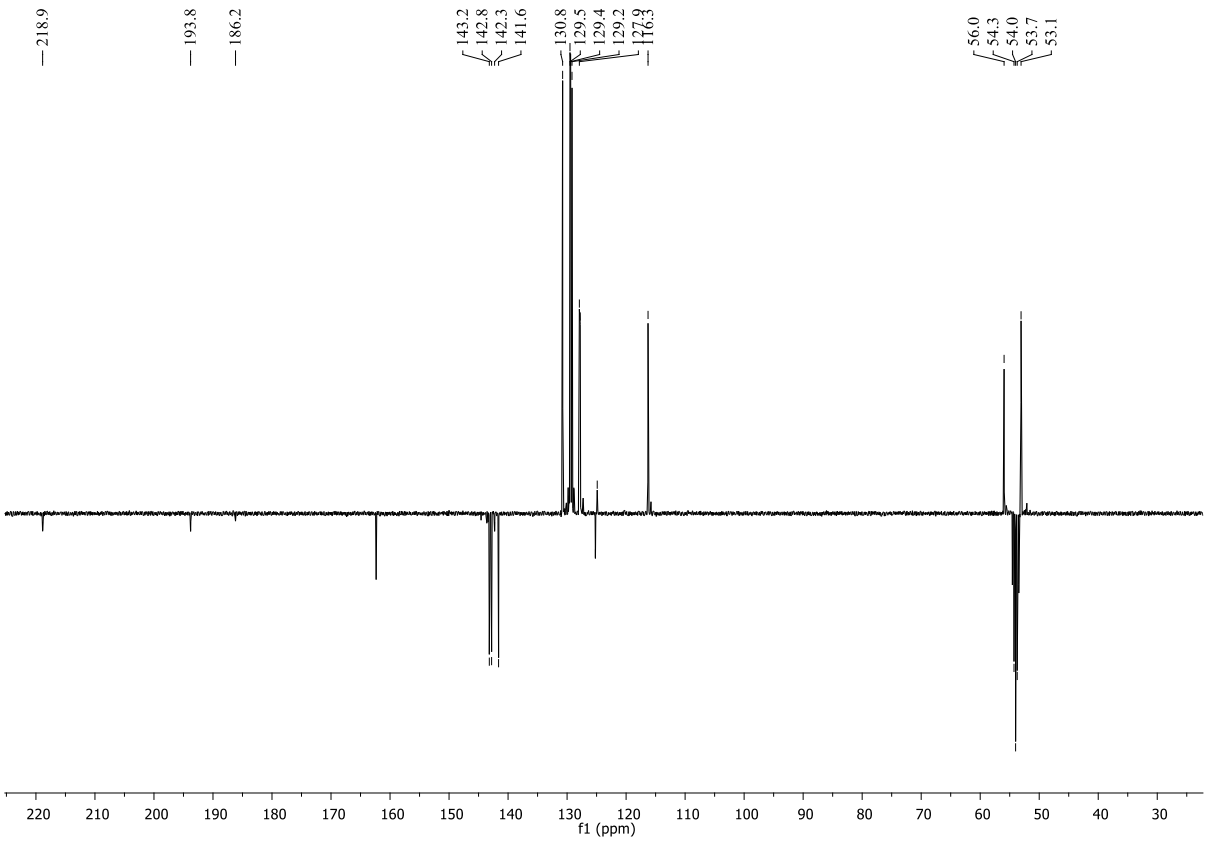

Figure S14. ^{13}C APT NMR spectrum (100 MHz, CD_2Cl_2, 298 K) of [$ReBr(CO)_3(S_2C{\cdot}IDip^*OMe)$] (**4**)

