# Hoveyda-Grubbs-type Precatalysts with Unsymmetrical N-Heterocyclic Carbenes as Effective Catalysts in Olefin Metathesis

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## Supporting Information

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NMR Characterization

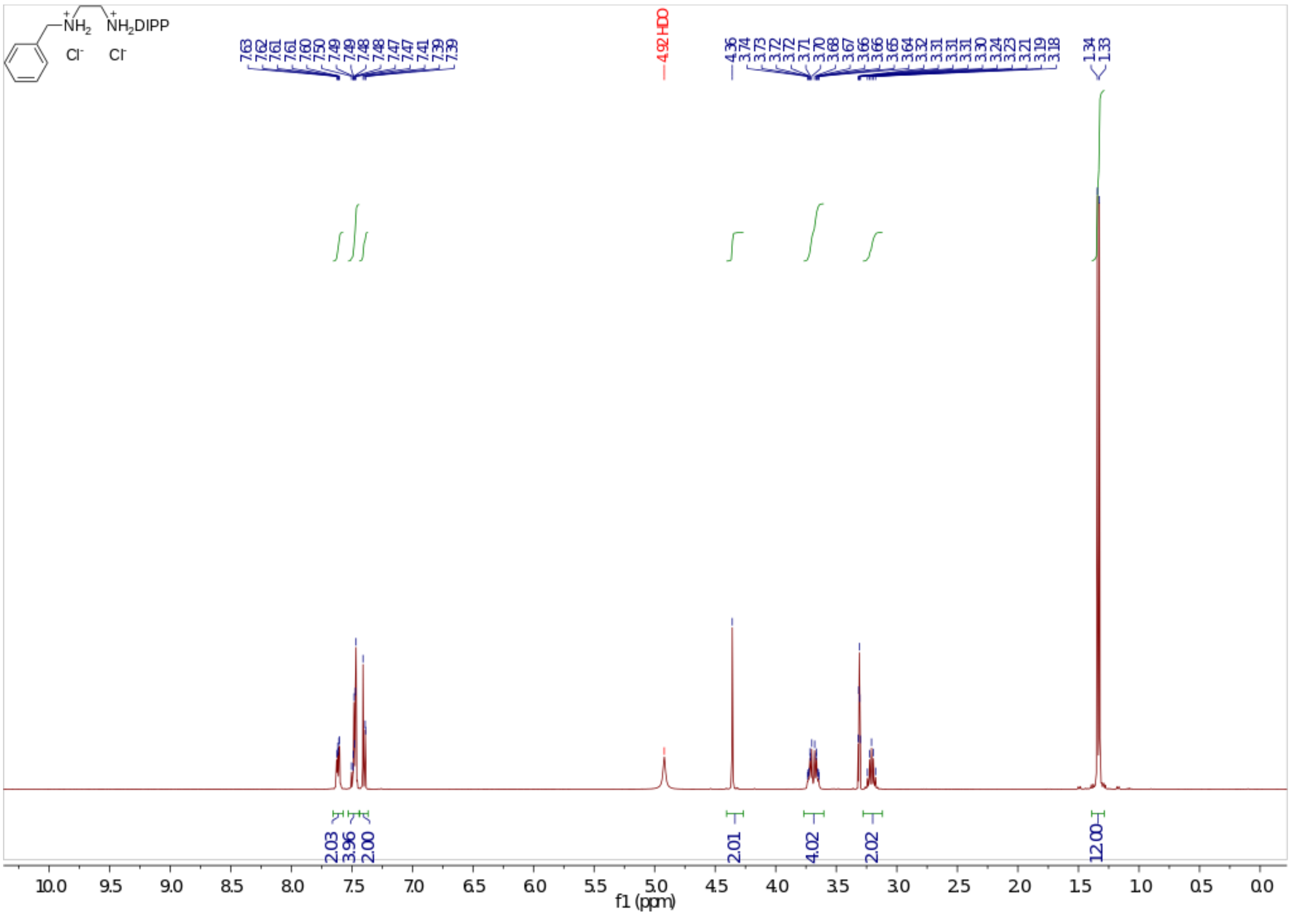


Figure S1. $^{1}H$ NMR spectrum of [4a] in $CD_3OD$, 400MHz.

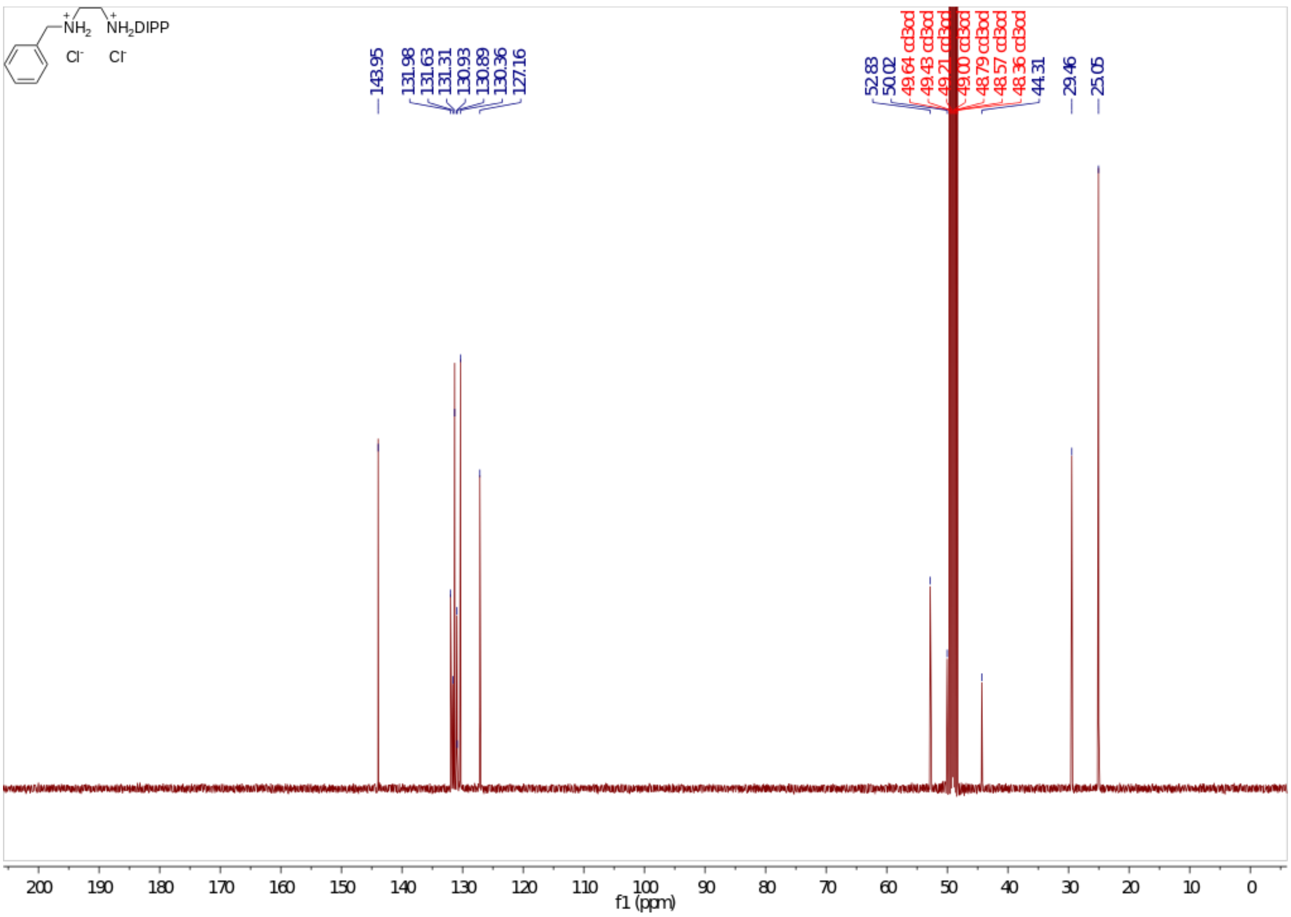


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of [4a] in $CD_3OD$, 100MHz.

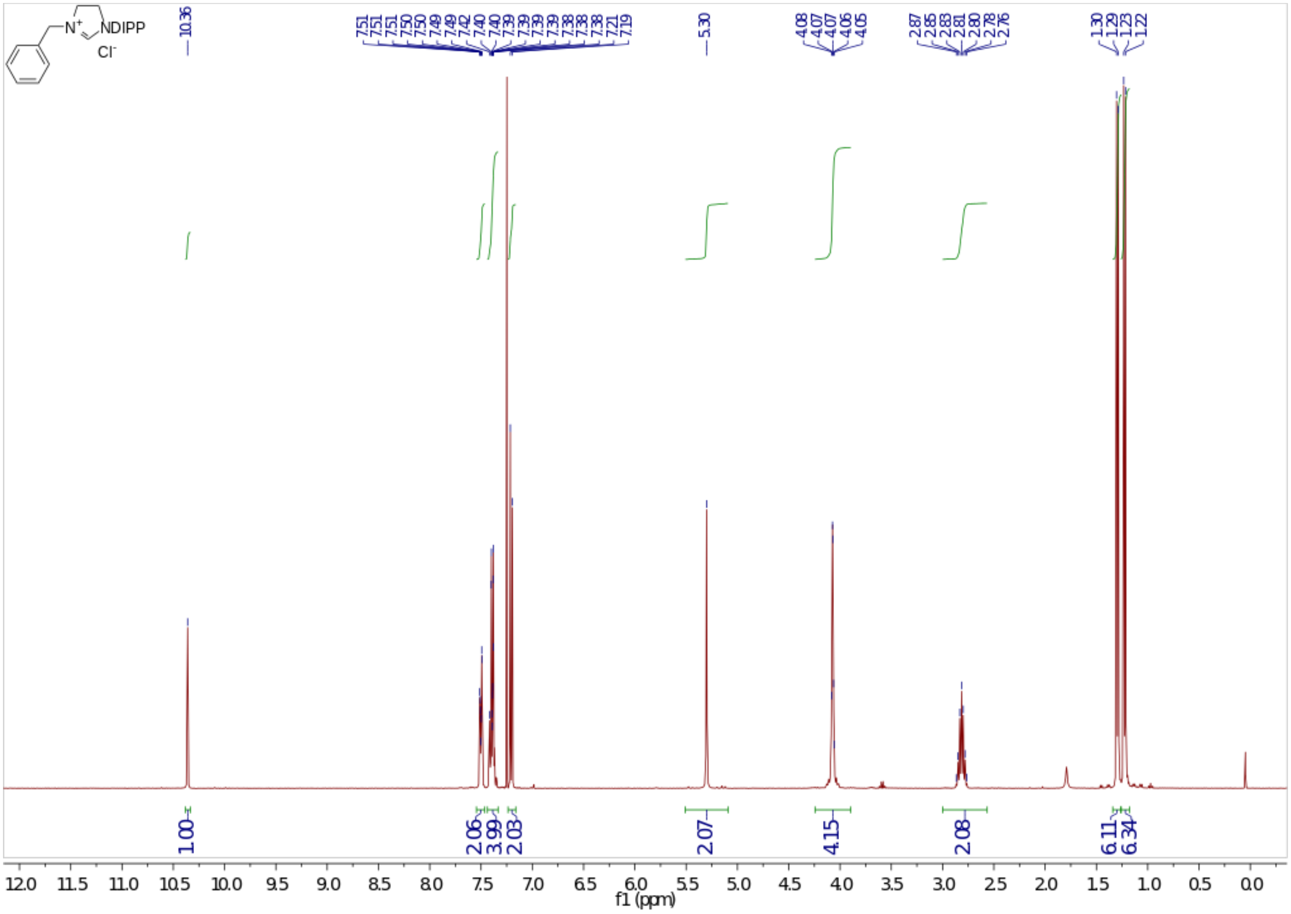


Figure S3. $^{1}H$ NMR spectrum of [5a] in $CDCl_3$, 400MHz.

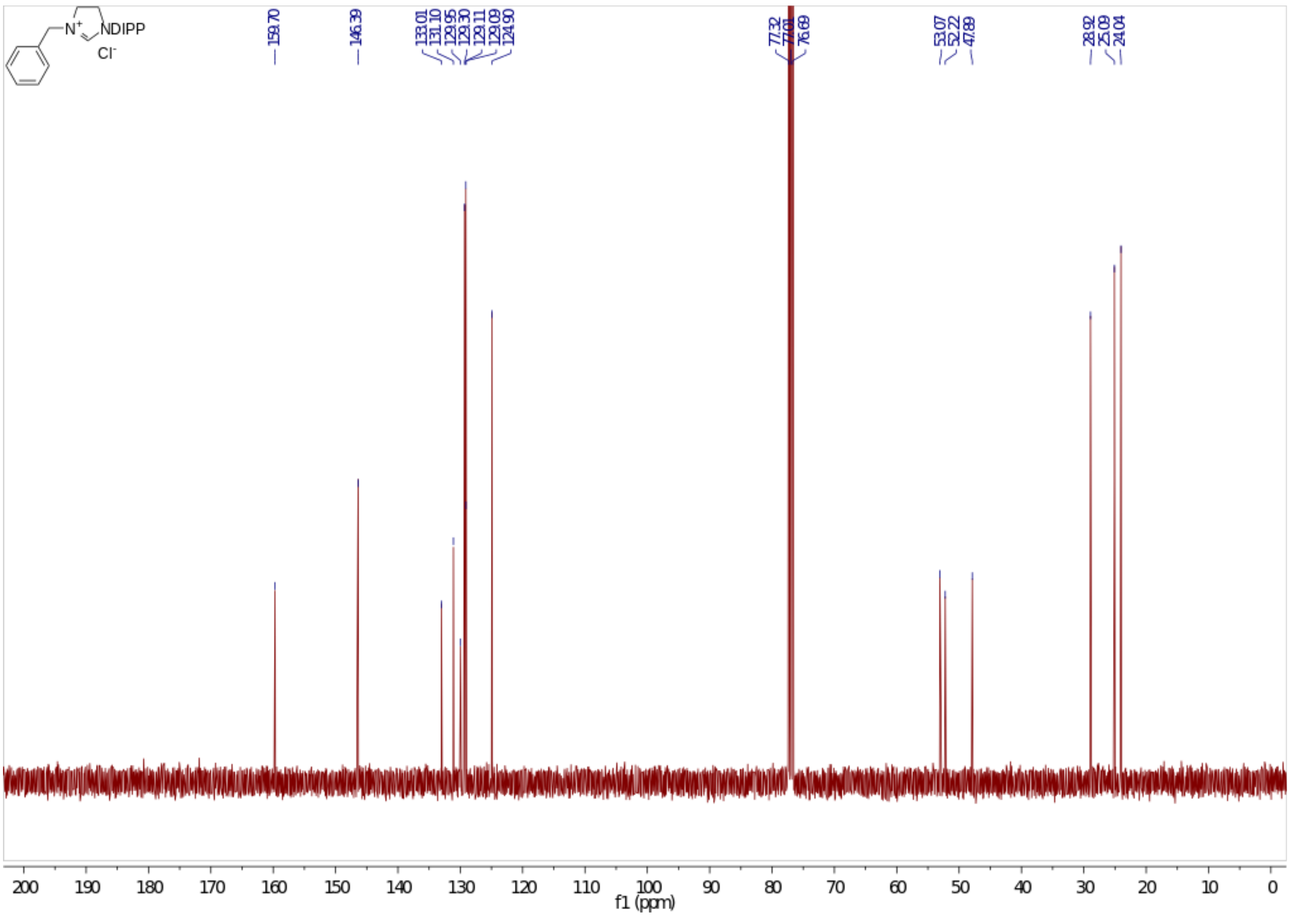


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of [5a] in $CDCl_3$, 100MHz.

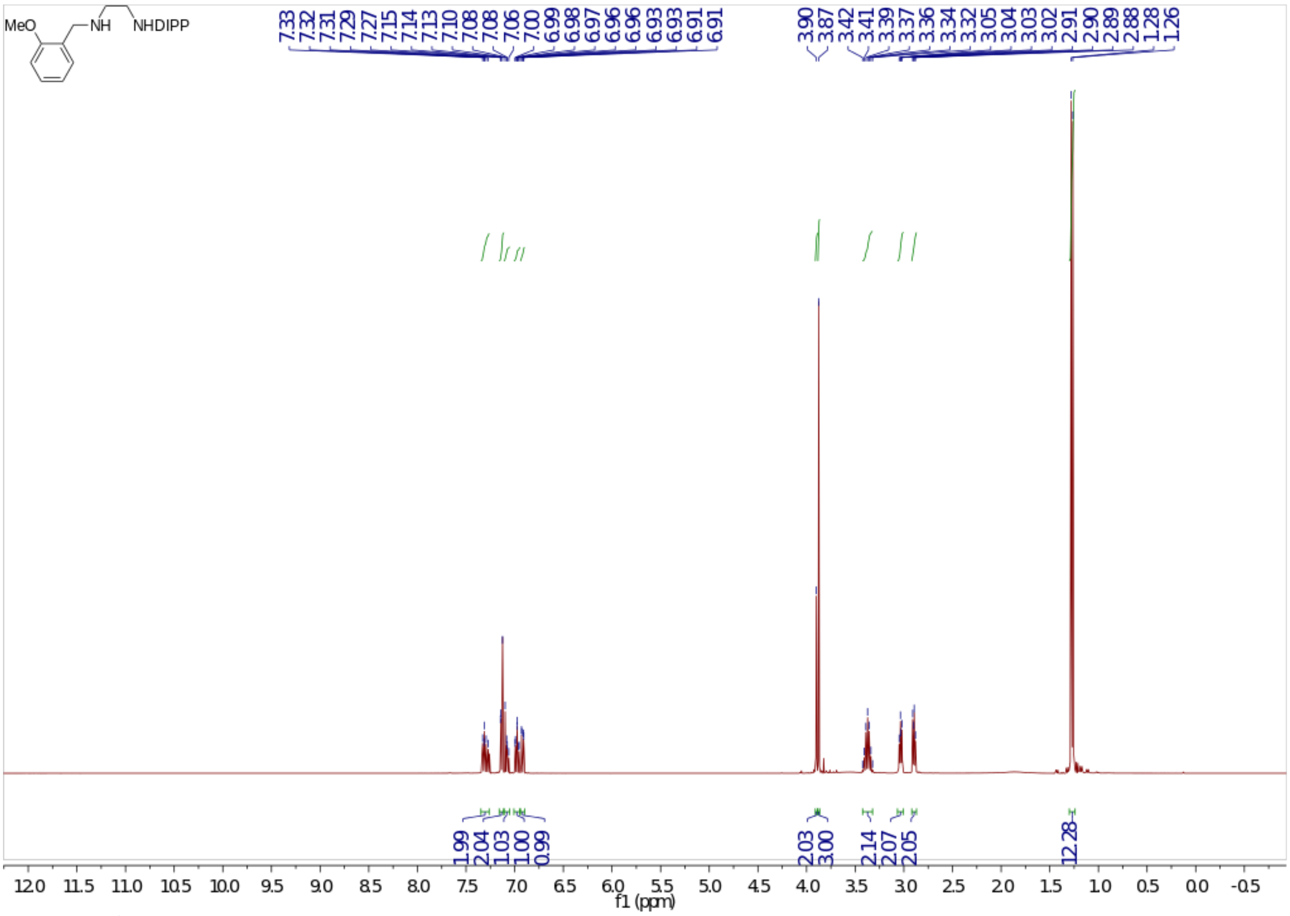


Figure S5. $^{1}$H NMR spectrum of [4b] in $CDCl_3$, 400MHz.

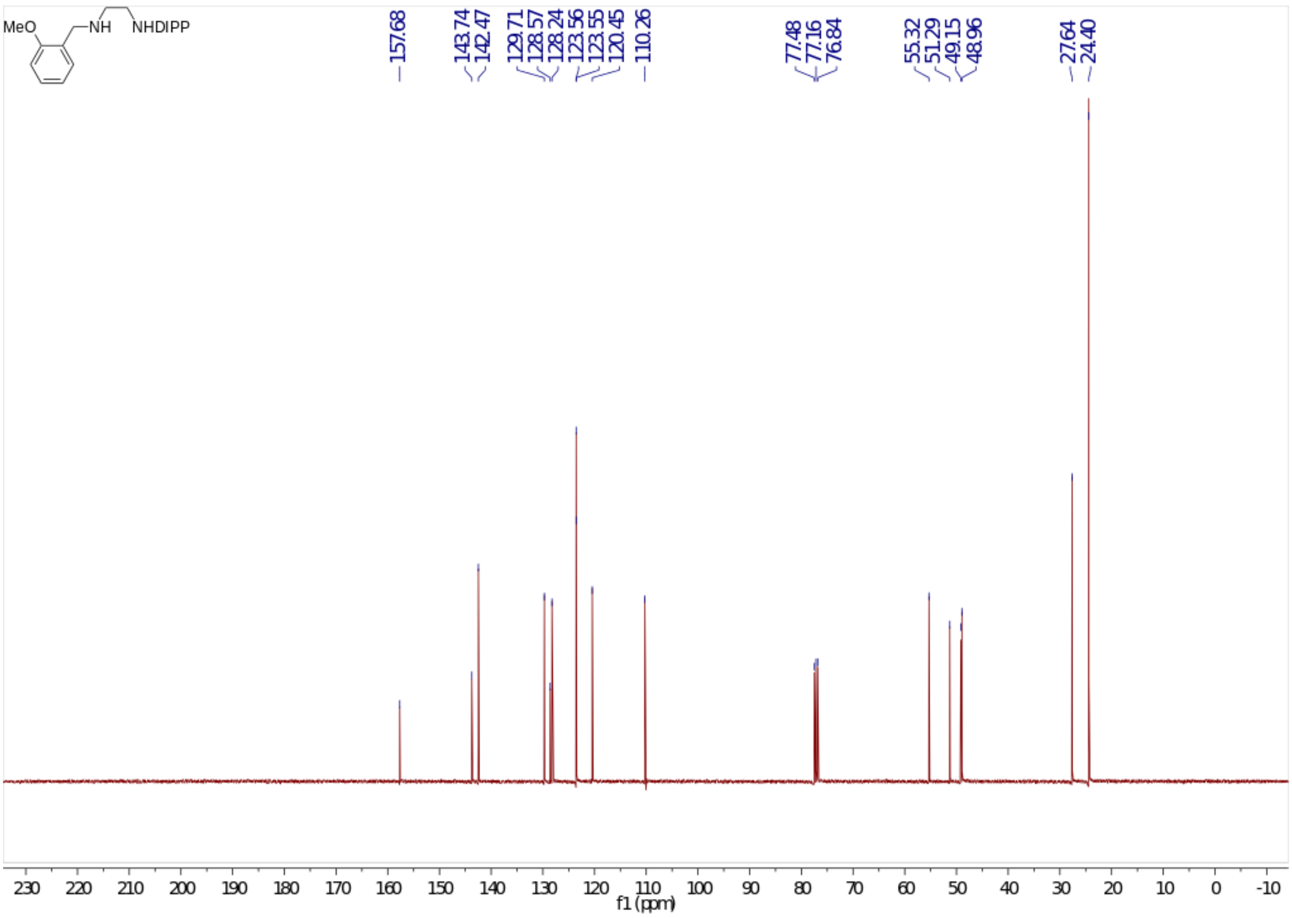


Figure S6. $^{13}$C{$^{1}$H} NMR spectrum of [4b] in $CDCl_3$, 100MHz.

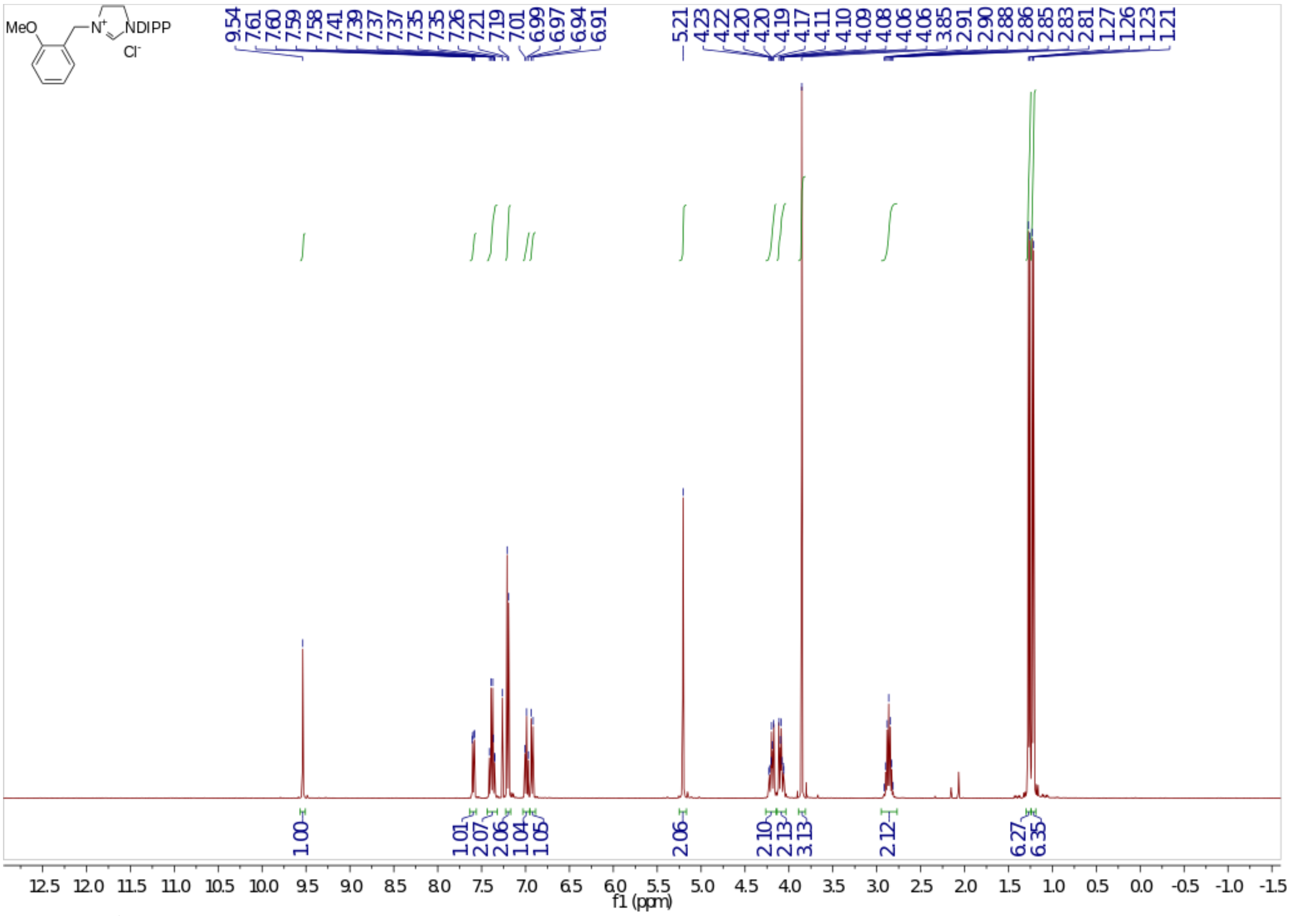


Figure S7. [1]H NMR spectrum of [5b] in $CDCl_3$, 400MHz.

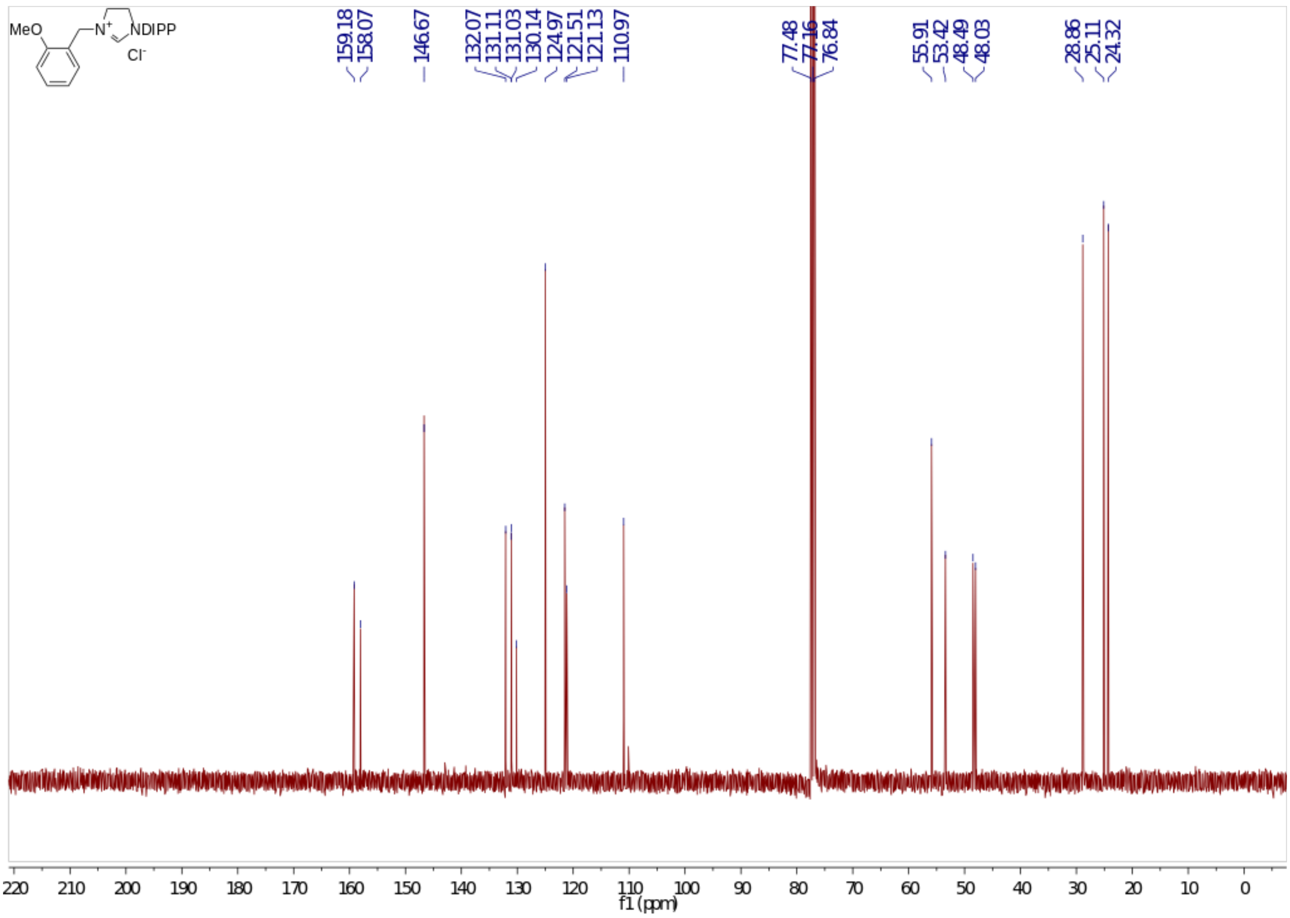


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of [5b] in $CDCl_3$, 100MHz.

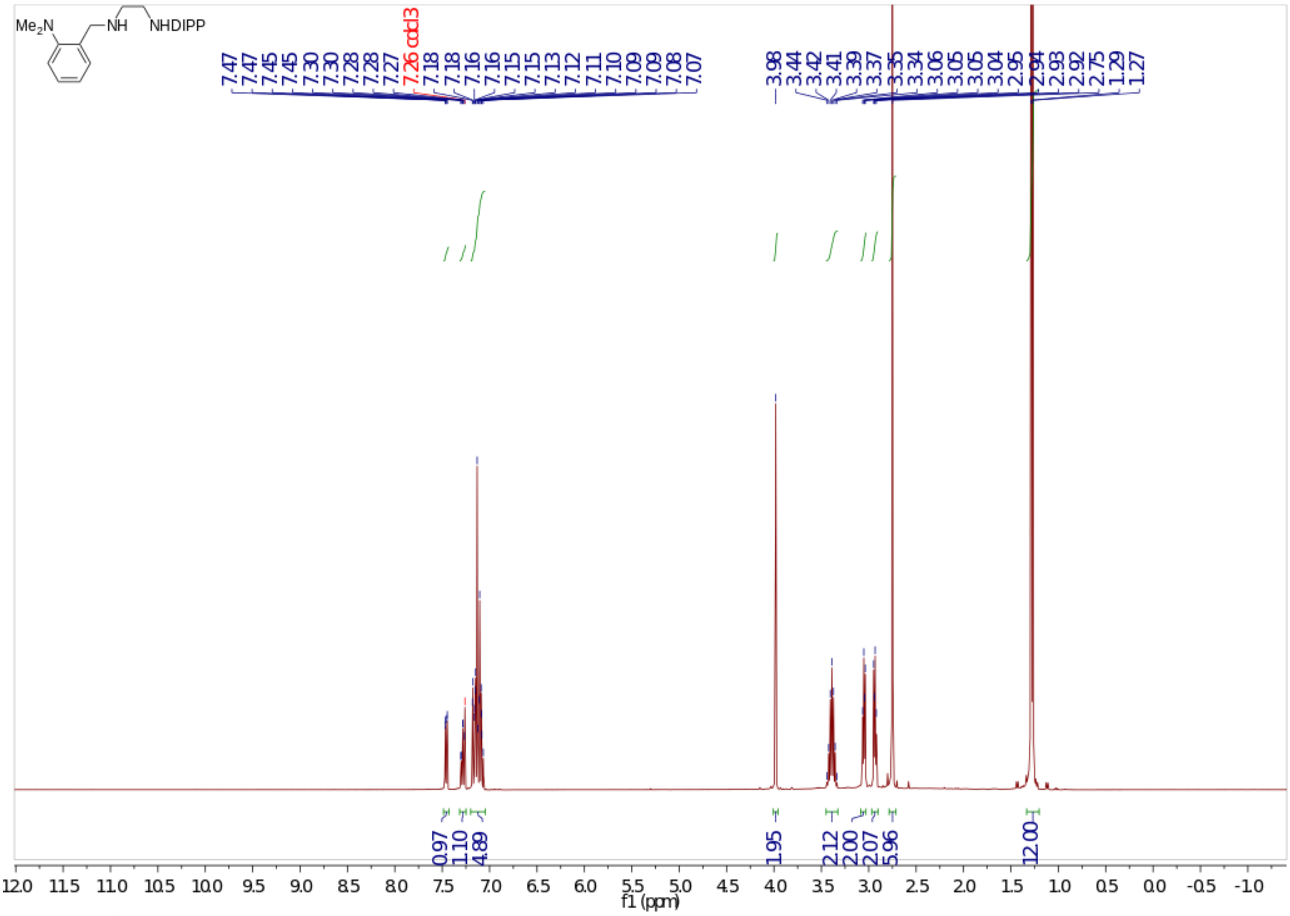

Figure S9. $^{1}H$ NMR spectrum of [4c] in $CDCl_3$, 400MHz.

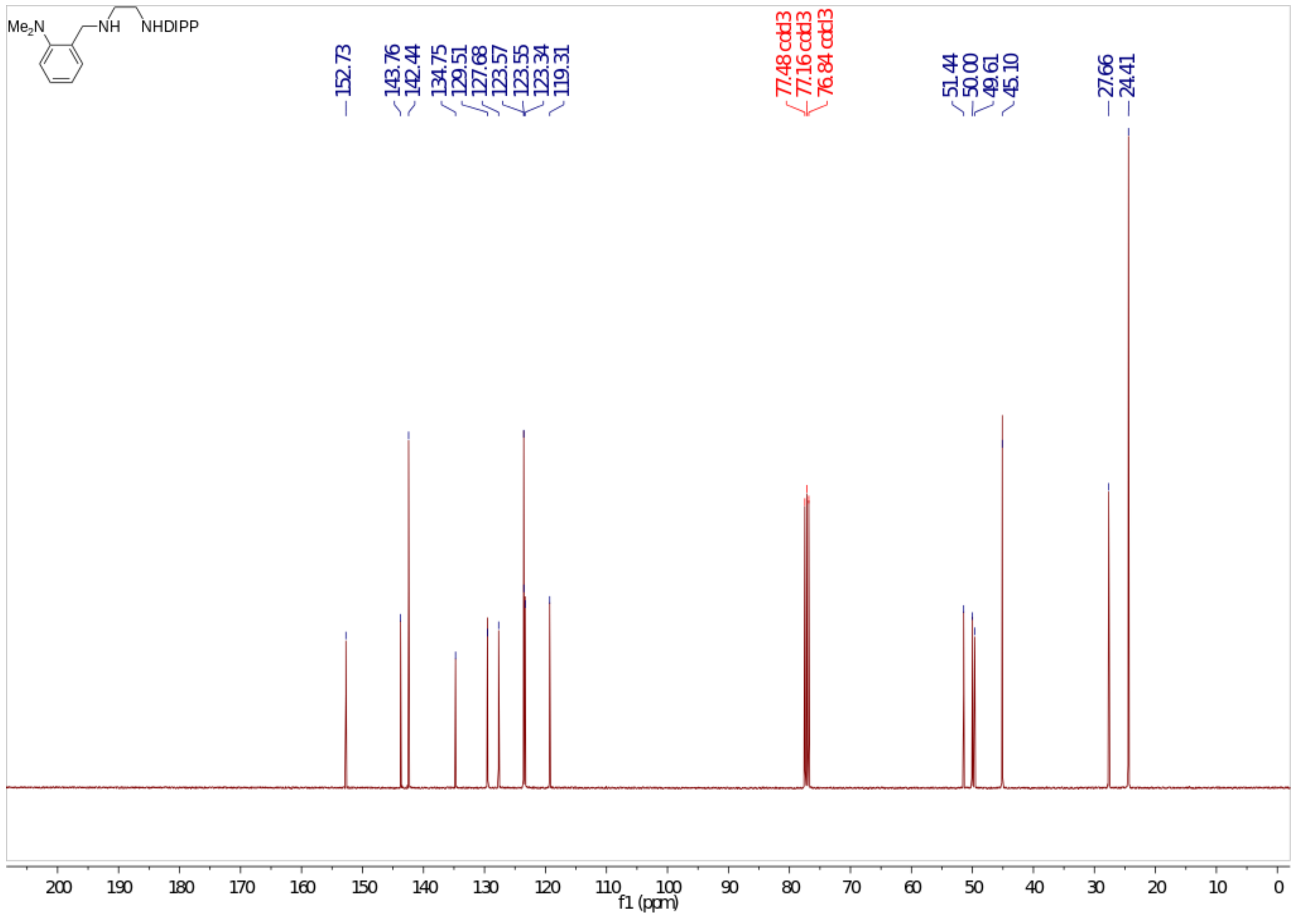

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of [4c] in $CDCl_3$, 100MHz.

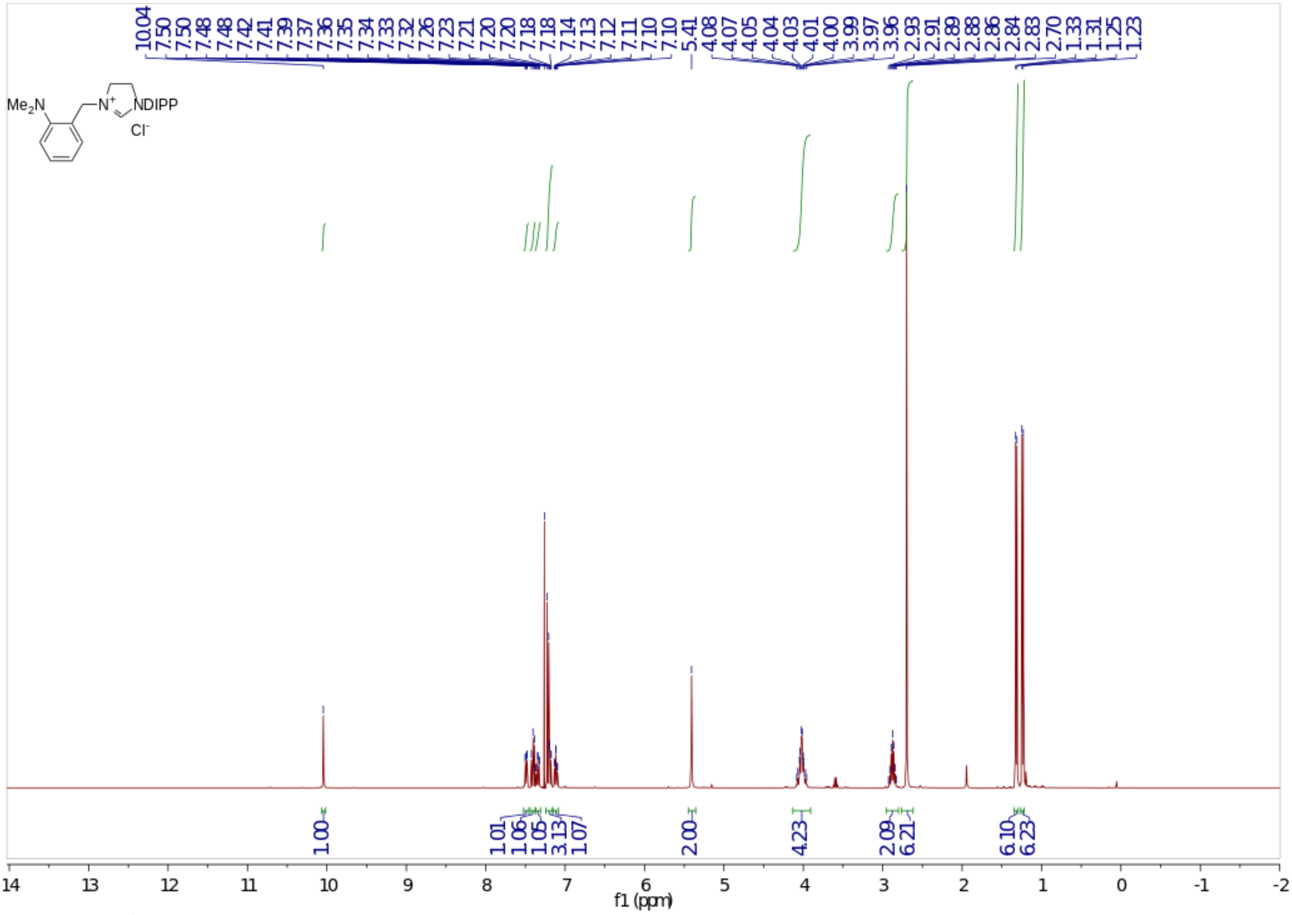

Figure S11. $^{1}$H NMR spectrum of [5c] in $CDCl_3$, 400MHz.

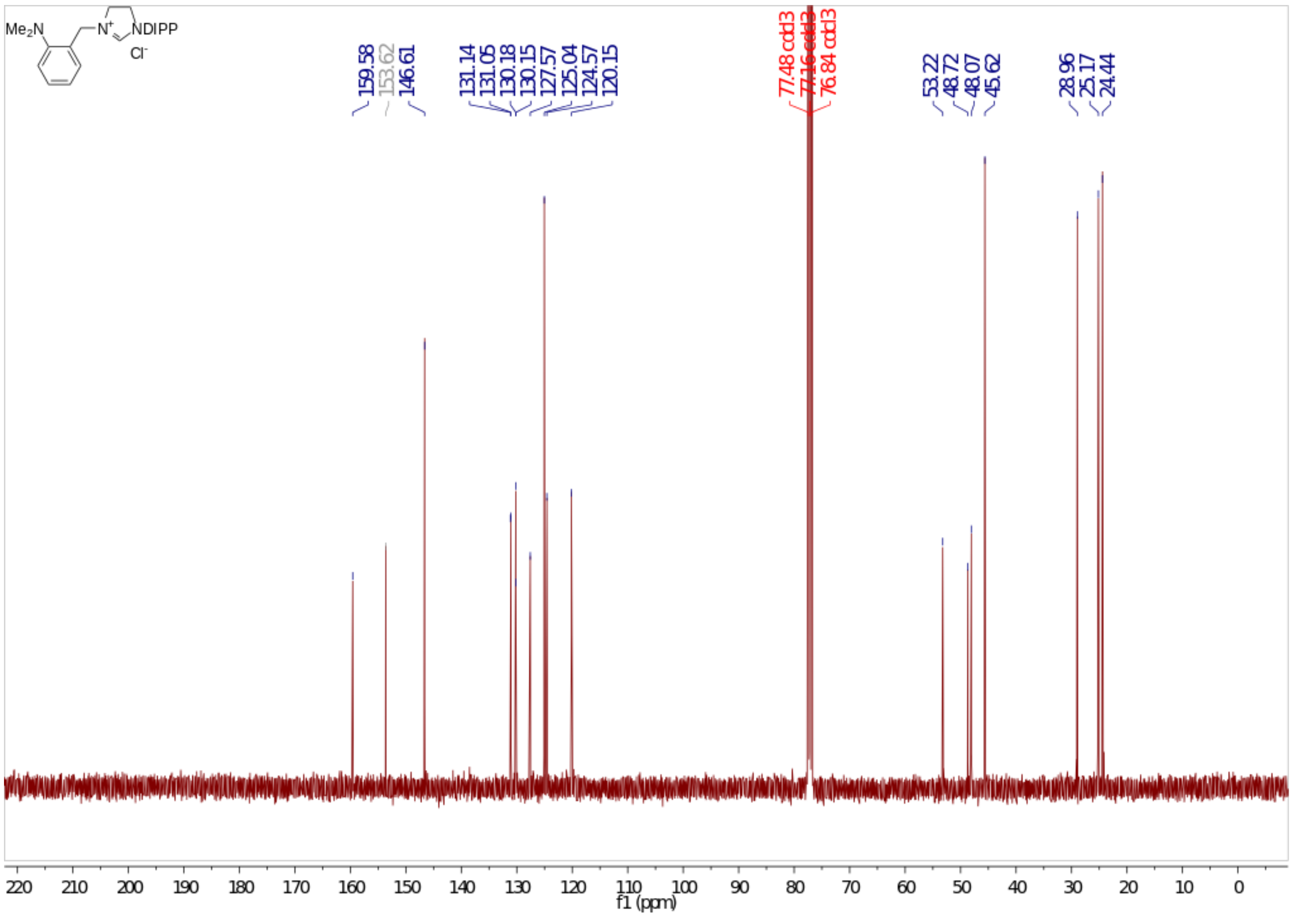

Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of [5c] in $CDCl_3$, 100MHz.

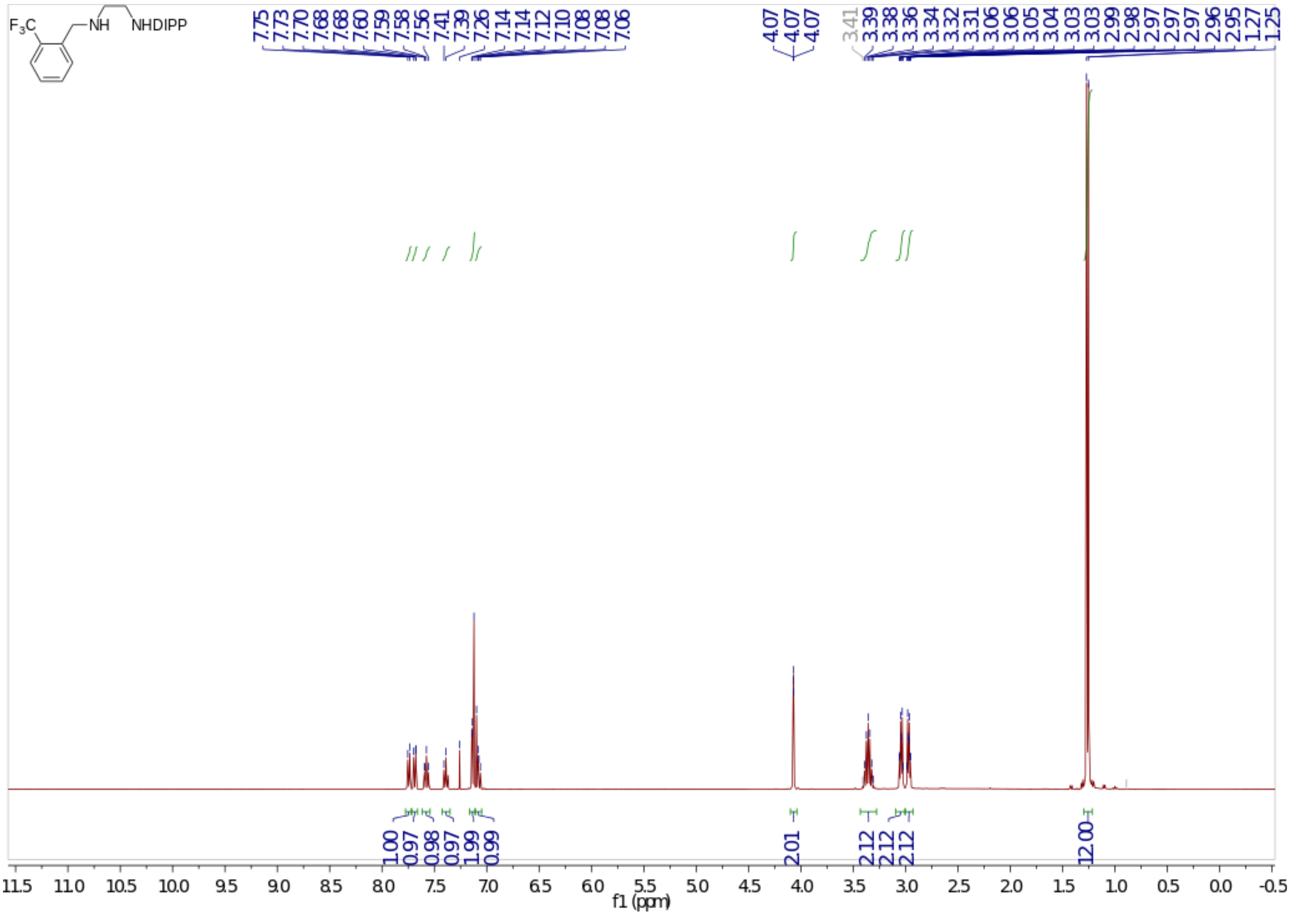


Figure S13. $^{1}$H NMR spectrum of [4d] in $CDCl_3$, 400MHz.