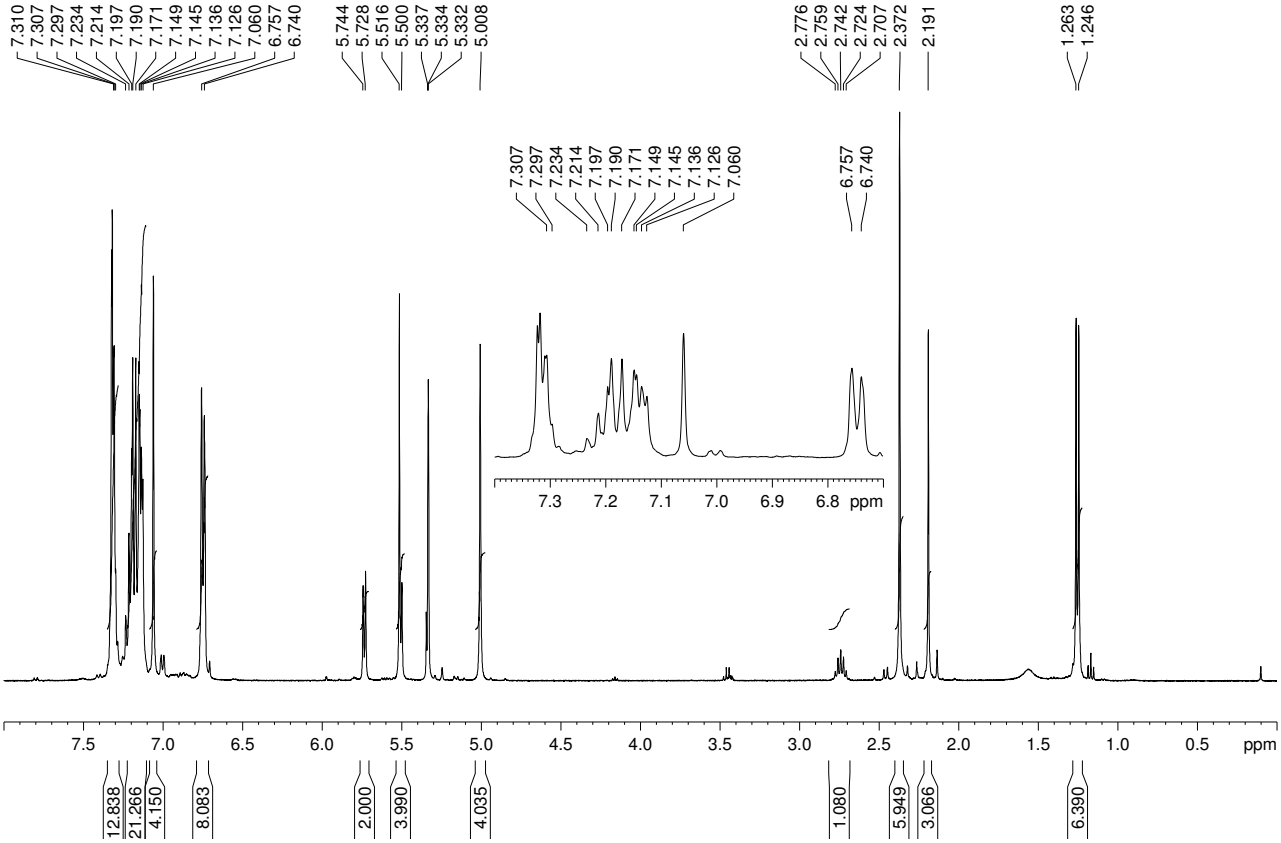

Figure S15. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2, 298 K) of [RuCl(*p*-cym)(S_2C·IDip*Me)]PF_6 (**5**)