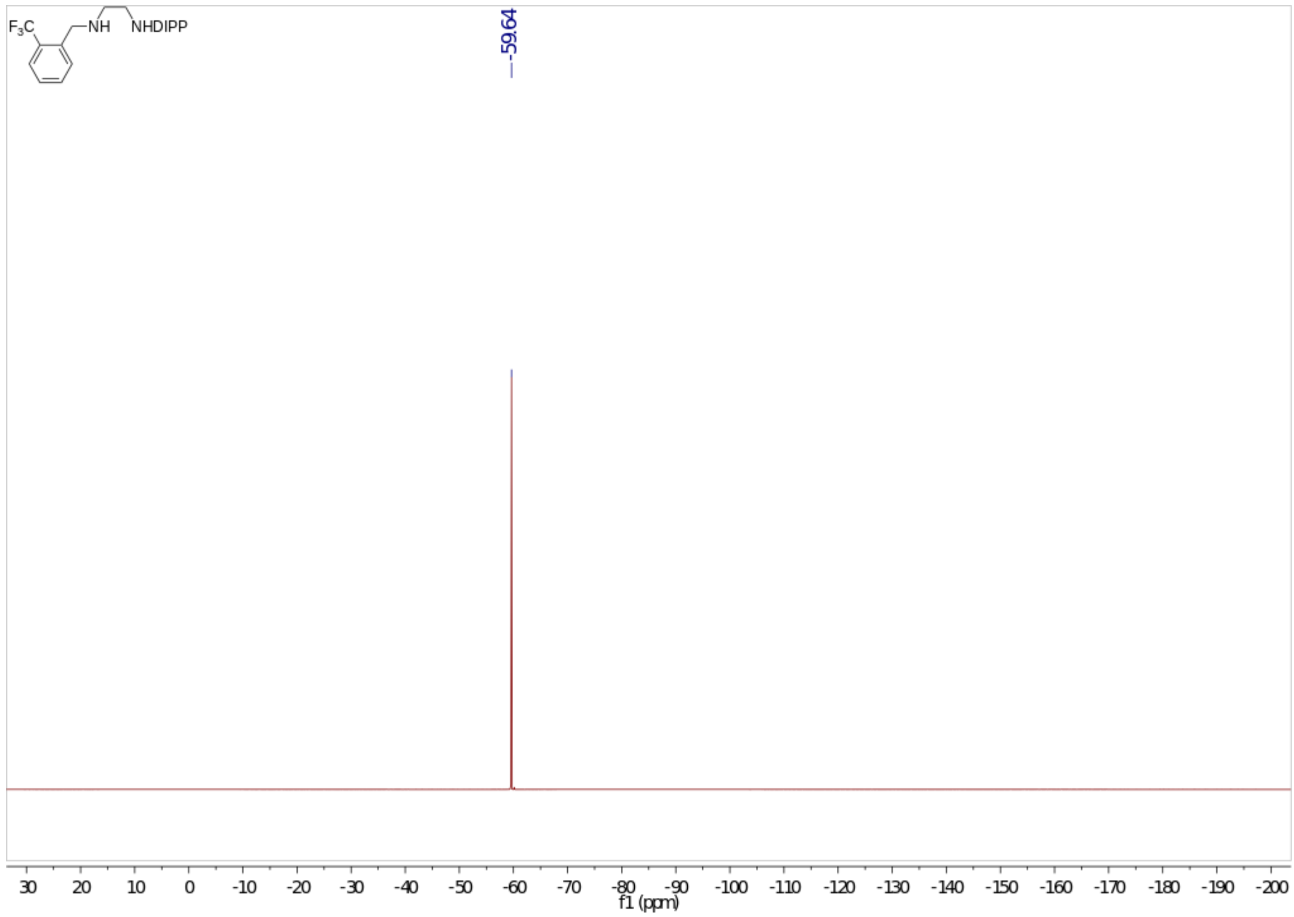


Figure S14. $^{19}$F NMR spectrum of [4d] in $CDCl_3$, 376MHz.

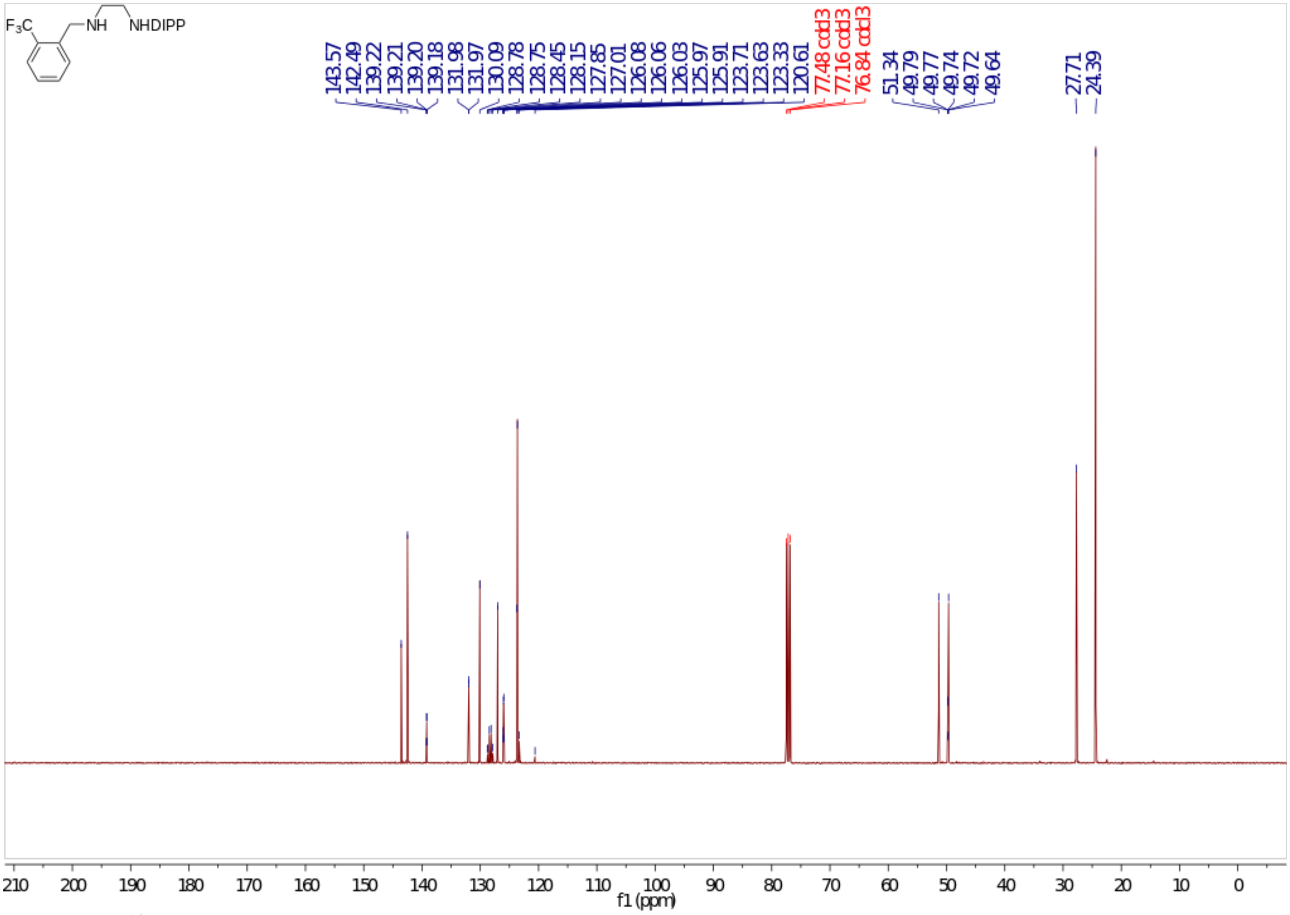


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of [4d] in $CDCl_3$, 100MHz.

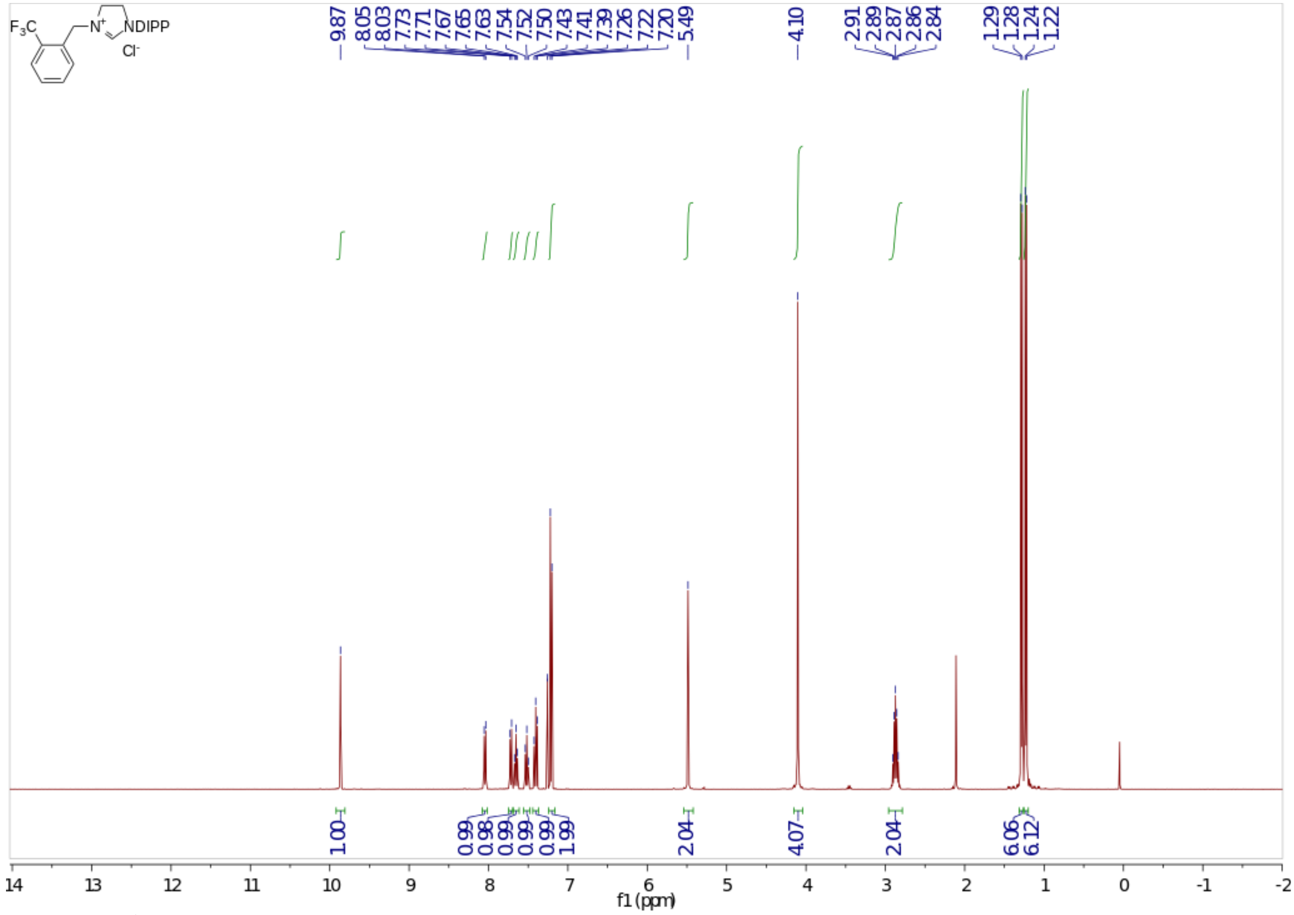

Figure S16. $^{1}$H NMR spectrum of [5d] in $CDCl_3$, 400MHz.

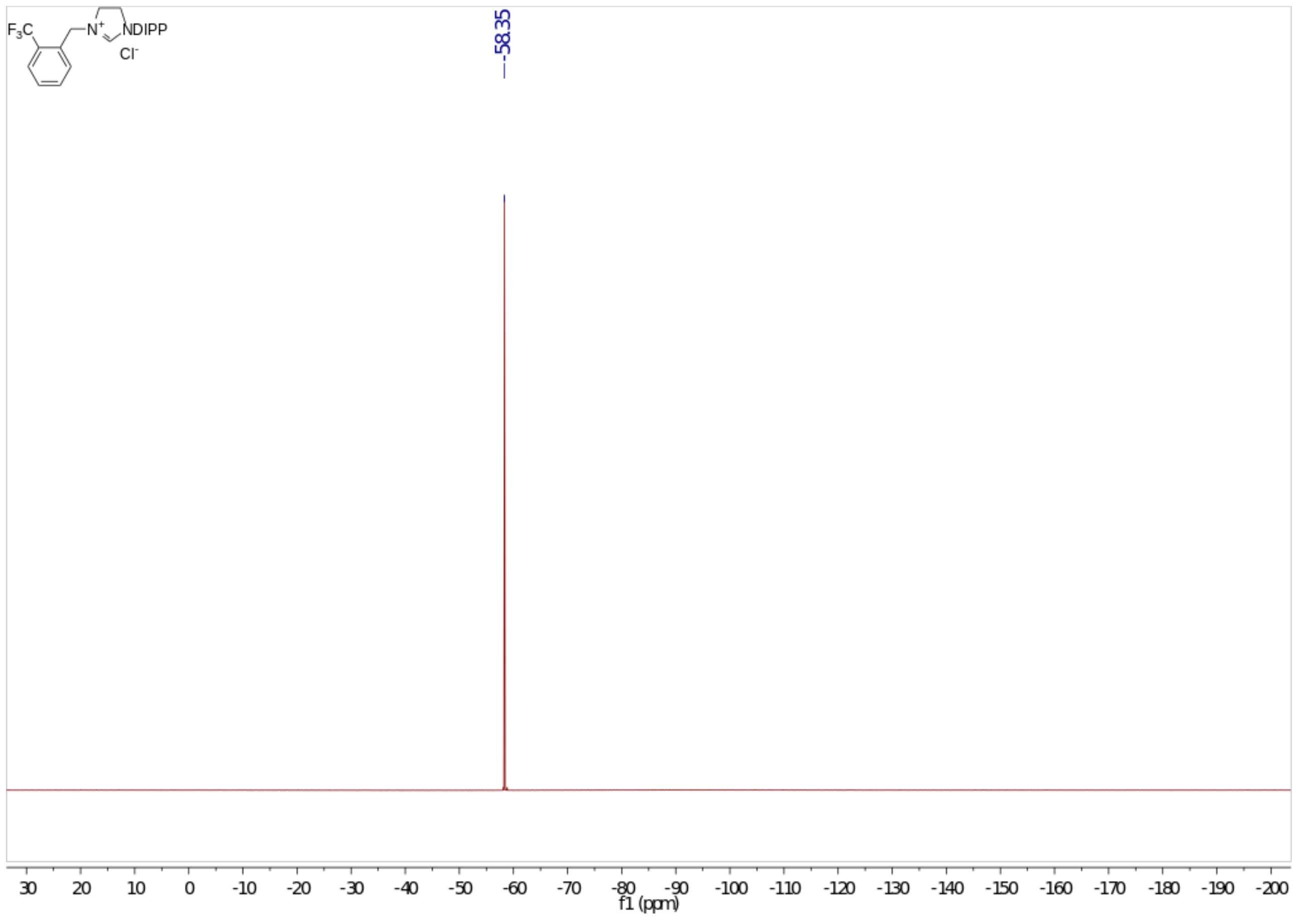

Figure S17. $^{19}$F NMR spectrum of [5d] in $CDCl_3$, 376MHz.

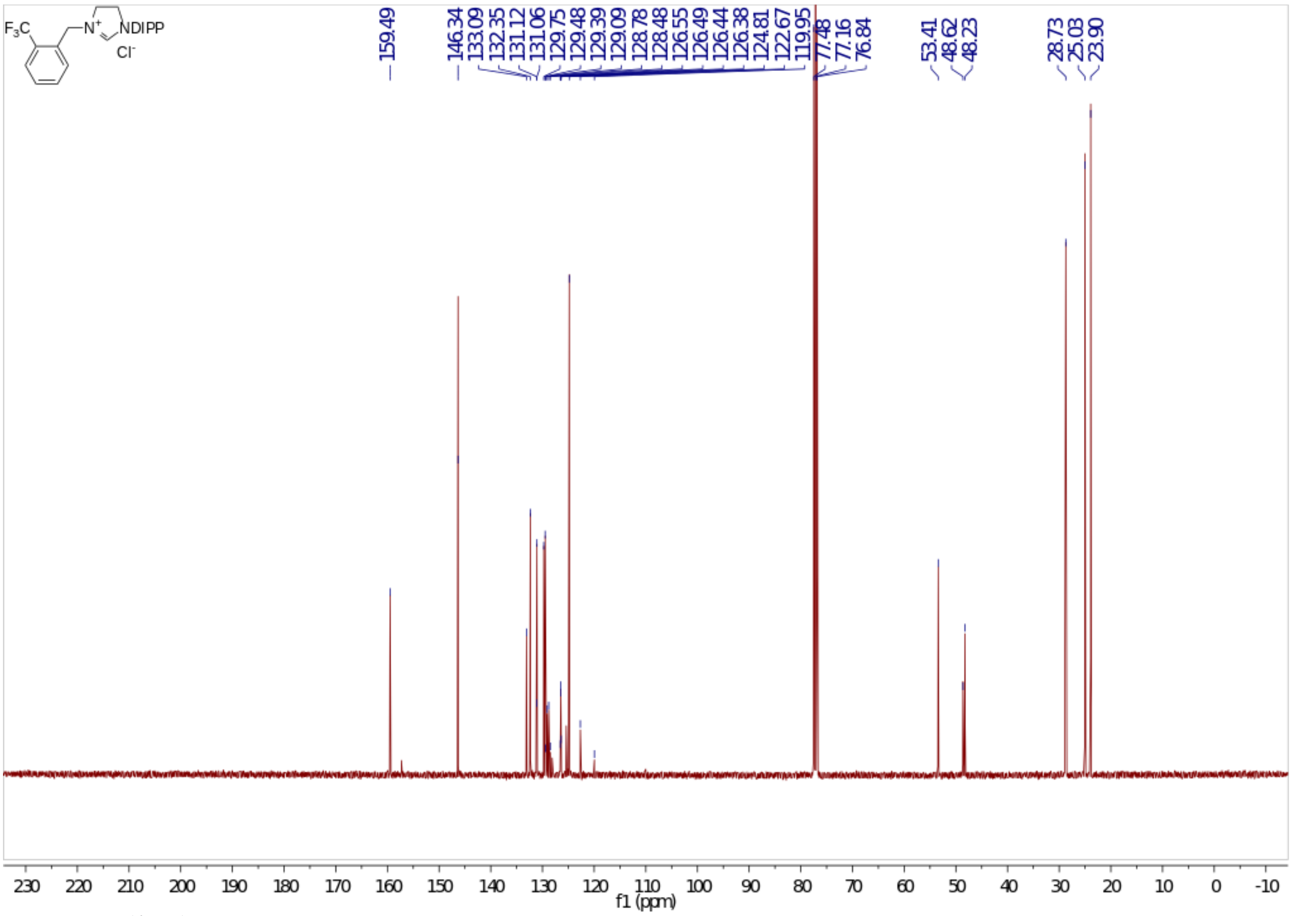


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of [5d] in $CDCl_3$, 100MHz.

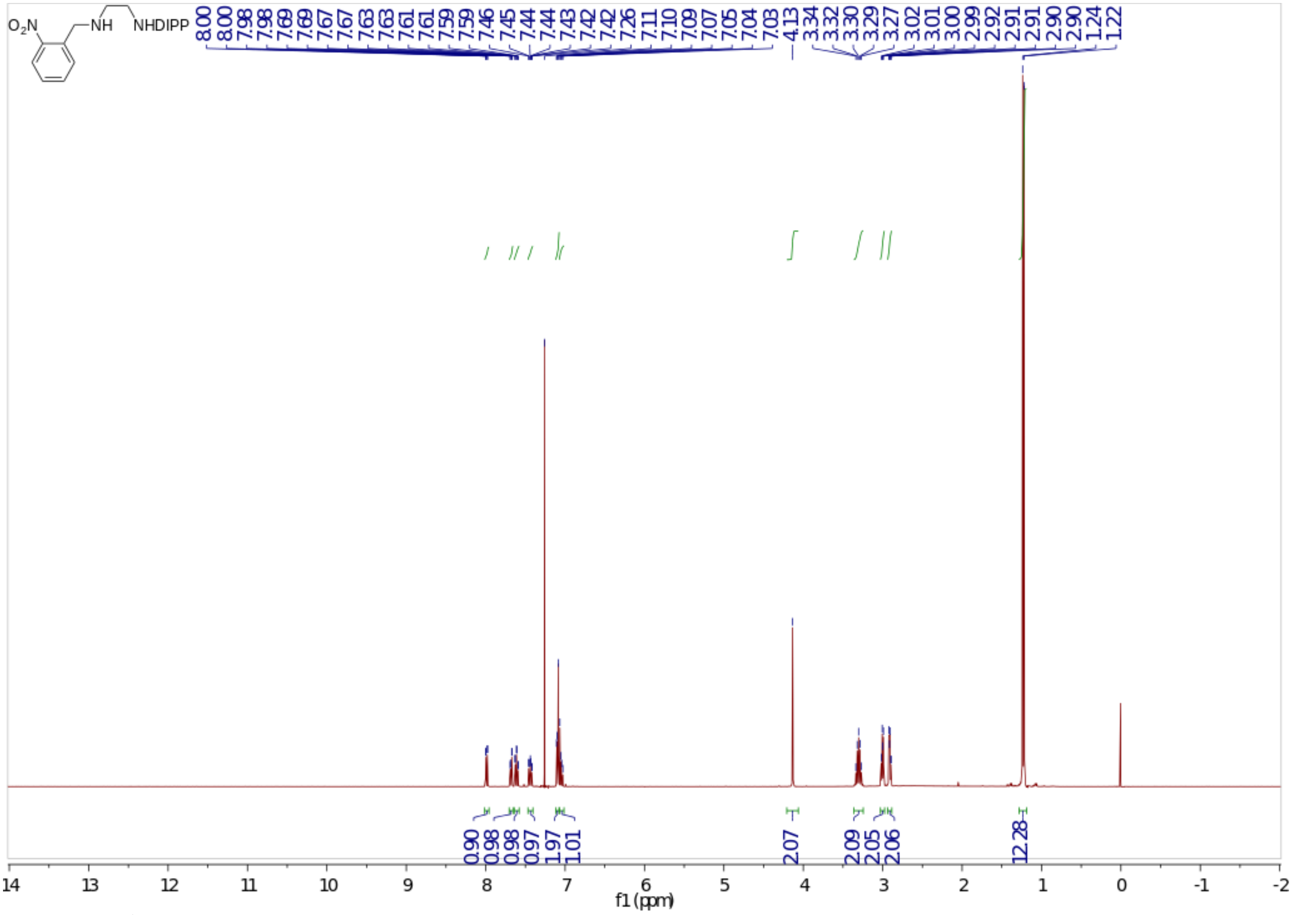

Figure S19. $^{1}H$ NMR spectrum of [4e] in $CDCl_3$, 400MHz.

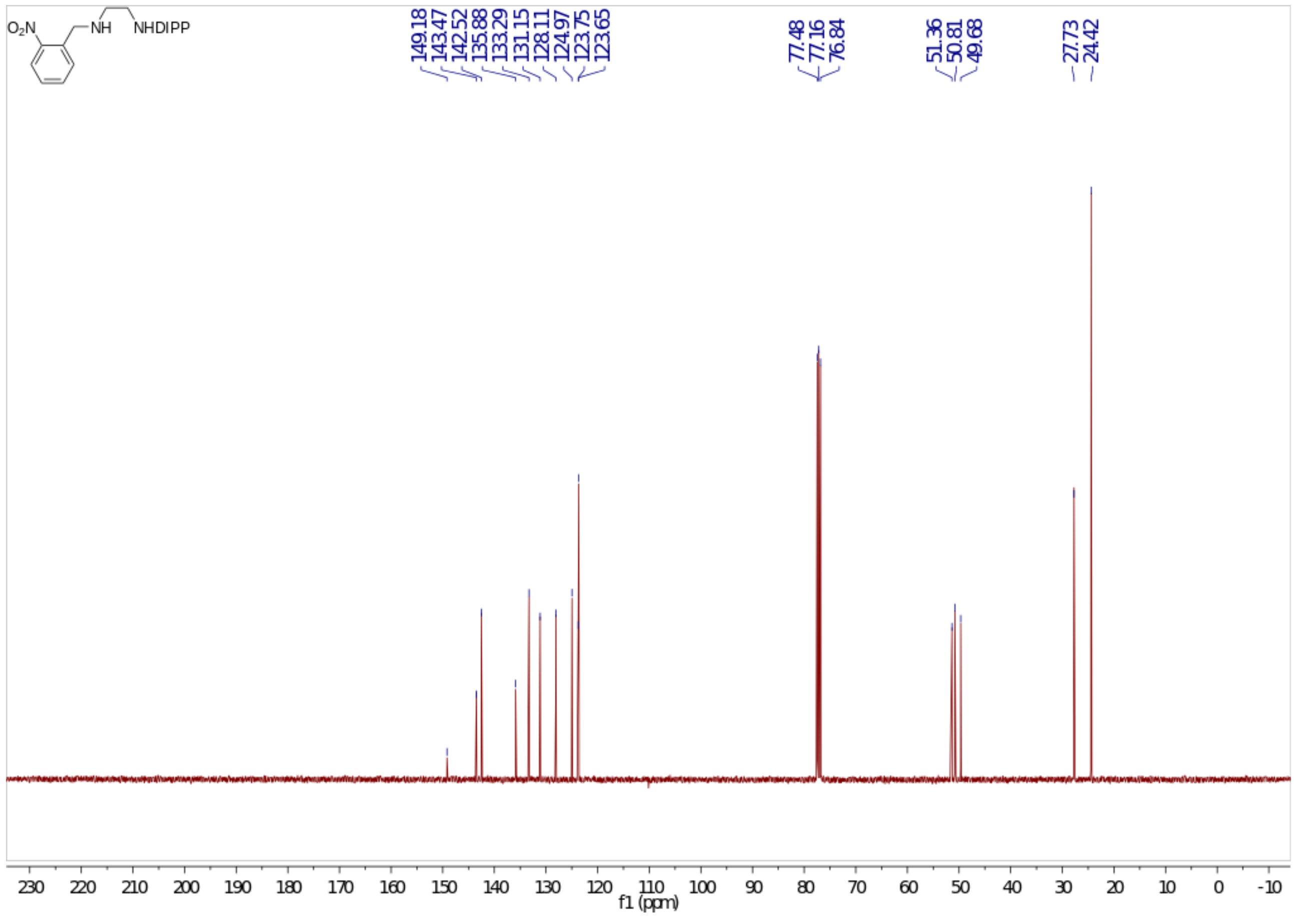

Figure S20. $^{13}C\{^{1}H\}$ NMR spectrum of [4e] in $CDCl_3$, 100MHz.

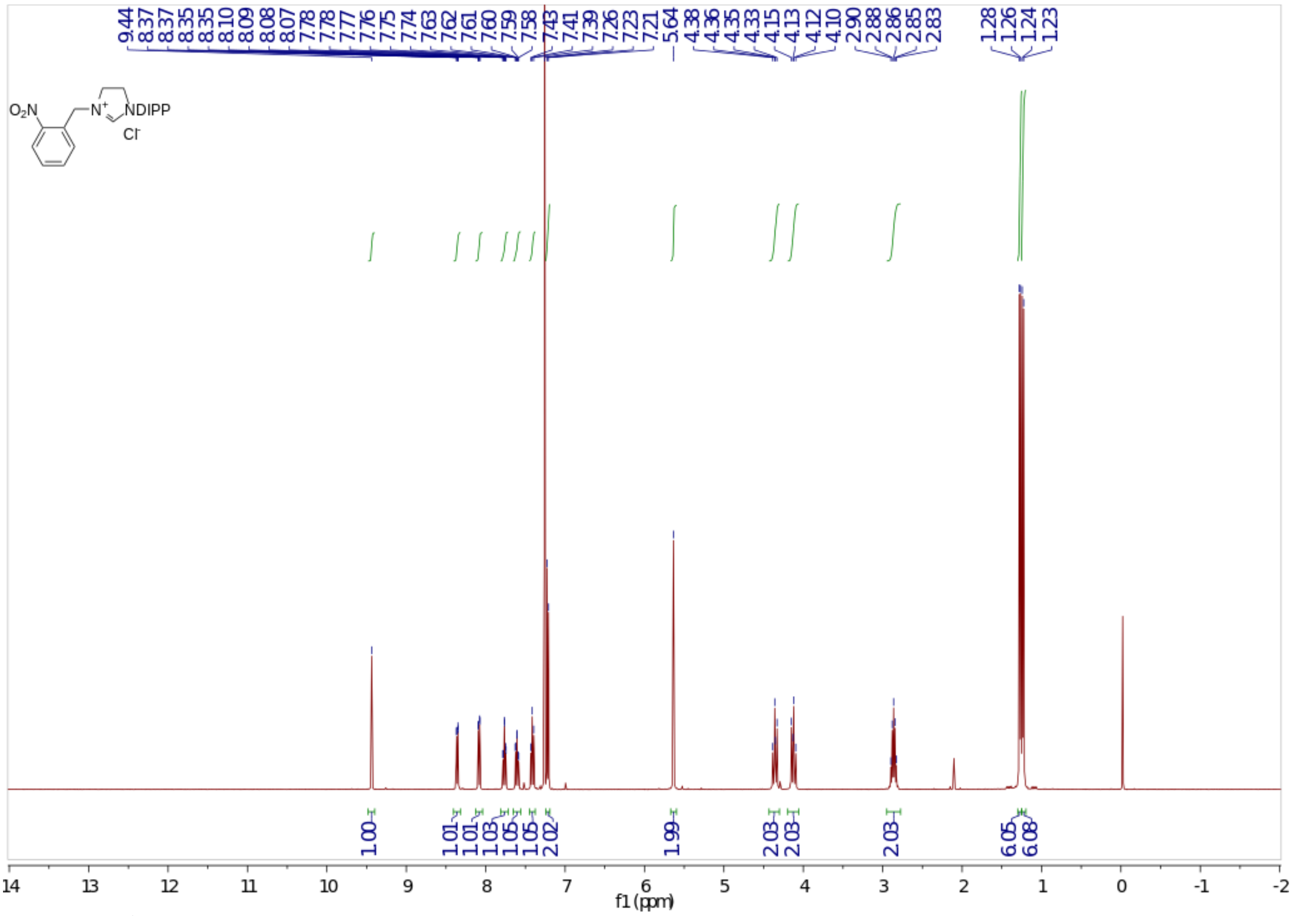

Figure S21. $^{1}H$ NMR spectrum of [5e] in $CDCl_3$, 400MHz.

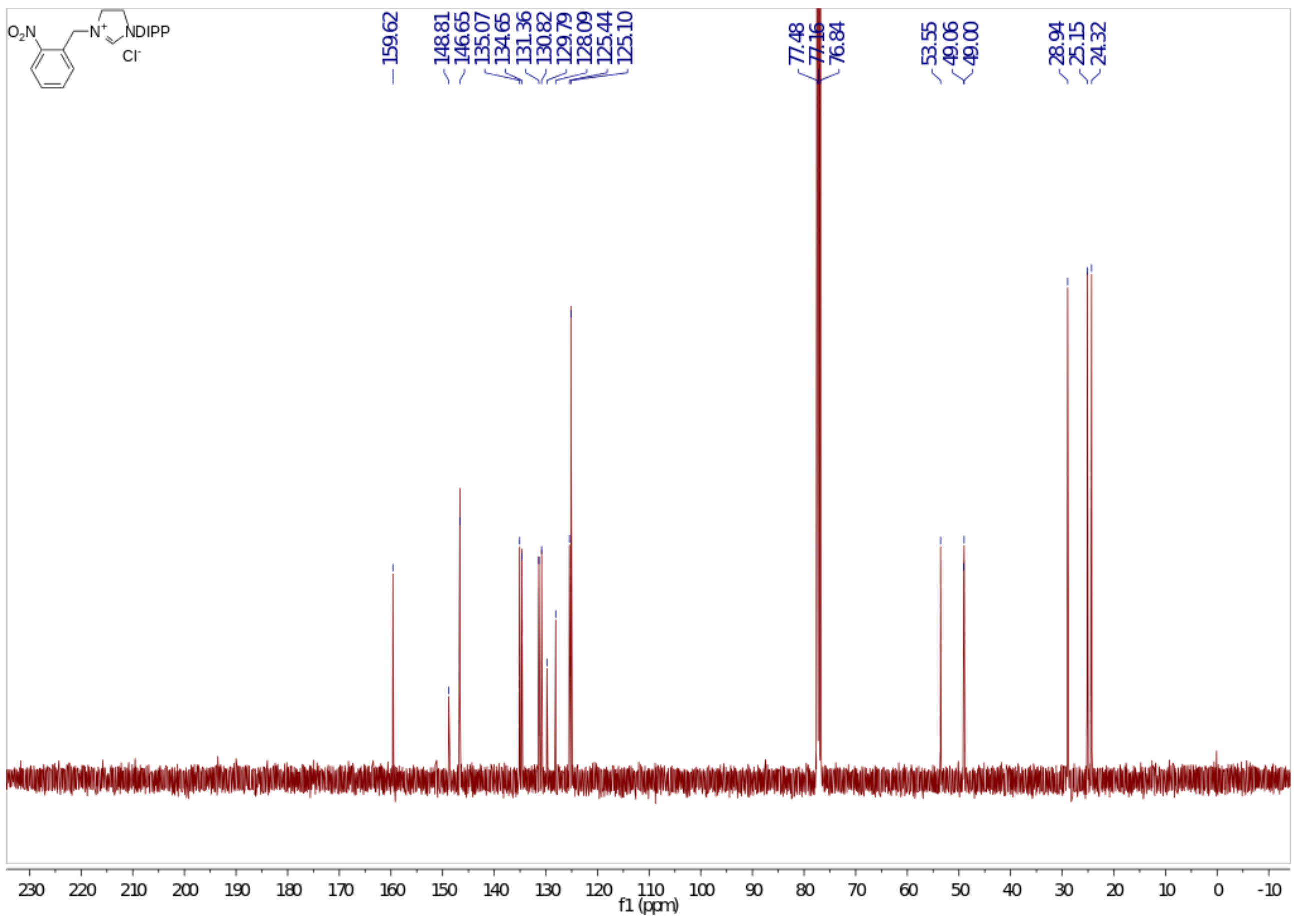

Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of [5e] in $CDCl_3$, 100MHz.

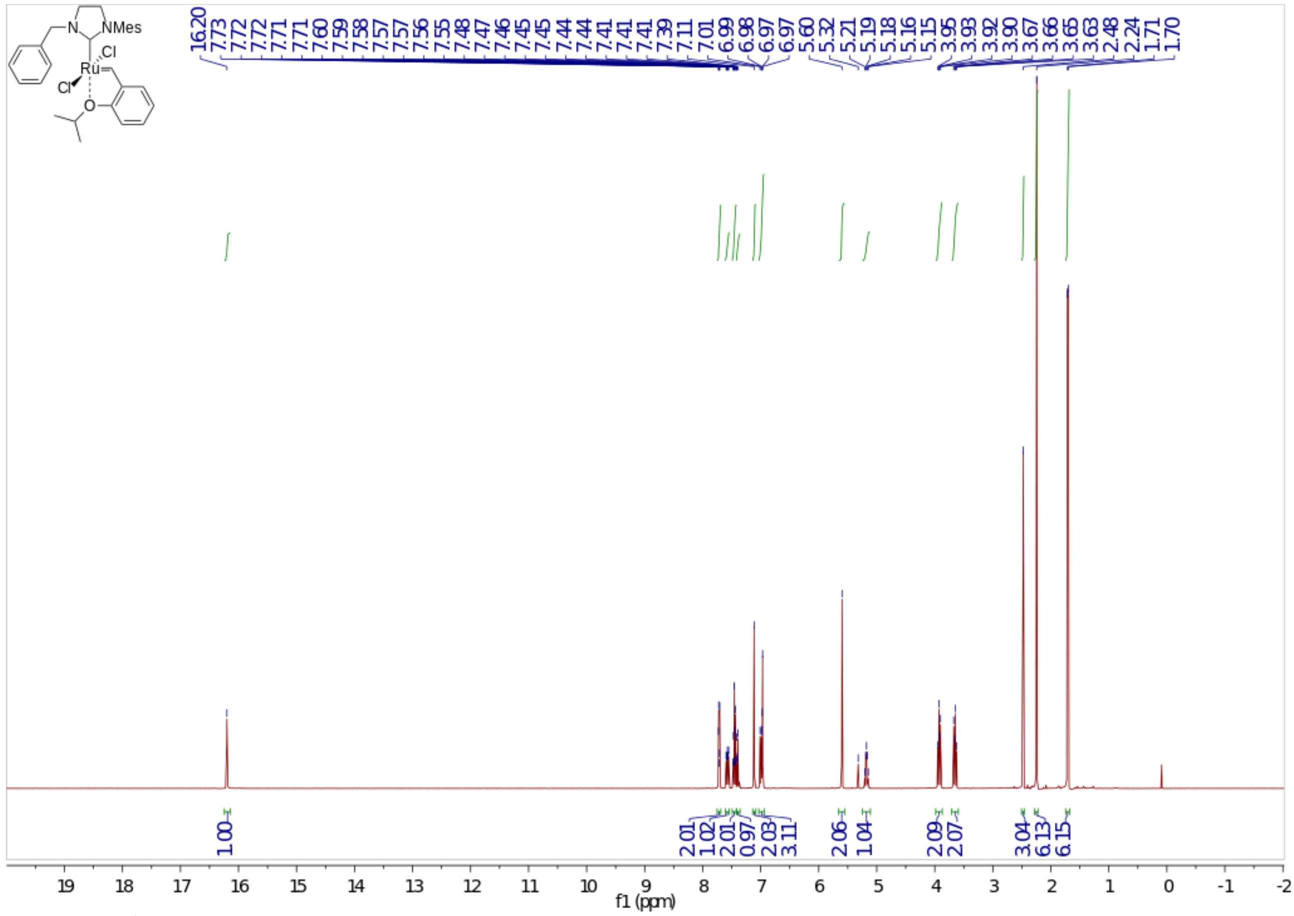

Figure S23. $^{1}$H NMR spectrum of [Ru-1] in $CD_2Cl_2$, 400MHz.

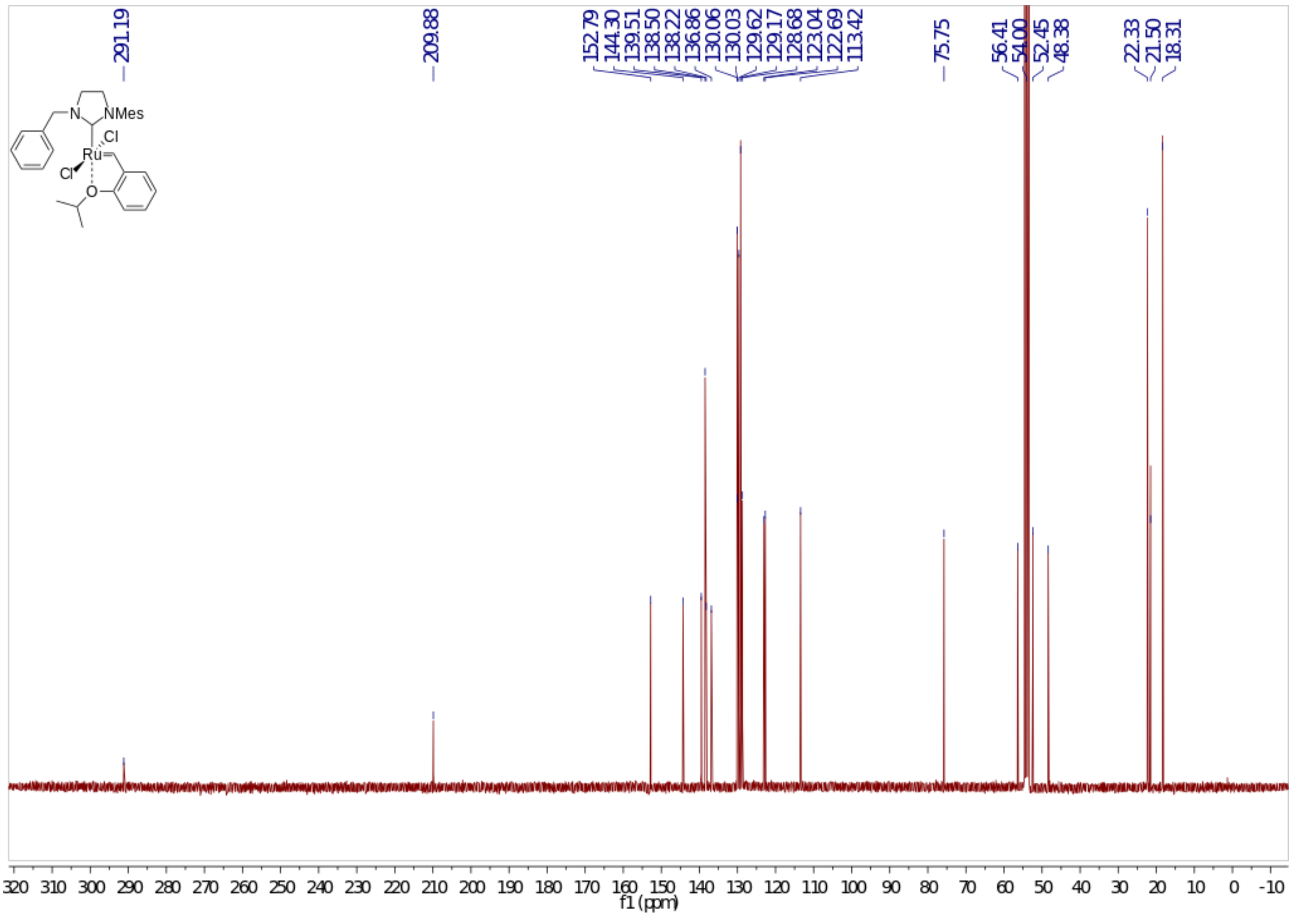

Figure S24. $^{13}C\{^{1}H\}$ NMR spectrum of [Ru-1] in $CD_2Cl_2$, 100MHz.

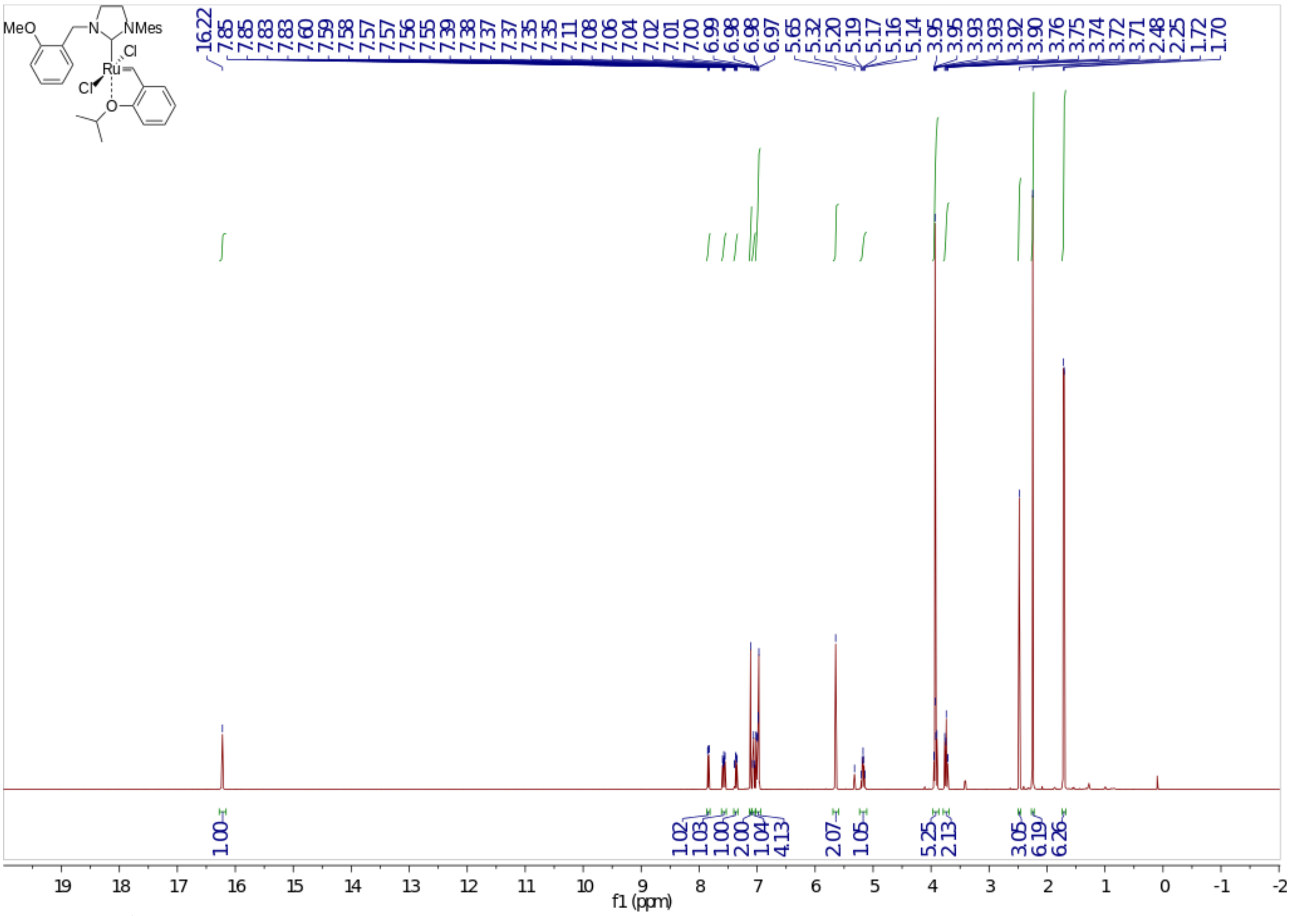

Figure S25. $^{1}H$ NMR spectrum of [Ru-2] in $CD_2Cl_2$, 400MHz.