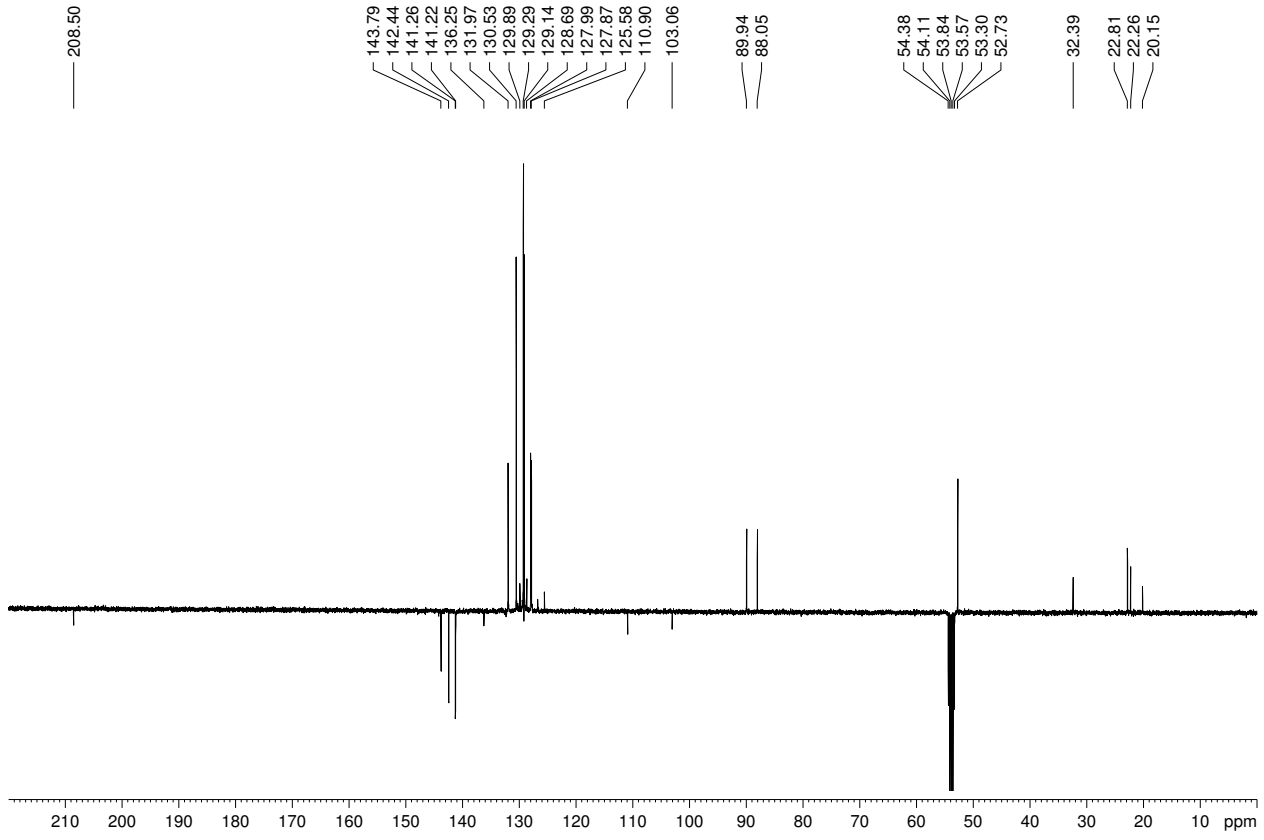

Figure S16. ^{13}C APT NMR spectrum (100 MHz, CD_2Cl_2, 298 K) of [RuCl(*p*-cym)(S_2C·IDip*Me)]PF_6 (**5**)