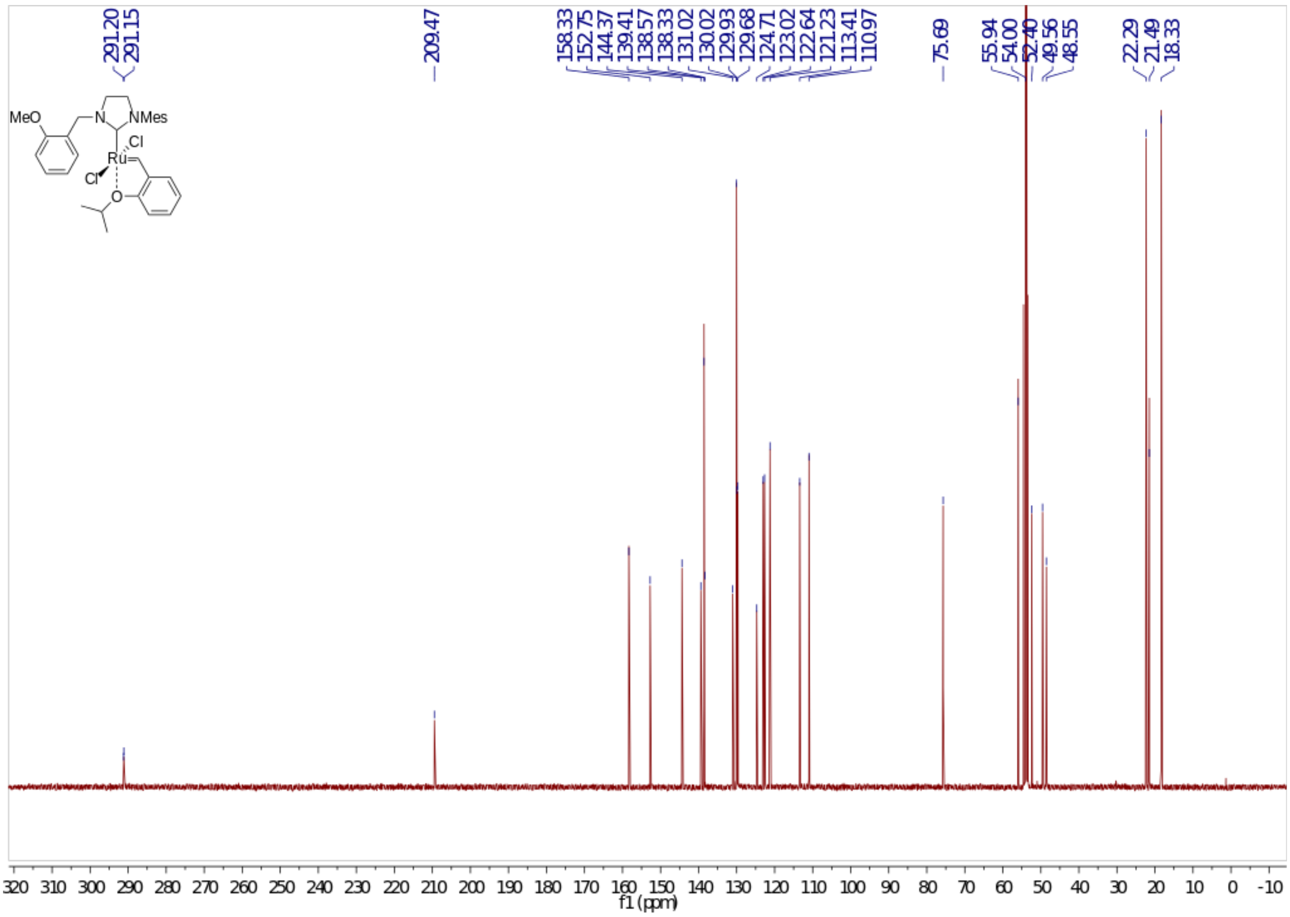

Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of [Ru-2] in $CD_2Cl_2$, 100MHz.

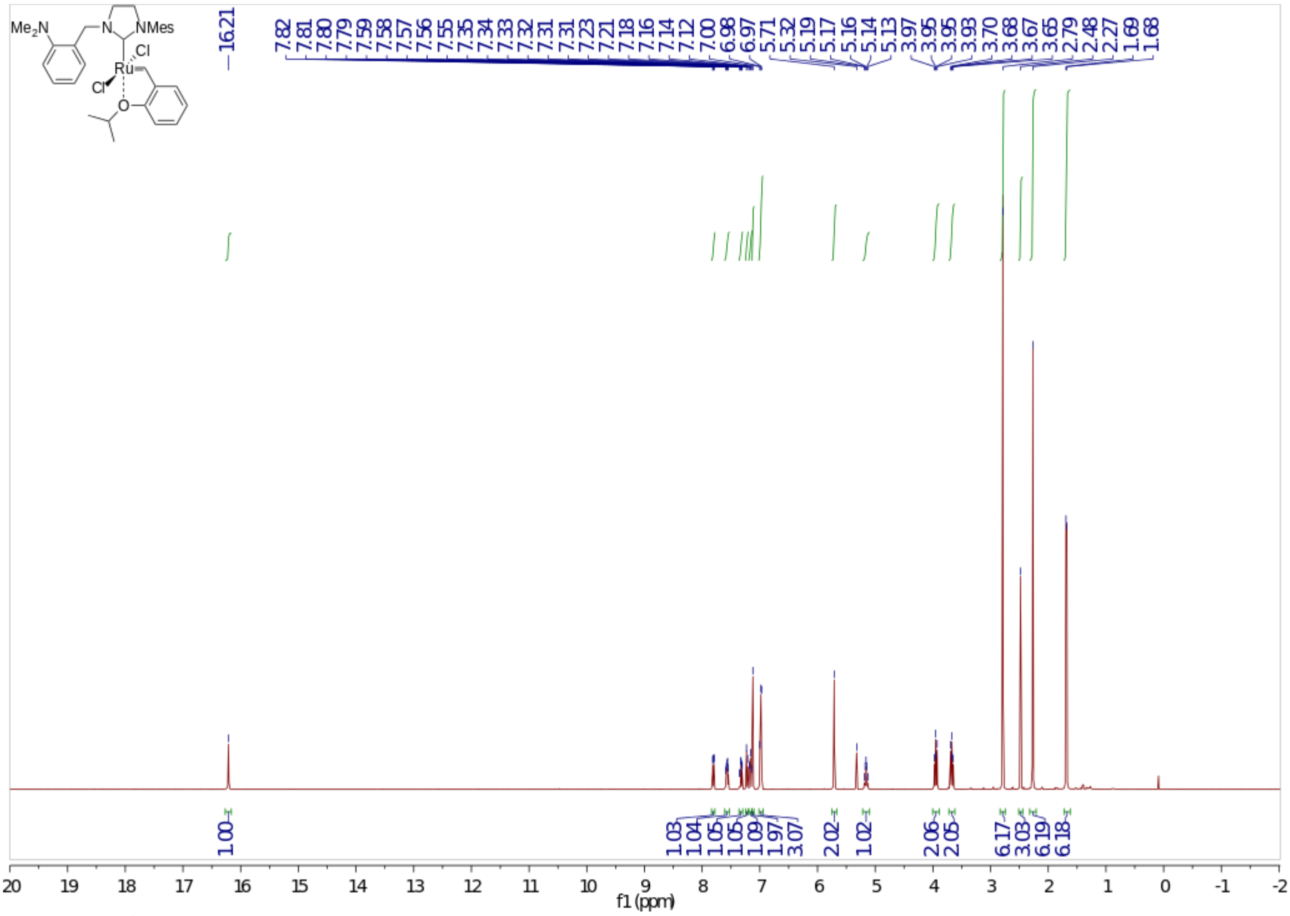


Figure S27. $^{1}H$ NMR spectrum of [Ru-3] in $CD_2Cl_2$, 400MHz.

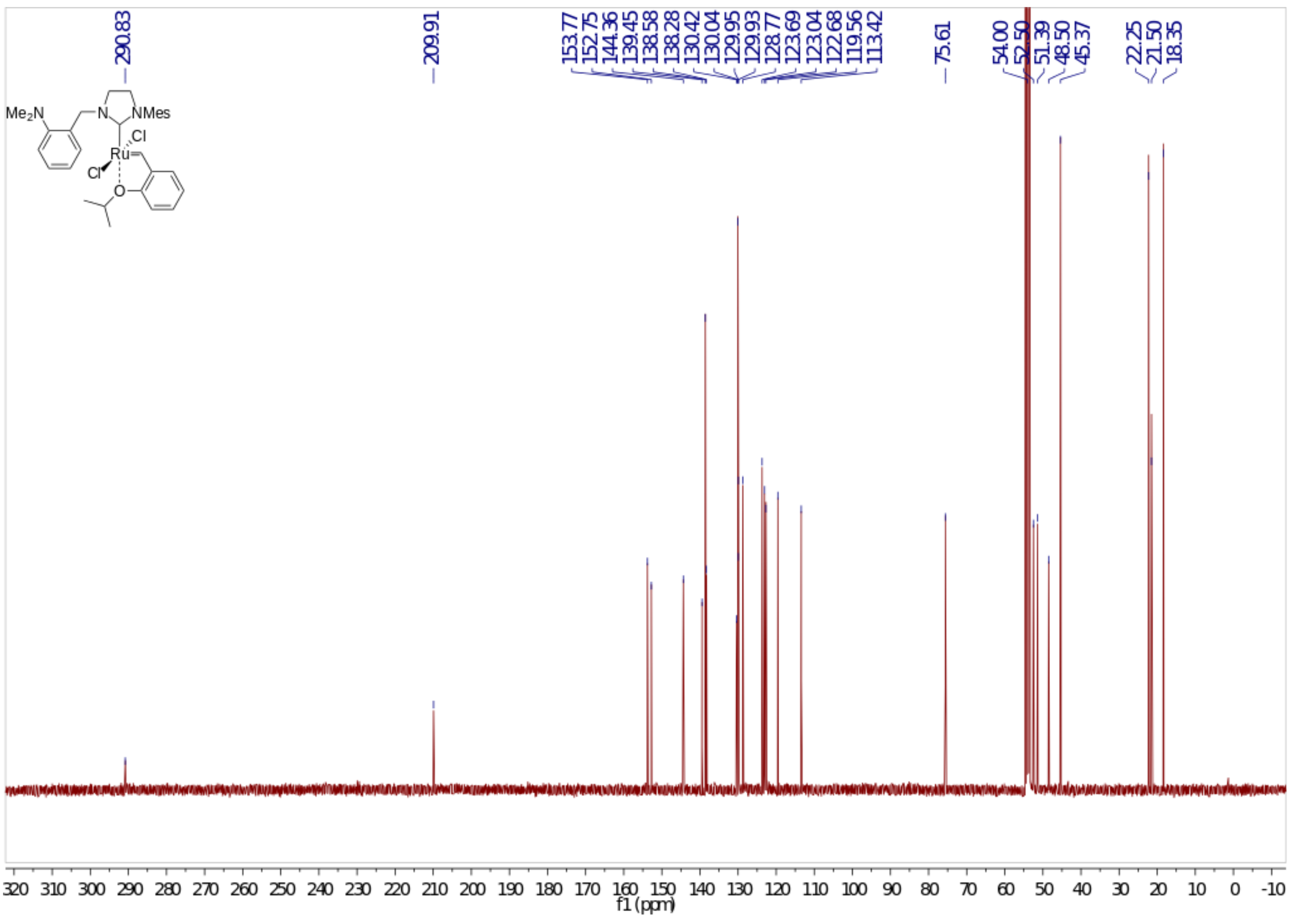


Figure S28. $^{13}C\{^{1}H\}$ NMR spectrum of [Ru-3] in $CD_2Cl_2$, 100MHz.

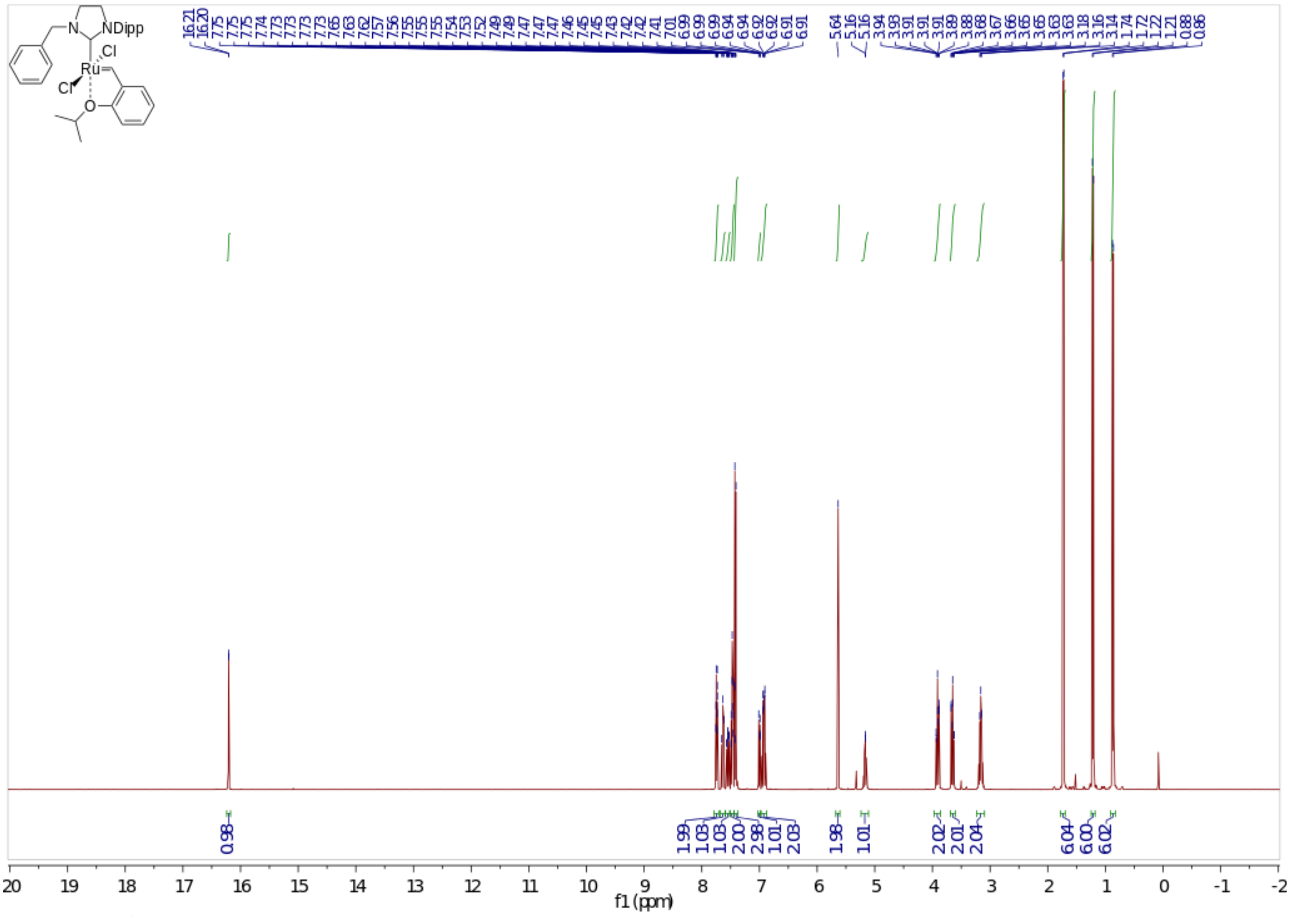

Figure S29. $^{1}H$ NMR spectrum of [Ru-4] in $CD_2Cl_2$, 400MHz.

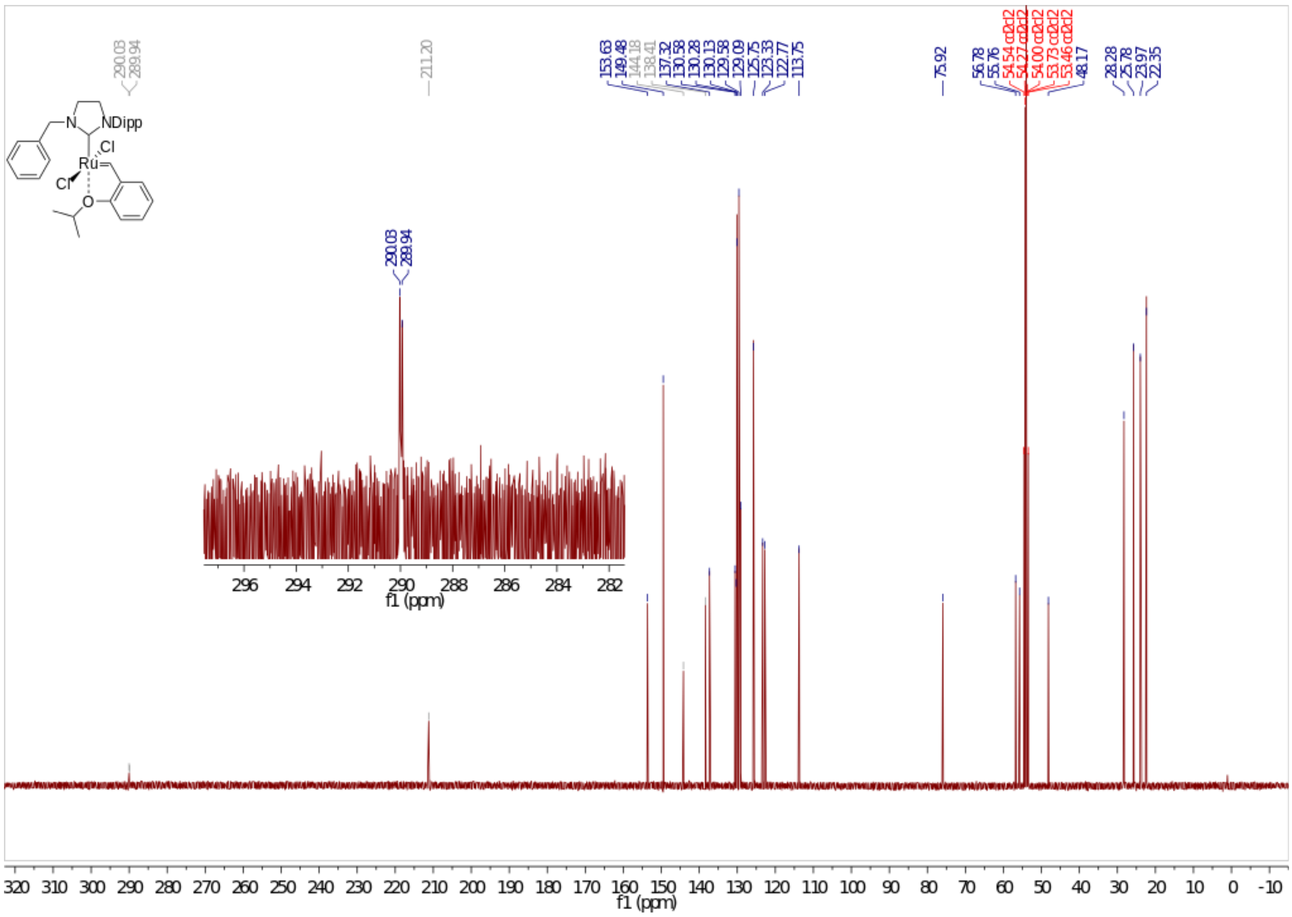

Figure S30. $^{13}C\{^{1}H\}$ NMR spectrum of [Ru-4], $CD_2Cl_2$, 100MHz.

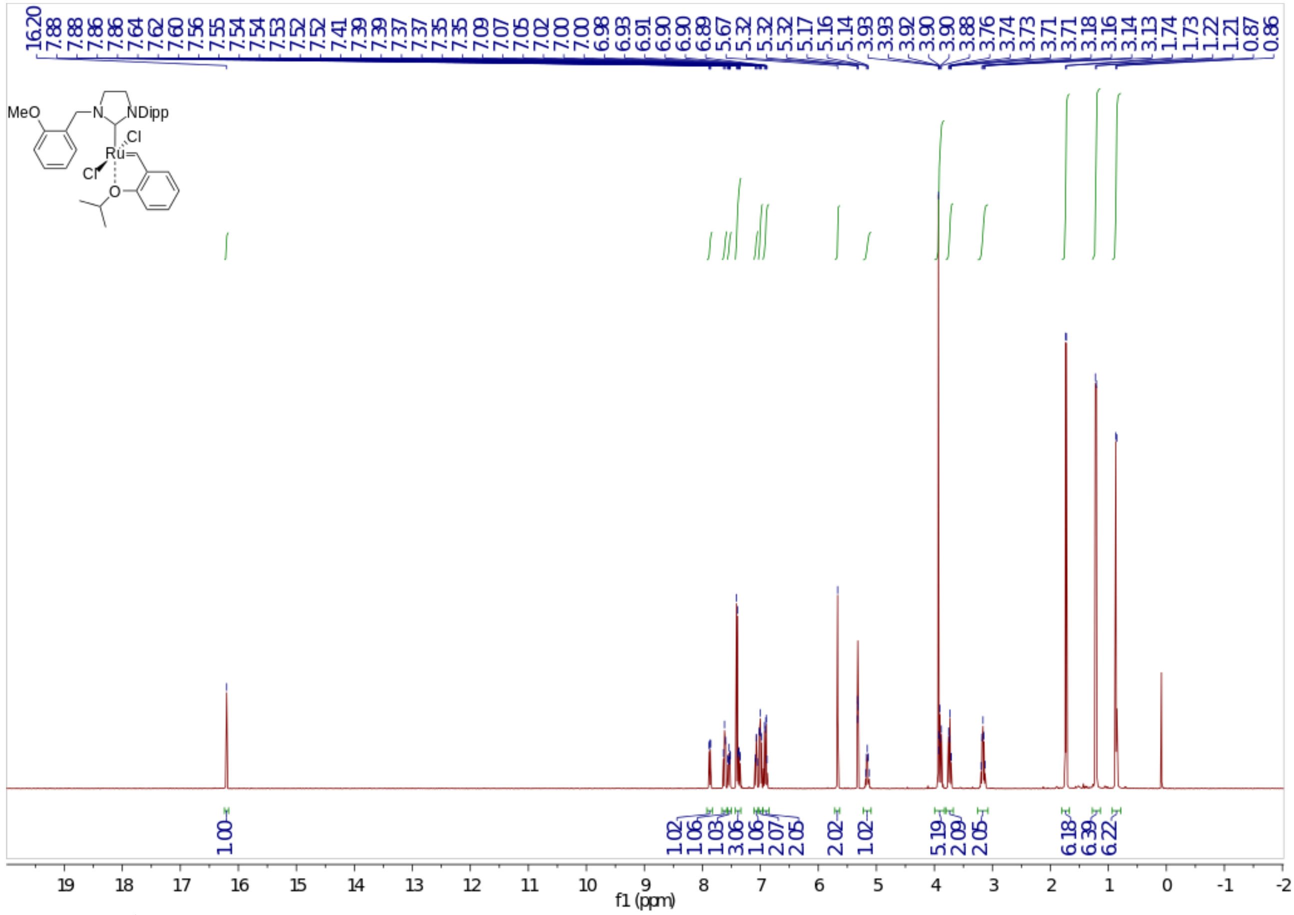

Figure S31. $^{1}H$ NMR spectrum of [Ru-5] in $CD_2Cl_2$, 400MHz.

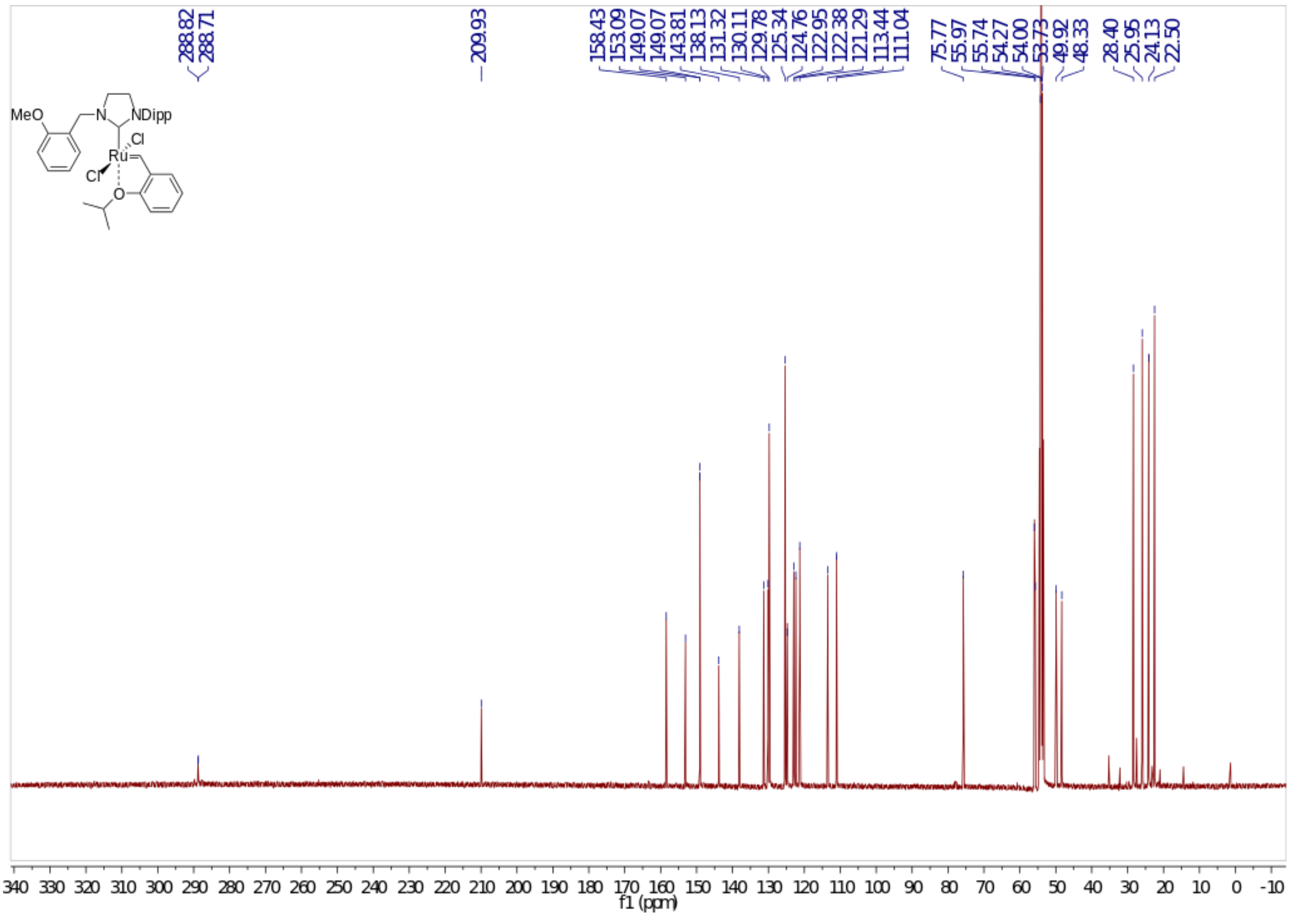

Figure S32. $^{13}C\{^{1}H\}$ NMR spectrum of [Ru-5] in $CD_2Cl_2$, 100MHz.

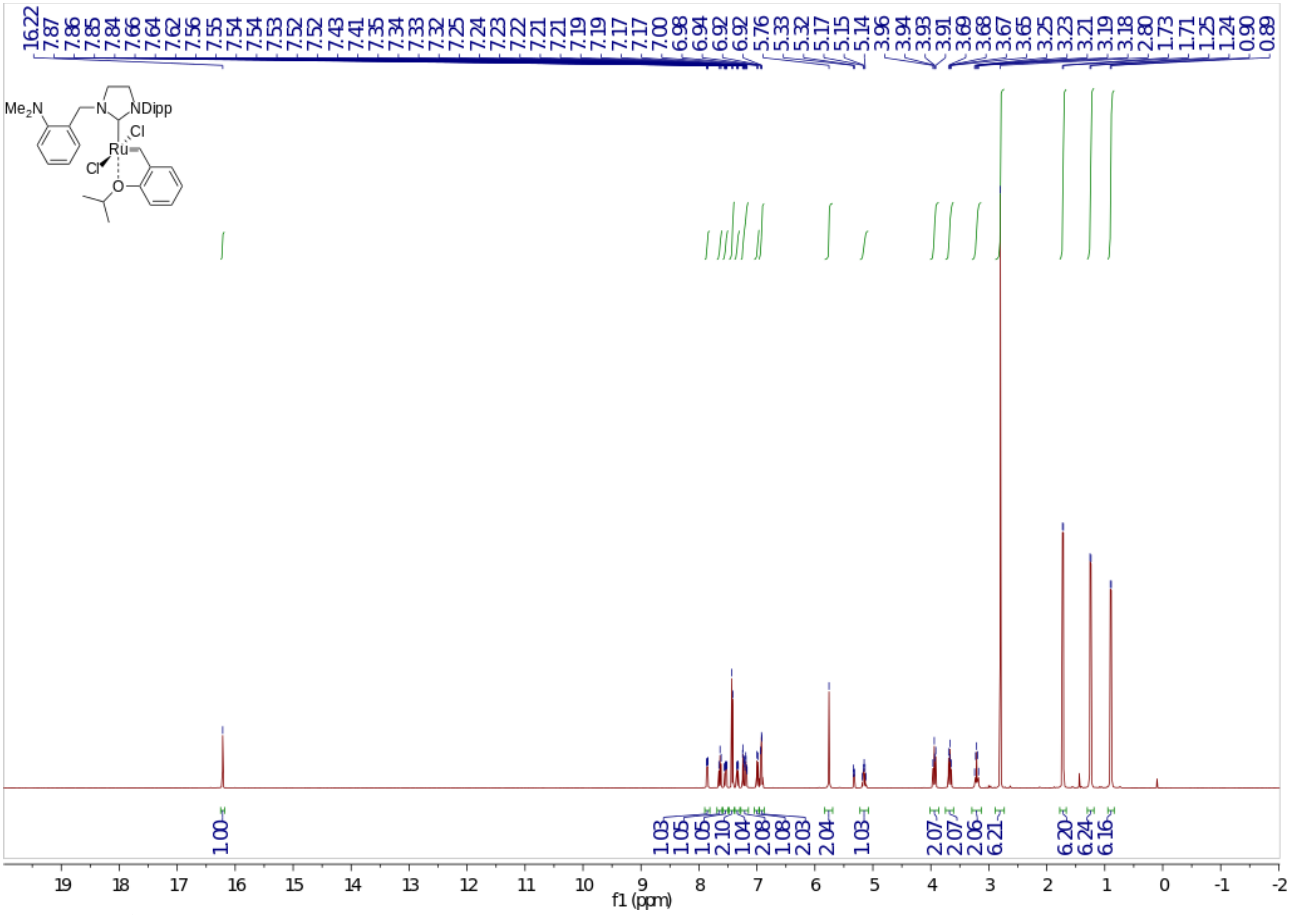

Figure S33. $^{1}H$ NMR spectrum of [Ru-6] in $CD_2Cl_2$, 400MHz.

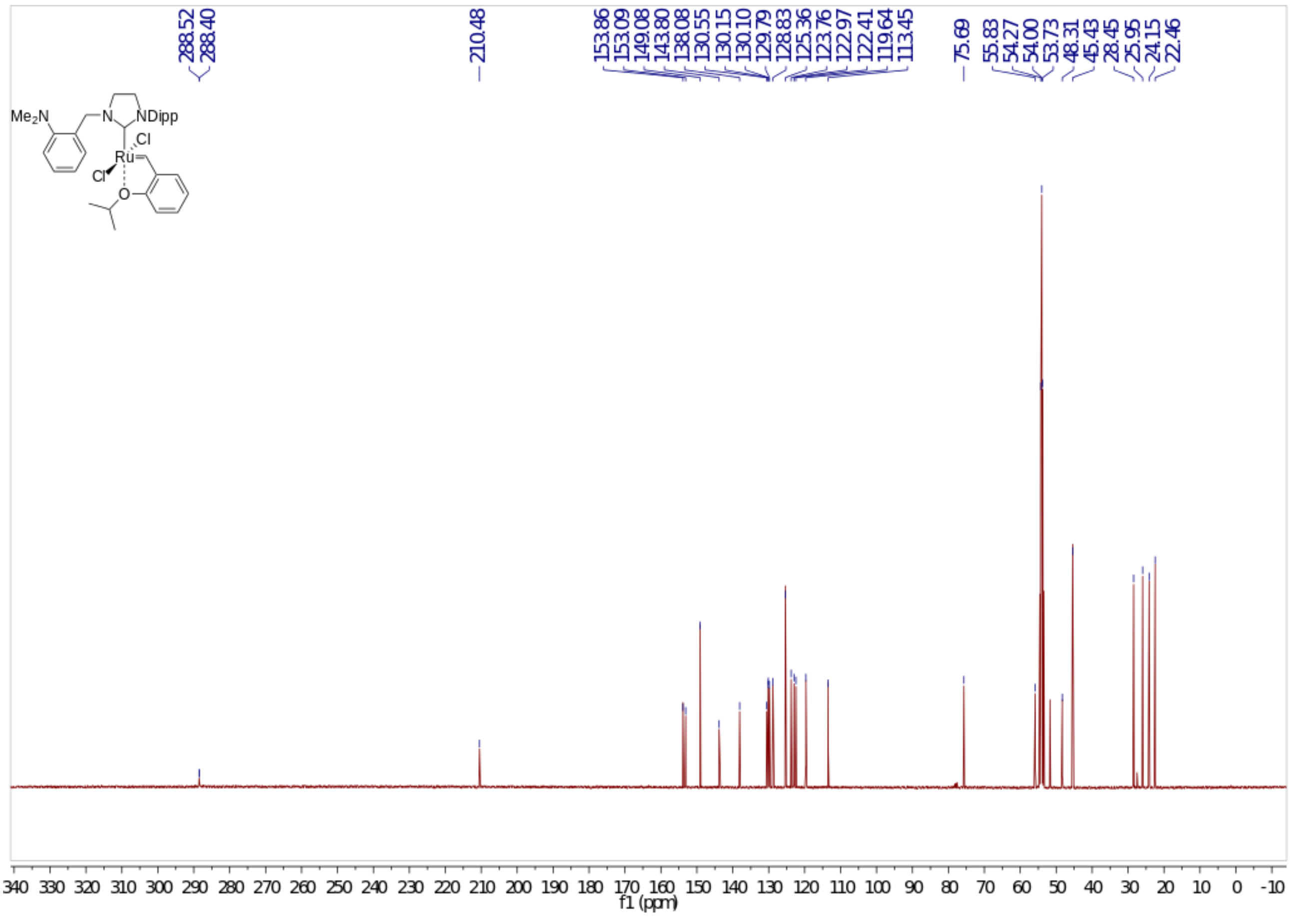

Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum of [Ru-6] in $CD_2Cl_2$, 100MHz.

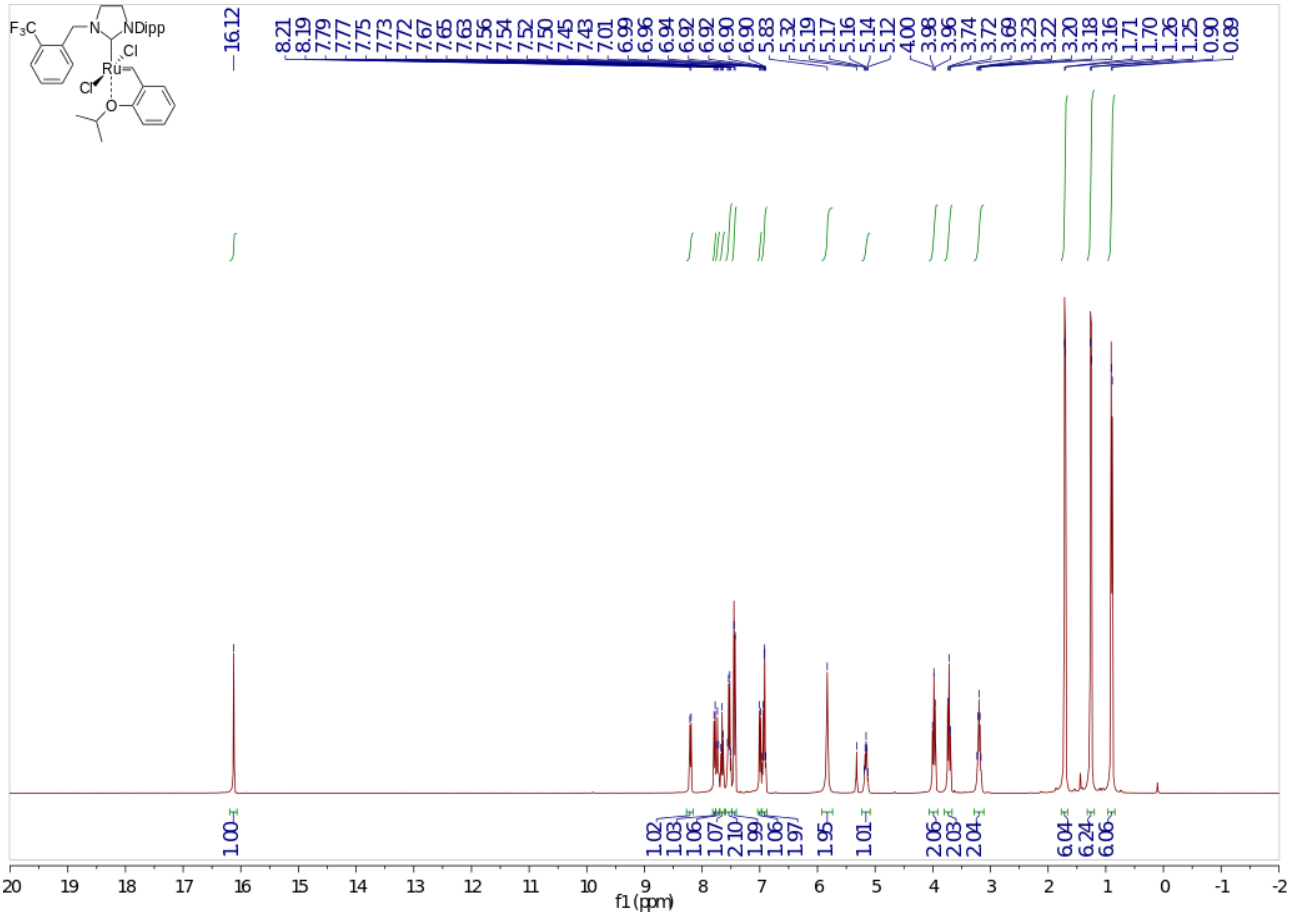


Figure S35. $^{1}$H NMR spectrum of [Ru-7] in $CD_2Cl_2$, 400MHz.

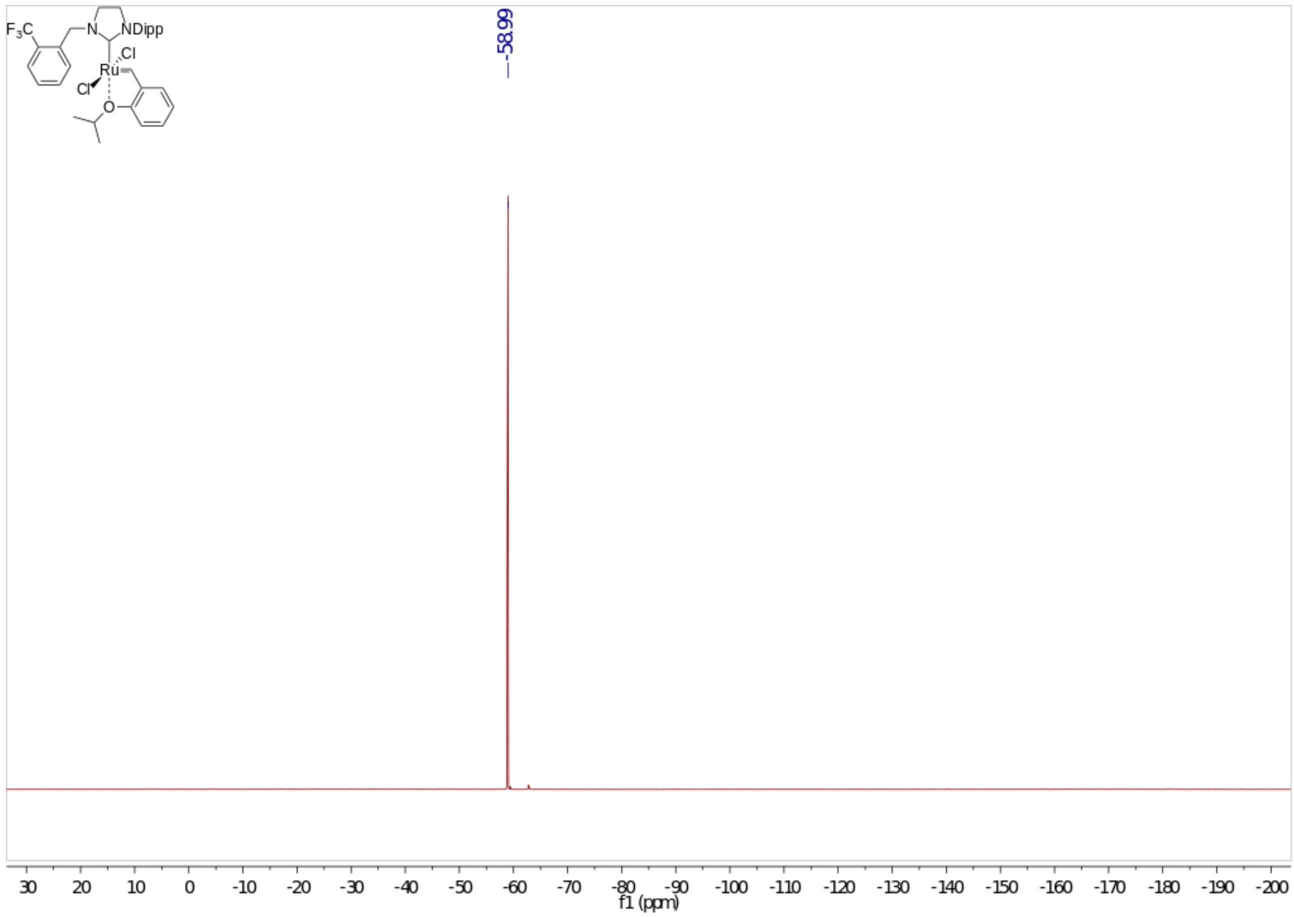


Figure S36. $^{19}$F NMR spectrum of [Ru-7] in $CD_2Cl_2$, 376MHz.

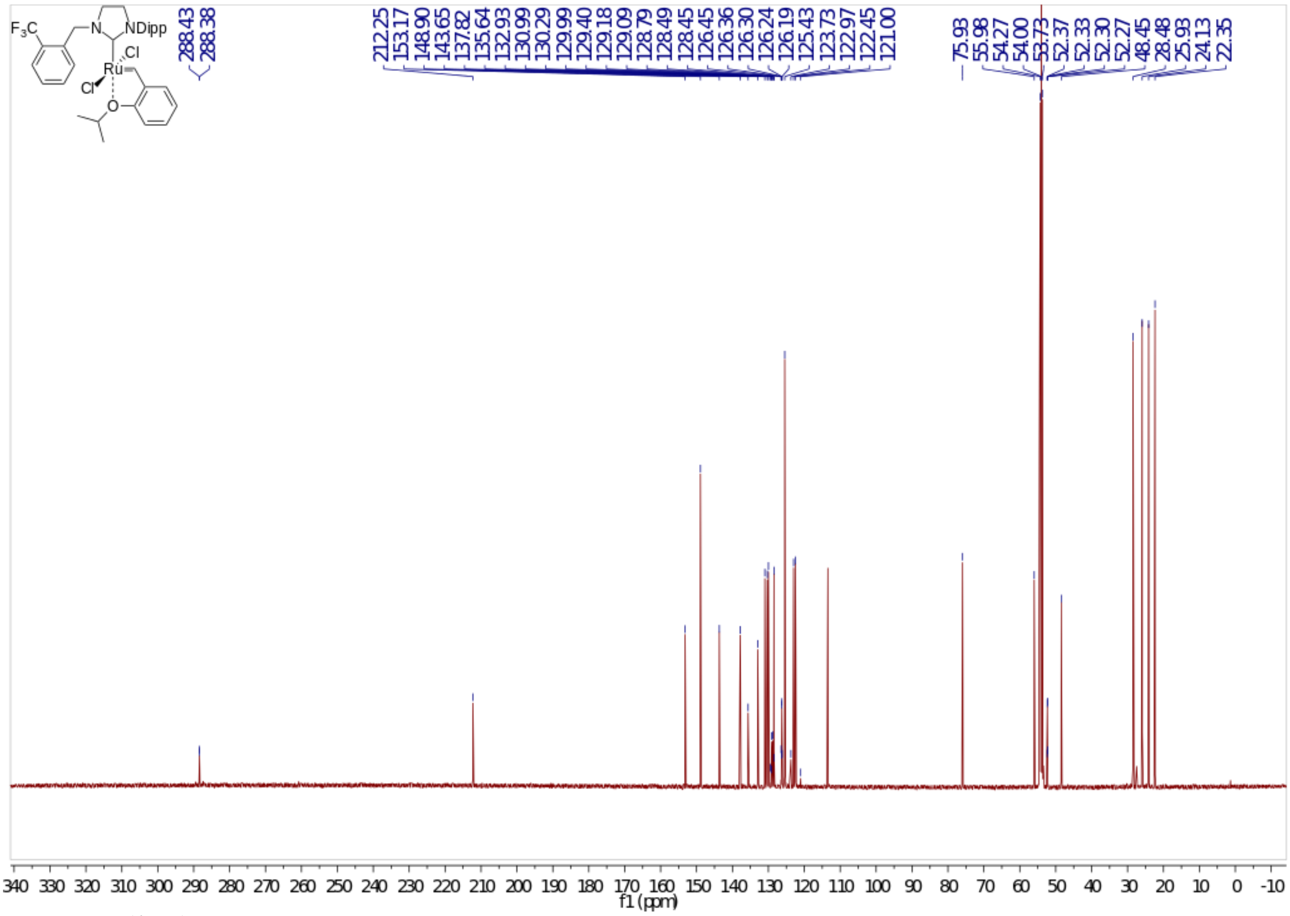

Figure S37. $^{13}C\{^{1}H\}$ NMR spectrum of [Ru-7] in $CD_2Cl_2$, 100MHz.

Crystallographic Information

The single crystal diffraction data collection for **Ru-1** was performed on a KUMA Xcalibur diffractometer, **Ru-2** and **Ru-3** on a Bruker Apex II Ultra, **Ru-4** was performed on a SuperNova diffractometer. Molecular structures of investigated compounds are presented on Figure 1. All experiments were carried out with Mo Kα radiation. The diffractometers were equipped with an Oxford Cryosystem nitrogen gas-flow apparatus and measurements were conducted at 100K, except the **Ru-4** measurement which was conducted at room temperature. Multi-scan absorption correction was applied for **Ru-1**, **Ru-2** and **Ru-3** data. In the case of **Ru-4** the analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid was used [1]. Indexing, integration and initial scaling were performed with SAINT [2] and SADABS [3] software (Bruker, 2008) for **Ru-2** and **Ru-3** structures. CrysAlis PRO program was applied for the data collection and its further reduction [4] for **Ru-1** and **Ru-4** structures. The structures were solved by direct methods and refined using SHELXL [5] program in cooperation with the Olex2 program [6]. The refinements were based on $F^2$. The data collection and processing statistics are reported in tables for according structures.

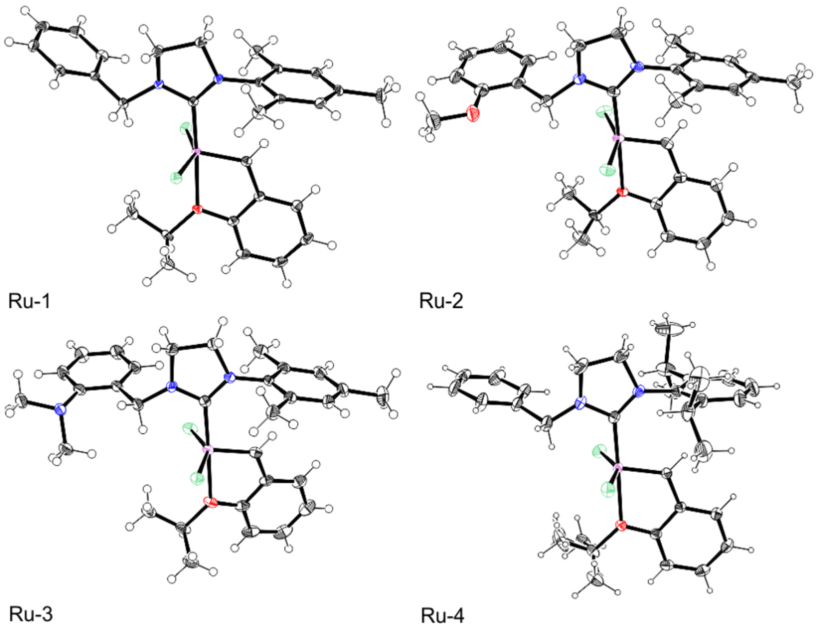


Figure S38. ORTEP drawing showing 50% thermal ellipsoids of the **Ru-1**, **Ru-2**, **Ru-3**, except **Ru-4** drawn at 20% thermal ellipsoids. One of two molecules from asymmetric unit is presented for **Ru-2**.