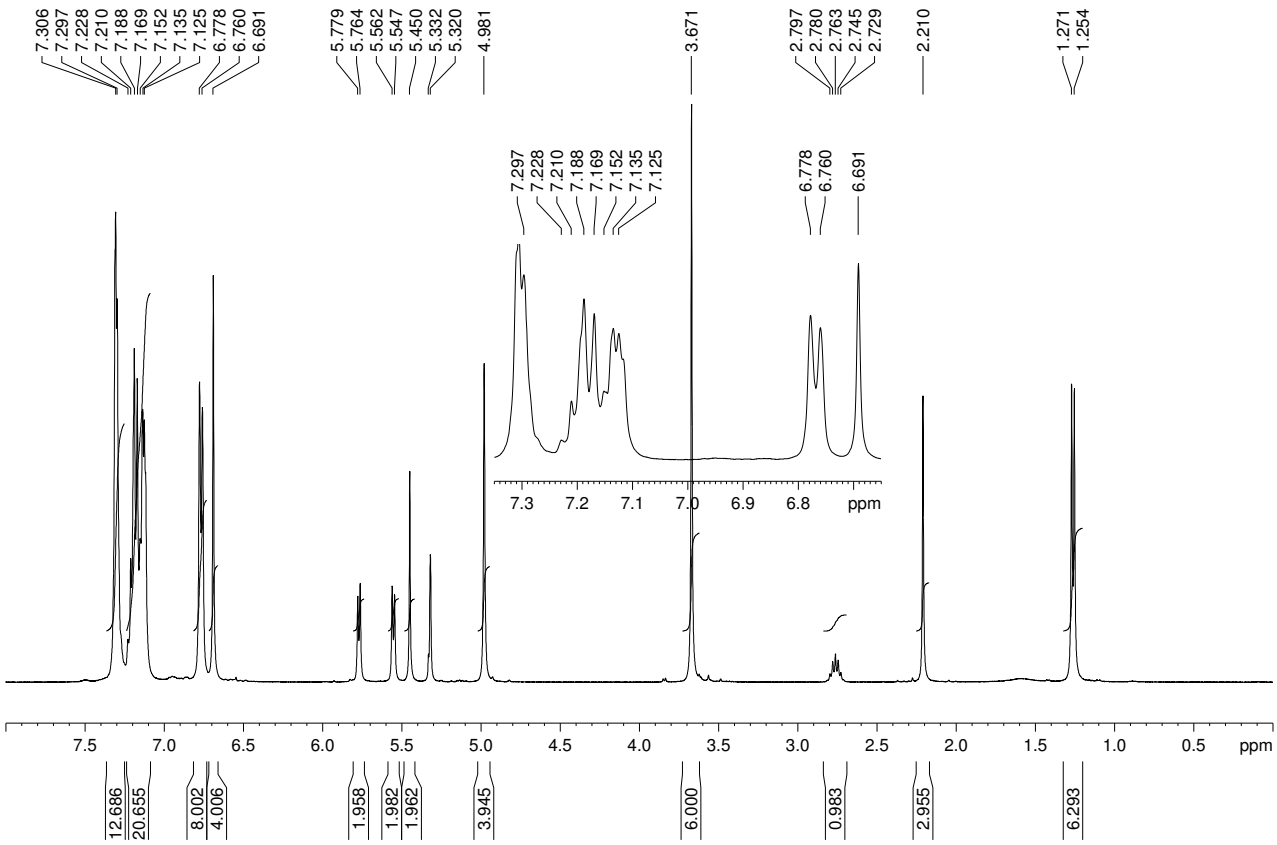

Figure S17. ^{1}H NMR spectrum (400 MHz, CD_2Cl_2, 298 K) of [RuCl(*p*-cym)(S_2C·IDip*OMe)]PF_6 (**6**)

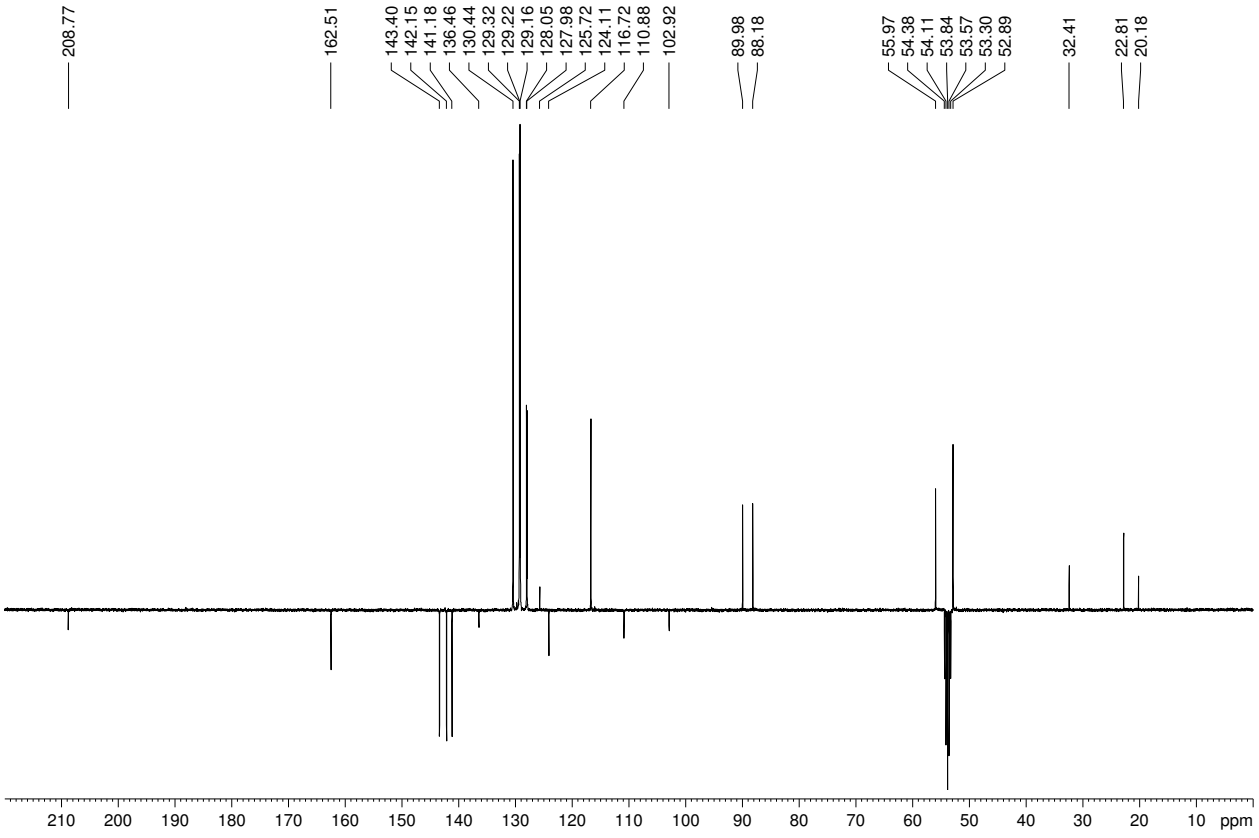

Figure S18. ^{13}C APT NMR spectrum (100 MHz, CD_2Cl_2, 298 K) of [RuCl(*p*-cym)(S_2C·IDip*OMe)]PF_6 (**6**)