Table S1. Experimental details. For all structures: Z = 4.

| | **Ru-1** | **Ru-2** | **Ru-3** | **Ru-4** |
|---|---|---|---|---|
| **Crystal data** | | | | |
| Chemical formula | $C_{29}H_{34}Cl_2N_2ORu$ | $C_{30}H_{36}Cl_2N_2O_2Ru$ | $C_{31}H_{39}Cl_2N_3ORu$ | $C_{32}H_{40}Cl_2N_2ORu$ |
| $M_r$ | 598.55 | 628.58 | 641.62 | 640.63 |
| Crystal system, space group | Monoclinic, $P2_1/n$ | Triclinic, P-1 | Monoclinic, $P2_1/c$ | Monoclinic, $P2_1/c$ |
| Temperature (K) | 100 | 100 | 100 | 293 |
| a, b, c (Å) | 12.1453 (2), 14.3472 (3), 15.7196 (3) | 11.3218 (4), 13.7468 (6), 20.1108 (9) | 8.9252 (4), 14.3998 (7), 23.802 (1) | 19.2104 (5), 10.1892 (3), 16.3430 (5) |
| α, β, γ,(°) | 90, 92.156 (2), 90 | 74.926 (2), 74.027 (2), 81.863 (2) | 90, 90.787 (2), 90 | 90, 96.427 (3), 90 |
| V ($Å^3$) | 2737.22 (9) | 2897.4 (2) | 3058.8 (2) | 3178.83 (15) |
| μ ($mm^{-1}$) | 0.79 | 0.76 | 0.72 | 0.69 |
| Crystal size (mm) | 0.40 × 0.30 × 0.30 | 0.20 × 0.10 × 0.10 | 0.30 × 0.10 × 0.10 | 0.26 × 0.12 × 0.07 |

| Data collection | | | | |
|---|---|---|---|---|
| Diffractometer | Xcalibur, Opal | Kappa ApexII Ultra CCD | Kappa ApexII Ultra CCD | SuperNova, Single source at offset, Eos |
| Absorption correction | Multi-scan CrysAlis PRO, Agilent | Multi-scan SADABS2008/1 - Bruker Nonius | Multi-scan SADABS2008/1 - Bruker Nonius | Analytical CrysAlis PRO, Agilent |
| $T_{min}$, $T_{max}$ | 0.992, 1.000 | 0.627, 0.745 | 0.673, 0.745 | 0.861, 0.958 |
| No. of measured, independent and observed [I > 2σ(I)] reflections | 23043, 5590, 4832 | 34175, 10996, 8578 | 41448, 5790, 5346 | 83367, 9706, 7778 |
| $R_{int}$ | 0.026 | 0.040 | 0.030 | 0.053 |
| $(\sin \theta/\lambda)_{max}$ (Å$^{-1}$) | 0.625 | 0.610 | 0.610 | 0.714 |
| **Refinement** | | | | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S | 0.022, 0.053, 1.04 | 0.041, 0.105, 1.04 | 0.023, 0.069, 1.08 | 0.049, 0.095, 1.11 |
| No. of reflections | 5590 | 10996 | 5790 | 9706 |
| No. of parameters | 321 | 679 | 350 | 374 |
| H-atom treatment | H-atom parameters constrained | H-atom parameters constrained | H-atom parameters constrained | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.34, -0.38 | 1.63, -0.91 | 0.33, -0.27 | 0.41, -0.31 |
| CCDC Number | 1539095 | 1539096 | 1539097 | 1539098 |

Table S2. Selected geometric parameters for **Ru-1** (Å, º)

| | | | |
|---|---|---|---|
| C1—N2 | 1.343 (2) | C16—C17 | 1.385 (3) |
| C1—N1 | 1.357 (2) | C17—C18 | 1.388 (3) |
| C1—Ru1 | 1.9676 (18) | C18—C19 | 1.380 (3) |
| C2—N1 | 1.467 (2) | C19—C20 | 1.389 (3) |
| C2—C3 | 1.521 (3) | C22—C23 | 1.451 (3) |
| C3—N2 | 1.476 (2) | C22—Ru1 | 1.8303 (18) |
| C4—C9 | 1.396 (3) | C23—C24 | 1.400 (3) |
| C4—C5 | 1.400 (3) | C23—C28 | 1.402 (3) |
| C4—N2 | 1.432 (2) | C24—O1 | 1.381 (2) |
| C5—C6 | 1.390 (3) | C24—C25 | 1.387 (3) |
| C5—C10 | 1.506 (3) | C25—C26 | 1.388 (3) |
| C6—C7 | 1.392 (3) | C26—C27 | 1.387 (3) |
| C7—C8 | 1.391 (3) | C27—C28 | 1.385 (3) |
| C7—C11 | 1.504 (3) | C29—O1 | 1.475 (2) |
| C8—C9 | 1.398 (3) | C29—C30 | 1.511 (3) |
| C9—C12 | 1.504 (3) | C29—C31 | 1.513 (3) |
| C14—N1 | 1.457 (2) | O1—Ru1 | 2.2666 (12) |
| C14—C15 | 1.507 (2) | Cl1—Ru1 | 2.3415 (5) |
| C15—C20 | 1.388 (3) | Cl2—Ru1 | 2.3456 (4) |

| | | | |
|---|---|---|---|
| C15—C16 | 1.390 (3) | | |
| | | | |
| N2—C1—N1 | 107.34 (15) | C28—C23—C22 | 123.28 (17) |
| N2—C1—Ru1 | 133.85 (13) | O1—C24—C25 | 125.15 (17) |
| N1—C1—Ru1 | 118.50 (13) | O1—C24—C23 | 113.00 (16) |
| N1—C2—C3 | 101.49 (14) | C25—C24—C23 | 121.83 (17) |
| N2—C3—C2 | 101.94 (14) | C24—C25—C26 | 118.14 (19) |
| C9—C4—C5 | 122.13 (17) | C27—C26—C25 | 121.68 (19) |
| C9—C4—N2 | 119.17 (16) | C28—C27—C26 | 119.45 (19) |
| C5—C4—N2 | 118.67 (16) | C27—C28—C23 | 120.60 (19) |
| C6—C5—C4 | 118.06 (17) | O1—C29—C30 | 105.77 (15) |
| C6—C5—C10 | 121.00 (17) | O1—C29—C31 | 109.83 (15) |
| C4—C5—C10 | 120.94 (16) | C30—C29—C31 | 113.24 (17) |
| C5—C6—C7 | 121.59 (17) | C1—N1—C14 | 123.66 (15) |
| C8—C7—C6 | 118.66 (17) | C1—N1—C2 | 112.24 (14) |
| C8—C7—C11 | 120.83 (18) | C14—N1—C2 | 118.23 (14) |
| C6—C7—C11 | 120.50 (18) | C1—N2—C4 | 126.04 (15) |
| C7—C8—C9 | 121.86 (18) | C1—N2—C3 | 112.49 (15) |
| C4—C9—C8 | 117.55 (17) | C4—N2—C3 | 119.56 (14) |
| C4—C9—C12 | 121.93 (17) | C24—O1—C29 | 119.19 (14) |
| C8—C9—C12 | 120.50 (17) | C24—O1—Ru1 | 110.19 (10) |
| N1—C14—C15 | 111.11 (15) | C29—O1—Ru1 | 127.76 (10) |
| C20—C15—C16 | 119.38 (17) | C22—Ru1—C1 | 102.75 (8) |
| C20—C15—C14 | 120.36 (17) | C22—Ru1—O1 | 79.12 (7) |
| C16—C15—C14 | 120.26 (17) | C1—Ru1—O1 | 177.31 (6) |
| C17—C16—C15 | 120.20 (18) | C22—Ru1—Cl1 | 103.52 (6) |
| C16—C17—C18 | 119.90 (19) | C1—Ru1—Cl1 | 93.27 (5) |
| C19—C18—C17 | 120.34 (18) | O1—Ru1—Cl1 | 88.13 (3) |
| C18—C19—C20 | 119.61 (18) | C22—Ru1—Cl2 | 102.66 (6) |
| C15—C20—C19 | 120.55 (18) | C1—Ru1—Cl2 | 86.84 (5) |
| C23—C22—Ru1 | 119.25 (14) | O1—Ru1—Cl2 | 90.88 (3) |
| C24—C23—C28 | 118.27 (17) | Cl1—Ru1—Cl2 | 153.121 (17) |
| C24—C23—C22 | 118.44 (16) | | |
| | | | |
| N1—C2—C3—N2 | -19.64 (18) | C24—C25—C26—C27 | 0.0 (3) |
| C9—C4—C5—C6 | -4.0 (3) | C25—C26—C27—C28 | -1.0 (3) |
| N2—C4—C5—C6 | 177.81 (16) | C26—C27—C28—C23 | 0.6 (3) |
| C9—C4—C5—C10 | 176.40 (17) | C24—C23—C28—C27 | 0.7 (3) |
| N2—C4—C5—C10 | -1.8 (3) | C22—C23—C28—C27 | 179.59 (17) |
| C4—C5—C6—C7 | 1.9 (3) | N2—C1—N1—C14 | -163.93 (16) |
| C10—C5—C6—C7 | -178.48 (17) | Ru1—C1—N1—C14 | 10.5 (2) |
| C5—C6—C7—C8 | 1.4 (3) | N2—C1—N1—C2 | -11.5 (2) |

| | | | |
|---|---|---|---|
| C5—C6—C7—C11 | -179.48 (18) | Ru1—C1—N1—C2 | 162.90 (13) |
| C6—C7—C8—C9 | -2.8 (3) | C15—C14—N1—C1 | -154.18 (17) |
| C11—C7—C8—C9 | 178.03 (18) | C15—C14—N1—C2 | 54.9 (2) |
| C5—C4—C9—C8 | 2.6 (3) | C3—C2—N1—C1 | 20.2 (2) |
| N2—C4—C9—C8 | -179.20 (16) | C3—C2—N1—C14 | 174.25 (16) |
| C5—C4—C9—C12 | -179.10 (17) | N1—C1—N2—C4 | -167.06 (16) |
| N2—C4—C9—C12 | -0.9 (3) | Ru1—C1—N2—C4 | 19.7 (3) |
| C7—C8—C9—C4 | 0.9 (3) | N1—C1—N2—C3 | -3.0 (2) |
| C7—C8—C9—C12 | -177.41 (18) | Ru1—C1—N2—C3 | -176.20 (14) |
| N1—C14—C15—C20 | -118.43 (18) | C9—C4—N2—C1 | 78.4 (2) |
| N1—C14—C15—C16 | 61.1 (2) | C5—C4—N2—C1 | -103.3 (2) |
| C20—C15—C16—C17 | -1.5 (3) | C9—C4—N2—C3 | -84.6 (2) |
| C14—C15—C16—C17 | 178.98 (17) | C5—C4—N2—C3 | 93.6 (2) |
| C15—C16—C17—C18 | 0.9 (3) | C2—C3—N2—C1 | 15.1 (2) |
| C16—C17—C18—C19 | 0.0 (3) | C2—C3—N2—C4 | -179.72 (15) |
| C17—C18—C19—C20 | -0.4 (3) | C25—C24—O1—C29 | 18.8 (3) |
| C16—C15—C20—C19 | 1.2 (3) | C23—C24—O1—C29 | -162.46 (15) |
| C14—C15—C20—C19 | -179.33 (17) | C25—C24—O1—Ru1 | -178.87 (15) |
| C18—C19—C20—C15 | -0.2 (3) | C23—C24—O1—Ru1 | -0.13 (18) |
| Ru1—C22—C23—C24 | -0.7 (2) | C30—C29—O1—C24 | -171.66 (15) |
| Ru1—C22—C23—C28 | -179.51 (14) | C31—C29—O1—C24 | 65.8 (2) |
| C28—C23—C24—O1 | 179.38 (15) | C30—C29—O1—Ru1 | 29.5 (2) |
| C22—C23—C24—O1 | 0.5 (2) | C31—C29—O1—Ru1 | -93.06 (17) |
| C28—C23—C24—C25 | -1.8 (3) | C23—C22—Ru1—C1 | 178.45 (13) |
| C22—C23—C24—C25 | 179.26 (17) | C23—C22—Ru1—O1 | 0.42 (13) |
| O1—C24—C25—C26 | -179.88 (17) | C23—C22—Ru1—Cl1 | -84.97 (14) |
| C23—C24—C25—C26 | 1.5 (3) | C23—C22—Ru1—Cl2 | 88.86 (14) |

Table S3. Selected geometric parameters for **Ru-2**(Å, º)

| | | | |
|---|---|---|---|
| C24—O1 | 1.362 (5) | C63—C68 | 1.395 (6) |
| C24—C25 | 1.381 (6) | C63—C62 | 1.447 (5) |
| C24—C23 | 1.410 (5) | C68—C67 | 1.385 (6) |
| C25—C26 | 1.382 (6) | C67—C66 | 1.389 (6) |
| C26—C27 | 1.388 (6) | C66—C65 | 1.384 (6) |
| C27—C29 | 1.383 (6) | C62—Ru2 | 1.827 (4) |
| C29—C23 | 1.396 (6) | C69—O2 | 1.472 (5) |
| C23—C22 | 1.441 (5) | C69—C70 | 1.496 (6) |
| C22—Ru1 | 1.828 (4) | C69—C71 | 1.518 (6) |
| C30—O1 | 1.479 (5) | C41—N4 | 1.342 (5) |
| C30—C32 | 1.494 (6) | C41—N3 | 1.351 (5) |
| C30—C31 | 1.503 (6) | C41—Ru2 | 1.974 (4) |
| C1—N2 | 1.347 (5) | C53—N4 | 1.446 (5) |
| C1—N1 | 1.348 (5) | C53—C54 | 1.510 (6) |
| C1—Ru1 | 1.960 (4) | C54—C59 | 1.376 (6) |
| C4—C9 | 1.389 (6) | C54—C55 | 1.392 (6) |
| C4—C5 | 1.399 (6) | C59—C58 | 1.390 (6) |
| C4—N1 | 1.429 (5) | C58—C57 | 1.376 (7) |
| C9—C8 | 1.394 (6) | C57—C56 | 1.381 (7) |
| C9—C12 | 1.508 (6) | C56—C55 | 1.398 (7) |
| C8—C7 | 1.388 (6) | C55—O4 | 1.369 (6) |
| C7—C6 | 1.391 (6) | C60—O4 | 1.427 (6) |
| C7—C11 | 1.508 (6) | C43—N4 | 1.467 (5) |
| C6—C5 | 1.388 (6) | C43—C42 | 1.517 (6) |
| C5—C10 | 1.501 (6) | C42—N3 | 1.473 (5) |
| C2—N1 | 1.470 (5) | C44—C49 | 1.389 (6) |
| C2—C3 | 1.517 (6) | C44—C45 | 1.404 (6) |
| C3—N2 | 1.467 (5) | C44—N3 | 1.423 (5) |
| C13—N2 | 1.451 (5) | C45—C46 | 1.383 (6) |
| C13—C14 | 1.514 (6) | C45—C50 | 1.509 (6) |
| C14—C15 | 1.384 (6) | C46—C47 | 1.385 (6) |
| C14—C19 | 1.398 (6) | C47—C48 | 1.385 (6) |
| C15—C16 | 1.390 (6) | C47—C51 | 1.503 (6) |
| C16—C17 | 1.366 (8) | C48—C49 | 1.386 (6) |
| C17—C18 | 1.383 (8) | C49—C52 | 1.502 (6) |
| C18—C19 | 1.395 (7) | O1—Ru1 | 2.285 (3) |
| C19—O3 | 1.364 (6) | O2—Ru2 | 2.274 (3) |
| C20—O3 | 1.432 (5) | Cl1—Ru1 | 2.3383 (10) |
| C64—O2 | 1.369 (5) | Cl2—Ru1 | 2.3246 (10) |
| C64—C65 | 1.372 (5) | Cl3—Ru2 | 2.3282 (10) |
| C64—C63 | 1.406 (5) | Cl4—Ru2 | 2.3426 (11) |

| | | | |
|---|---|---|---|
| | | | |
| O1—C24—C25 | 126.9 (4) | C55—C54—C53 | 119.4 (4) |
| O1—C24—C23 | 112.6 (3) | C54—C59—C58 | 121.6 (4) |
| C25—C24—C23 | 120.5 (4) | C57—C58—C59 | 118.9 (5) |
| C24—C25—C26 | 119.6 (4) | C58—C57—C56 | 120.9 (5) |
| C25—C26—C27 | 121.1 (4) | C57—C56—C55 | 119.6 (5) |
| C29—C27—C26 | 119.3 (4) | O4—C55—C54 | 115.9 (4) |
| C27—C29—C23 | 120.9 (4) | O4—C55—C56 | 124.0 (4) |
| C29—C23—C24 | 118.5 (4) | C54—C55—C56 | 120.1 (4) |
| C29—C23—C22 | 122.6 (4) | N4—C43—C42 | 102.4 (3) |
| C24—C23—C22 | 118.9 (4) | N3—C42—C43 | 103.0 (3) |
| C23—C22—Ru1 | 118.5 (3) | C49—C44—C45 | 121.7 (4) |
| O1—C30—C32 | 106.4 (3) | C49—C44—N3 | 118.2 (4) |
| O1—C30—C31 | 109.4 (3) | C45—C44—N3 | 120.1 (4) |
| C32—C30—C31 | 113.7 (4) | C46—C45—C44 | 118.1 (4) |
| N2—C1—N1 | 107.0 (3) | C46—C45—C50 | 121.1 (4) |
| N2—C1—Ru1 | 118.7 (3) | C44—C45—C50 | 120.8 (4) |
| N1—C1—Ru1 | 134.3 (3) | C45—C46—C47 | 122.0 (4) |
| C9—C4—C5 | 122.5 (4) | C48—C47—C46 | 118.0 (4) |
| C9—C4—N1 | 119.5 (4) | C48—C47—C51 | 121.2 (4) |
| C5—C4—N1 | 118.0 (4) | C46—C47—C51 | 120.8 (4) |
| C4—C9—C8 | 118.0 (4) | C47—C48—C49 | 122.7 (4) |
| C4—C9—C12 | 121.5 (4) | C48—C49—C44 | 117.6 (4) |
| C8—C9—C12 | 120.4 (4) | C48—C49—C52 | 120.6 (4) |
| C7—C8—C9 | 121.6 (4) | C44—C49—C52 | 121.8 (4) |
| C8—C7—C6 | 118.2 (4) | C1—N1—C4 | 126.1 (3) |
| C8—C7—C11 | 121.4 (4) | C1—N1—C2 | 112.8 (3) |
| C6—C7—C11 | 120.5 (4) | C4—N1—C2 | 121.1 (3) |
| C5—C6—C7 | 122.6 (4) | C1—N2—C13 | 123.3 (3) |
| C6—C5—C4 | 117.0 (4) | C1—N2—C3 | 113.0 (3) |
| C6—C5—C10 | 121.7 (4) | C13—N2—C3 | 118.8 (3) |
| C4—C5—C10 | 121.3 (4) | C41—N3—C44 | 127.4 (3) |
| N1—C2—C3 | 102.4 (3) | C41—N3—C42 | 112.3 (3) |
| N2—C3—C2 | 101.6 (3) | C44—N3—C42 | 120.2 (3) |
| N2—C13—C14 | 113.0 (3) | C41—N4—C53 | 125.4 (3) |
| C15—C14—C19 | 119.3 (4) | C41—N4—C43 | 113.1 (3) |
| C15—C14—C13 | 121.3 (4) | C53—N4—C43 | 120.0 (3) |
| C19—C14—C13 | 119.3 (4) | C24—O1—C30 | 119.2 (3) |
| C14—C15—C16 | 121.0 (5) | C24—O1—Ru1 | 109.1 (2) |
| C17—C16—C15 | 119.3 (5) | C30—O1—Ru1 | 130.3 (2) |
| C16—C17—C18 | 121.0 (5) | C64—O2—C69 | 119.4 (3) |

| | | | |
|---|---|---|---|
| C17—C18—C19 | 120.0 (5) | C64—O2—Ru2 | 110.2 (2) |
| O3—C19—C18 | 124.8 (4) | C69—O2—Ru2 | 129.8 (2) |
| O3—C19—C14 | 115.8 (4) | C19—O3—C20 | 117.8 (4) |
| C18—C19—C14 | 119.4 (5) | C55—O4—C60 | 117.9 (4) |
| O2—C64—C65 | 126.1 (4) | C22—Ru1—C1 | 102.97 (17) |
| O2—C64—C63 | 112.8 (3) | C22—Ru1—O1 | 78.78 (14) |
| C65—C64—C63 | 121.0 (4) | C1—Ru1—O1 | 176.96 (13) |
| C68—C63—C64 | 118.6 (4) | C22—Ru1—Cl2 | 100.22 (12) |
| C68—C63—C62 | 122.7 (4) | C1—Ru1—Cl2 | 89.46 (11) |
| C64—C63—C62 | 118.7 (4) | O1—Ru1—Cl2 | 87.77 (7) |
| C67—C68—C63 | 120.6 (4) | C22—Ru1—Cl1 | 103.14 (12) |
| C68—C67—C66 | 119.2 (4) | C1—Ru1—Cl1 | 90.49 (11) |
| C65—C66—C67 | 121.2 (4) | O1—Ru1—Cl1 | 91.52 (7) |
| C64—C65—C66 | 119.2 (4) | Cl2—Ru1—Cl1 | 156.03 (4) |
| C63—C62—Ru2 | 119.1 (3) | C62—Ru2—C41 | 102.42 (17) |
| O2—C69—C70 | 106.6 (3) | C62—Ru2—O2 | 78.99 (14) |
| O2—C69—C71 | 108.5 (3) | C41—Ru2—O2 | 176.59 (13) |
| C70—C69—C71 | 114.5 (4) | C62—Ru2—Cl3 | 101.46 (12) |
| N4—C41—N3 | 108.0 (3) | C41—Ru2—Cl3 | 89.73 (11) |
| N4—C41—Ru2 | 119.0 (3) | O2—Ru2—Cl3 | 86.94 (8) |
| N3—C41—Ru2 | 133.0 (3) | C62—Ru2—Cl4 | 102.99 (12) |
| N4—C53—C54 | 112.9 (3) | C41—Ru2—Cl4 | 91.78 (11) |
| C59—C54—C55 | 118.9 (4) | O2—Ru2—Cl4 | 90.91 (8) |
| C59—C54—C53 | 121.7 (4) | Cl3—Ru2—Cl4 | 154.56 (4) |
| | | | |
| O1—C24—C25—C26 | 176.7 (4) | C50—C45—C46—C47 | -179.7 (4) |
| C23—C24—C25—C26 | -1.4 (6) | C45—C46—C47—C48 | 0.9 (6) |
| C24—C25—C26—C27 | -1.8 (6) | C45—C46—C47—C51 | -178.4 (4) |
| C25—C26—C27—C29 | 2.3 (6) | C46—C47—C48—C49 | 0.5 (6) |
| C26—C27—C29—C23 | 0.4 (6) | C51—C47—C48—C49 | 179.8 (4) |
| C27—C29—C23—C24 | -3.5 (6) | C47—C48—C49—C44 | -0.7 (6) |
| C27—C29—C23—C22 | 174.9 (4) | C47—C48—C49—C52 | 177.9 (4) |
| O1—C24—C23—C29 | -174.3 (3) | C45—C44—C49—C48 | -0.5 (6) |
| C25—C24—C23—C29 | 4.0 (6) | N3—C44—C49—C48 | 179.1 (3) |
| O1—C24—C23—C22 | 7.2 (5) | C45—C44—C49—C52 | -179.1 (4) |
| C25—C24—C23—C22 | -174.5 (4) | N3—C44—C49—C52 | 0.5 (5) |
| C29—C23—C22—Ru1 | -172.9 (3) | N2—C1—N1—C4 | 179.9 (4) |
| C24—C23—C22—Ru1 | 5.6 (5) | Ru1—C1—N1—C4 | 2.6 (6) |
| C5—C4—C9—C8 | 2.6 (6) | N2—C1—N1—C2 | -1.9 (5) |
| N1—C4—C9—C8 | -176.9 (3) | Ru1—C1—N1—C2 | -179.2 (3) |
| C5—C4—C9—C12 | -179.8 (4) | C9—C4—N1—C1 | 87.1 (5) |
| N1—C4—C9—C12 | 0.7 (6) | C5—C4—N1—C1 | -92.4 (5) |

| | | | |
|---|---|---|---|
| C4—C9—C8—C7 | -0.9 (6) | C9—C4—N1—C2 | -90.9 (5) |
| C12—C9—C8—C7 | -178.6 (4) | C5—C4—N1—C2 | 89.6 (5) |
| C9—C8—C7—C6 | -0.5 (6) | C3—C2—N1—C1 | 12.3 (5) |
| C9—C8—C7—C11 | 179.9 (4) | C3—C2—N1—C4 | -169.4 (4) |
| C8—C7—C6—C5 | 0.2 (6) | N1—C1—N2—C13 | -165.2 (3) |
| C11—C7—C6—C5 | 179.8 (4) | Ru1—C1—N2—C13 | 12.5 (5) |
| C7—C6—C5—C4 | 1.3 (6) | N1—C1—N2—C3 | -10.3 (4) |
| C7—C6—C5—C10 | 178.8 (4) | Ru1—C1—N2—C3 | 167.5 (3) |
| C9—C4—C5—C6 | -2.8 (6) | C14—C13—N2—C1 | -132.5 (4) |
| N1—C4—C5—C6 | 176.7 (3) | C14—C13—N2—C3 | 73.9 (5) |
| C9—C4—C5—C10 | 179.8 (4) | C2—C3—N2—C1 | 17.4 (4) |
| N1—C4—C5—C10 | -0.7 (6) | C2—C3—N2—C13 | 173.6 (3) |
| N1—C2—C3—N2 | -16.5 (4) | N4—C41—N3—C44 | 176.2 (4) |
| N2—C13—C14—C15 | 33.8 (5) | Ru2—C41—N3—C44 | -2.8 (6) |
| N2—C13—C14—C19 | -149.2 (4) | N4—C41—N3—C42 | -1.1 (5) |
| C19—C14—C15—C16 | -0.7 (6) | Ru2—C41—N3—C42 | 179.9 (3) |
| C13—C14—C15—C16 | 176.2 (4) | C49—C44—N3—C41 | -92.0 (5) |
| C14—C15—C16—C17 | -0.4 (7) | C45—C44—N3—C41 | 87.6 (5) |
| C15—C16—C17—C18 | 0.9 (7) | C49—C44—N3—C42 | 85.1 (5) |
| C16—C17—C18—C19 | -0.4 (7) | C45—C44—N3—C42 | -95.3 (5) |
| C17—C18—C19—O3 | -179.8 (4) | C43—C42—N3—C41 | 7.7 (5) |
| C17—C18—C19—C14 | -0.7 (6) | C43—C42—N3—C44 | -169.8 (4) |
| C15—C14—C19—O3 | -179.6 (4) | N3—C41—N4—C53 | -172.6 (4) |
| C13—C14—C19—O3 | 3.4 (6) | Ru2—C41—N4—C53 | 6.6 (5) |
| C15—C14—C19—C18 | 1.2 (6) | N3—C41—N4—C43 | -6.6 (5) |
| C13—C14—C19—C18 | -175.8 (4) | Ru2—C41—N4—C43 | 172.6 (3) |
| O2—C64—C63—C68 | -180.0 (3) | C54—C53—N4—C41 | -124.5 (4) |
| C65—C64—C63—C68 | 2.1 (6) | C54—C53—N4—C43 | 70.4 (5) |
| O2—C64—C63—C62 | 2.5 (5) | C42—C43—N4—C41 | 11.0 (5) |
| C65—C64—C63—C62 | -175.4 (4) | C42—C43—N4—C53 | 177.8 (4) |
| C64—C63—C68—C67 | -2.5 (6) | C25—C24—O1—C30 | 0.2 (6) |
| C62—C63—C68—C67 | 174.9 (4) | C23—C24—O1—C30 | 178.5 (3) |
| C63—C68—C67—C66 | 0.7 (6) | C25—C24—O1—Ru1 | 168.3 (3) |
| C68—C67—C66—C65 | 1.7 (6) | C23—C24—O1—Ru1 | -13.5 (4) |
| O2—C64—C65—C66 | -177.5 (4) | C32—C30—O1—C24 | -151.3 (4) |
| C63—C64—C65—C66 | 0.2 (6) | C31—C30—O1—C24 | 85.5 (4) |
| C67—C66—C65—C64 | -2.1 (6) | C32—C30—O1—Ru1 | 43.5 (5) |
| C68—C63—C62—Ru2 | -174.8 (3) | C31—C30—O1—Ru1 | -79.7 (4) |
| C64—C63—C62—Ru2 | 2.6 (5) | C65—C64—O2—C69 | -15.9 (6) |
| N4—C53—C54—C59 | 27.2 (6) | C63—C64—O2—C69 | 166.3 (3) |
| N4—C53—C54—C55 | -155.4 (4) | C65—C64—O2—Ru2 | 172.5 (3) |
| C55—C54—C59—C58 | -0.2 (6) | C63—C64—O2—Ru2 | -5.3 (4) |

| | | | |
|---|---|---|---|
| C53—C54—C59—C58 | 177.3 (4) | C70—C69—O2—C64 | 157.8 (4) |
| C54—C59—C58—C57 | -0.8 (7) | C71—C69—O2—C64 | -78.3 (4) |
| C59—C58—C57—C56 | 1.5 (7) | C70—C69—O2—Ru2 | -32.5 (5) |
| C58—C57—C56—C55 | -1.0 (7) | C71—C69—O2—Ru2 | 91.3 (4) |
| C59—C54—C55—O4 | 179.9 (4) | C18—C19—O3—C20 | -5.1 (6) |
| C53—C54—C55—O4 | 2.4 (6) | C14—C19—O3—C20 | 175.7 (4) |
| C59—C54—C55—C56 | 0.7 (6) | C54—C55—O4—C60 | 174.9 (4) |
| C53—C54—C55—C56 | -176.9 (4) | C56—C55—O4—C60 | -5.9 (6) |
| C57—C56—C55—O4 | -179.2 (4) | C23—C22—Ru1—C1 | 167.7 (3) |
| C57—C56—C55—C54 | -0.1 (6) | C23—C22—Ru1—O1 | -9.7 (3) |
| N4—C43—C42—N3 | -10.4 (4) | C23—C22—Ru1—Cl2 | 75.9 (3) |
| C49—C44—C45—C46 | 1.8 (6) | C23—C22—Ru1—Cl1 | -98.7 (3) |
| N3—C44—C45—C46 | -177.8 (3) | C63—C62—Ru2—C41 | 172.8 (3) |
| C49—C44—C45—C50 | 179.5 (4) | C63—C62—Ru2—O2 | -4.1 (3) |
| N3—C44—C45—C50 | 0.0 (6) | C63—C62—Ru2—Cl3 | 80.5 (3) |
| C44—C45—C46—C47 | -2.0 (6) | C63—C62—Ru2—Cl4 | -92.5 (3) |

Table S4. Selected geometric parameters for **Ru-3** (Å, º).

| | | | |
|---|---|---|---|
| Ru1—C22 | 1.8293 (19) | C9—C12 | 1.507 (3) |
| Ru1—C1 | 1.9689 (18) | C2—C3 | 1.526 (3) |
| Ru1—O1 | 2.2452 (13) | C32—C30 | 1.504 (3) |
| Ru1—Cl1 | 2.3135 (5) | C21—N3 | 1.459 (2) |
| Ru1—Cl2 | 2.3387 (5) | C14—C15 | 1.389 (3) |
| O1—C24 | 1.371 (2) | C14—C19 | 1.411 (3) |
| O1—C30 | 1.474 (2) | C14—C13 | 1.517 (2) |
| N1—C1 | 1.344 (2) | C25—C24 | 1.390 (3) |
| N1—C4 | 1.434 (2) | C6—C5 | 1.389 (3) |
| N1—C3 | 1.470 (2) | C28—C23 | 1.400 (3) |
| N2—C1 | 1.349 (2) | C24—C23 | 1.400 (3) |
| N2—C13 | 1.449 (2) | C16—C17 | 1.384 (3) |
| N2—C2 | 1.462 (2) | C16—C15 | 1.389 (3) |
| C26—C25 | 1.385 (3) | C30—C31 | 1.510 (3) |
| C26—C27 | 1.389 (3) | C17—C18 | 1.382 (3) |
| C7—C6 | 1.384 (3) | C20—N3 | 1.466 (2) |
| C7—C8 | 1.392 (3) | C4—C5 | 1.399 (3) |
| C7—C11 | 1.509 (3) | C19—C18 | 1.394 (3) |
| C27—C28 | 1.380 (3) | C19—N3 | 1.418 (2) |
| C9—C4 | 1.392 (3) | C5—C10 | 1.505 (3) |
| C9—C8 | 1.396 (3) | C22—C23 | 1.451 (3) |
| | | | |
| C22—Ru1—C1 | 101.91 (8) | C15—C14—C13 | 120.34 (16) |
| C22—Ru1—O1 | 79.11 (7) | C19—C14—C13 | 120.18 (16) |
| C1—Ru1—O1 | 178.28 (6) | C26—C25—C24 | 118.4 (2) |
| C22—Ru1—Cl1 | 97.89 (6) | C7—C6—C5 | 122.02 (18) |
| C1—Ru1—Cl1 | 92.93 (5) | C27—C28—C23 | 120.1 (2) |
| O1—Ru1—Cl1 | 85.56 (4) | C7—C8—C9 | 121.53 (19) |
| C22—Ru1—Cl2 | 108.80 (6) | O1—C24—C25 | 126.01 (19) |
| C1—Ru1—Cl2 | 90.04 (5) | O1—C24—C23 | 112.87 (16) |
| O1—Ru1—Cl2 | 90.92 (4) | C25—C24—C23 | 121.10 (19) |
| Cl1—Ru1—Cl2 | 151.917 (18) | C17—C16—C15 | 119.39 (19) |
| C24—O1—C30 | 119.80 (15) | O1—C30—C32 | 106.66 (16) |
| C24—O1—Ru1 | 110.14 (11) | O1—C30—C31 | 108.75 (16) |
| C30—O1—Ru1 | 129.80 (12) | C32—C30—C31 | 113.38 (19) |
| C1—N1—C4 | 126.20 (15) | C18—C17—C16 | 120.32 (18) |
| C1—N1—C3 | 113.36 (15) | C9—C4—C5 | 121.99 (17) |
| C4—N1—C3 | 120.41 (14) | C9—C4—N1 | 119.65 (16) |
| C1—N2—C13 | 125.19 (15) | C5—C4—N1 | 118.34 (17) |
| C1—N2—C2 | 113.96 (15) | C18—C19—C14 | 118.69 (17) |
| C13—N2—C2 | 120.70 (15) | C18—C19—N3 | 122.27 (17) |

| | | | |
|---|---|---|---|
| | | | |
| C25—C26—C27 | 121.5 (2) | C14—C19—N3 | 119.00 (16) |
| N1—C1—N2 | 107.17 (15) | C6—C5—C4 | 117.82 (18) |
| N1—C1—Ru1 | 133.67 (13) | C6—C5—C10 | 121.43 (18) |
| N2—C1—Ru1 | 119.09 (13) | C4—C5—C10 | 120.68 (17) |
| C6—C7—C8 | 118.61 (18) | C17—C18—C19 | 121.03 (18) |
| C6—C7—C11 | 120.80 (19) | C23—C22—Ru1 | 118.32 (14) |
| C8—C7—C11 | 120.6 (2) | N2—C13—C14 | 114.14 (15) |
| C28—C27—C26 | 119.8 (2) | C28—C23—C24 | 119.05 (18) |
| C4—C9—C8 | 117.96 (18) | C28—C23—C22 | 122.95 (18) |
| C4—C9—C12 | 121.10 (17) | C24—C23—C22 | 118.00 (18) |
| C8—C9—C12 | 120.92 (18) | C19—N3—C21 | 115.67 (15) |
| N2—C2—C3 | 102.32 (15) | C19—N3—C20 | 114.56 (16) |
| N1—C3—C2 | 102.69 (15) | C21—N3—C20 | 110.79 (15) |
| C15—C14—C19 | 119.48 (17) | C14—C15—C16 | 121.05 (18) |
| | | | |
| C4—N1—C1—N2 | -174.21 (17) | C1—N1—C4—C5 | 86.2 (2) |
| C3—N1—C1—N2 | 4.0 (2) | C3—N1—C4—C5 | -91.9 (2) |
| C4—N1—C1—Ru1 | 9.2 (3) | C15—C14—C19—C18 | -1.5 (3) |
| C3—N1—C1—Ru1 | -172.61 (14) | C13—C14—C19—C18 | 178.93 (18) |
| C13—N2—C1—N1 | -174.71 (16) | C15—C14—C19—N3 | -179.37 (17) |
| C2—N2—C1—N1 | 0.8 (2) | C13—C14—C19—N3 | 1.1 (3) |
| C13—N2—C1—Ru1 | 2.5 (2) | C7—C6—C5—C4 | -1.0 (3) |
| C2—N2—C1—Ru1 | 178.05 (12) | C7—C6—C5—C10 | -178.05 (18) |
| C25—C26—C27—C28 | -0.5 (3) | C9—C4—C5—C6 | 2.6 (3) |
| C1—N2—C2—C3 | -4.9 (2) | N1—C4—C5—C6 | -176.21 (16) |
| C13—N2—C2—C3 | 170.87 (16) | C9—C4—C5—C10 | 179.69 (17) |
| C1—N1—C3—C2 | -6.8 (2) | N1—C4—C5—C10 | 0.9 (3) |
| C4—N1—C3—C2 | 171.50 (16) | C16—C17—C18—C19 | -0.6 (3) |
| N2—C2—C3—N1 | 6.49 (19) | C14—C19—C18—C17 | 1.9 (3) |
| C27—C26—C25—C24 | -0.4 (3) | N3—C19—C18—C17 | 179.65 (19) |
| C8—C7—C6—C5 | -1.3 (3) | C1—Ru1—C22—C23 | -168.37 (14) |
| C11—C7—C6—C5 | 178.5 (2) | O1—Ru1—C22—C23 | 10.22 (13) |
| C26—C27—C28—C23 | 1.2 (3) | Cl1—Ru1—C22—C23 | -73.67 (14) |
| C6—C7—C8—C9 | 2.1 (3) | Cl2—Ru1—C22—C23 | 97.46 (14) |
| C11—C7—C8—C9 | -177.7 (2) | C1—N2—C13—C14 | -116.66 (19) |
| C4—C9—C8—C7 | -0.6 (3) | C2—N2—C13—C14 | 68.1 (2) |
| C12—C9—C8—C7 | 177.67 (18) | C15—C14—C13—N2 | 27.8 (2) |
| C30—O1—C24—C25 | 2.6 (3) | C19—C14—C13—N2 | -152.66 (17) |
| Ru1—O1—C24—C25 | -171.99 (16) | C27—C28—C23—C24 | -1.1 (3) |
| C30—O1—C24—C23 | -175.98 (16) | C27—C28—C23—C22 | 179.93 (18) |
| Ru1—O1—C24—C23 | 9.40 (18) | O1—C24—C23—C28 | 178.83 (16) |

| | | | |
|---|---|---|---|
| C26—C25—C24—O1 | -177.91 (18) | C25—C24—C23—C28 | 0.1 (3) |
| C26—C25—C24—C23 | 0.6 (3) | O1—C24—C23—C22 | -2.1 (2) |
| C24—O1—C30—C32 | -161.11 (16) | C25—C24—C23—C22 | 179.21 (17) |
| Ru1—O1—C30—C32 | 12.3 (2) | Ru1—C22—C23—C28 | 170.38 (15) |
| C24—O1—C30—C31 | 76.3 (2) | Ru1—C22—C23—C24 | -8.6 (2) |
| Ru1—O1—C30—C31 | -110.31 (17) | C18—C19—N3—C21 | -20.4 (3) |
| C15—C16—C17—C18 | -0.9 (3) | C14—C19—N3—C21 | 157.35 (17) |
| C8—C9—C4—C5 | -1.8 (3) | C18—C19—N3—C20 | 110.3 (2) |
| C12—C9—C4—C5 | 179.92 (17) | C14—C19—N3—C20 | -71.9 (2) |
| C8—C9—C4—N1 | 176.96 (16) | C19—C14—C15—C16 | 0.0 (3) |
| C12—C9—C4—N1 | -1.3 (3) | C13—C14—C15—C16 | 179.52 (18) |
| C1—N1—C4—C9 | -92.7 (2) | C17—C16—C15—C14 | 1.3 (3) |
| C3—N1—C4—C9 | 89.2 (2) | | |

Table S5. Selected geometric parameters for **Ru-4**(Å, º)

| | | | |
|---|---|---|---|
| Ru1—Cl1 | 2.3300 (7) | C11—C16 | 1.398 (4) |
| Ru1—Cl2 | 2.3351 (7) | C12—C13 | 1.394 (5) |
| Ru1—O1 | 2.2845 (17) | C12—C17 | 1.510 (5) |
| Ru1—C1 | 1.967 (2) | C13—C14 | 1.370 (6) |
| Ru1—C23 | 1.823 (2) | C14—C15 | 1.360 (5) |
| O1—C25 | 1.370 (3) | C15—C16 | 1.390 (4) |
| O1—C30 | 1.465 (3) | C16—C20 | 1.500 (4) |
| N1—C1 | 1.346 (3) | C17—C18 | 1.551 (5) |
| N1—C2 | 1.451 (4) | C17—C19 | 1.535 (5) |
| N1—C4 | 1.448 (4) | C20—C21 | 1.537 (5) |
| N2—C1 | 1.343 (3) | C20—C22 | 1.529 (5) |
| N2—C3 | 1.476 (3) | C23—C24 | 1.450 (3) |
| N2—C11 | 1.431 (3) | C24—C25 | 1.402 (3) |
| C2—C3 | 1.496 (5) | C24—C29 | 1.390 (3) |
| C4—C5 | 1.512 (4) | C25—C26 | 1.385 (3) |
| C5—C6 | 1.373 (4) | C26—C27 | 1.382 (4) |
| C5—C10 | 1.364 (4) | C27—C28 | 1.374 (4) |
| C6—C7 | 1.391 (4) | C28—C29 | 1.387 (4) |
| C7—C8 | 1.333 (5) | C30—C32 | 1.476 (14) |
| C8—C9 | 1.361 (5) | C30—C31 | 1.664 (7) |
| C9—C10 | 1.386 (4) | C30—C32A | 1.725 (10) |
| C11—C12 | 1.394 (4) | C30—C31A | 1.390 (18) |
| | | | |
| Cl1—Ru1—Cl2 | 153.18 (3) | C12—C11—C16 | 122.1 (3) |
| O1—Ru1—Cl1 | 88.05 (5) | C16—C11—N2 | 118.4 (2) |
| O1—Ru1—Cl2 | 90.78 (5) | C11—C12—C17 | 122.2 (3) |
| C1—Ru1—Cl1 | 91.80 (6) | C13—C12—C11 | 117.3 (3) |
| C1—Ru1—Cl2 | 88.86 (7) | C13—C12—C17 | 120.5 (3) |
| C1—Ru1—O1 | 178.89 (8) | C14—C13—C12 | 121.5 (3) |
| C23—Ru1—Cl1 | 103.53 (7) | C15—C14—C13 | 120.0 (3) |
| C23—Ru1—Cl2 | 102.50 (7) | C14—C15—C16 | 121.8 (3) |
| C23—Ru1—O1 | 78.79 (8) | C11—C16—C20 | 122.5 (2) |
| C23—Ru1—C1 | 102.32 (10) | C15—C16—C11 | 117.3 (3) |
| C25—O1—Ru1 | 109.89 (13) | C15—C16—C20 | 120.1 (3) |
| C25—O1—C30 | 120.1 (2) | C12—C17—C18 | 109.5 (3) |
| C30—O1—Ru1 | 129.97 (18) | C12—C17—C19 | 112.0 (3) |
| C1—N1—C2 | 113.3 (2) | C19—C17—C18 | 111.3 (3) |
| C1—N1—C4 | 124.7 (2) | C16—C20—C21 | 109.2 (3) |
| C4—N1—C2 | 119.3 (2) | C16—C20—C22 | 112.1 (3) |
| C1—N2—C3 | 112.4 (2) | C22—C20—C21 | 111.5 (3) |
| C1—N2—C11 | 128.79 (19) | C24—C23—Ru1 | 119.67 (17) |

| | | | |
|---|---|---|---|
| C11—N2—C3 | 118.1 (2) | C25—C24—C23 | 118.3 (2) |
| N1—C1—Ru1 | 118.75 (18) | C29—C24—C23 | 123.5 (2) |
| N2—C1—Ru1 | 134.09 (17) | C29—C24—C25 | 118.2 (2) |
| N2—C1—N1 | 107.1 (2) | O1—C25—C24 | 113.2 (2) |
| N1—C2—C3 | 102.8 (2) | O1—C25—C26 | 125.5 (2) |
| N2—C3—C2 | 102.8 (2) | C26—C25—C24 | 121.2 (2) |
| N1—C4—C5 | 113.7 (2) | C27—C26—C25 | 118.7 (3) |
| C6—C5—C4 | 120.6 (3) | C28—C27—C26 | 121.4 (3) |
| C10—C5—C4 | 121.0 (2) | C27—C28—C29 | 119.6 (3) |
| C10—C5—C6 | 118.3 (3) | C28—C29—C24 | 120.8 (2) |
| C5—C6—C7 | 120.7 (3) | O1—C30—C32 | 107.1 (6) |
| C8—C7—C6 | 120.1 (3) | O1—C30—C31 | 102.3 (3) |
| C7—C8—C9 | 120.1 (3) | O1—C30—C32A | 100.1 (3) |
| C8—C9—C10 | 120.4 (4) | C32—C30—C31 | 105.8 (7) |
| C5—C10—C9 | 120.3 (3) | C31A—C30—O1 | 112.4 (8) |
| C12—C11—N2 | 119.3 (2) | C31A—C30—C32A | 100.4 (10) |
| | | | |
| Ru1—O1—C25—C24 | 4.0 (2) | C7—C8—C9—C10 | 2.2 (6) |
| Ru1—O1—C25—C26 | -176.9 (2) | C8—C9—C10—C5 | -0.5 (5) |
| Ru1—O1—C30—C32 | -19.6 (8) | C10—C5—C6—C7 | 2.1 (5) |
| Ru1—O1—C30—C31 | 91.4 (4) | C11—N2—C1—Ru1 | 12.3 (4) |
| Ru1—O1—C30—C32A | -98.1 (4) | C11—N2—C1—N1 | -170.9 (2) |
| Ru1—O1—C30—C31A | 7.7 (11) | C11—N2—C3—C2 | 179.4 (2) |
| Ru1—C23—C24—C25 | 2.3 (3) | C11—C12—C13—C14 | 0.2 (5) |
| Ru1—C23—C24—C29 | -178.11 (18) | C11—C12—C17—C18 | 112.2 (4) |
| Cl1—Ru1—C23—C24 | -85.15 (18) | C11—C12—C17—C19 | -123.9 (3) |
| Cl2—Ru1—C23—C24 | 88.36 (18) | C11—C16—C20—C21 | -111.0 (3) |
| O1—Ru1—C23—C24 | 0.06 (17) | C11—C16—C20—C22 | 124.9 (3) |
| O1—C25—C26—C27 | -176.5 (2) | C12—C11—C16—C15 | -1.3 (4) |
| N1—C2—C3—N2 | -11.3 (3) | C12—C11—C16—C20 | 176.0 (3) |
| N1—C4—C5—C6 | -133.0 (3) | C12—C13—C14—C15 | -0.5 (6) |
| N1—C4—C5—C10 | 51.2 (4) | C13—C12—C17—C18 | -66.6 (4) |
| N2—C11—C12—C13 | 176.2 (2) | C13—C12—C17—C19 | 57.3 (4) |
| N2—C11—C12—C17 | -2.7 (4) | C13—C14—C15—C16 | -0.1 (6) |
| N2—C11—C16—C15 | -176.8 (2) | C14—C15—C16—C11 | 1.0 (5) |
| N2—C11—C16—C20 | 0.5 (4) | C14—C15—C16—C20 | -176.4 (3) |
| C1—Ru1—C23—C24 | 179.94 (17) | C15—C16—C20—C21 | 66.3 (4) |
| C1—N1—C2—C3 | 12.3 (3) | C15—C16—C20—C22 | -57.8 (4) |
| C1—N1—C4—C5 | -137.9 (3) | C16—C11—C12—C13 | 0.8 (4) |
| C1—N2—C3—C2 | 8.1 (3) | C16—C11—C12—C17 | -178.1 (3) |

| | | | |
|---|---|---|---|
| C1—N2—C11—C12 | 85.1 (3) | C17—C12—C13—C14 | 179.0 (3) |
| C1—N2—C11—C16 | -99.3 (3) | C23—C24—C25—O1 | -4.4 (3) |
| C2—N1—C1—Ru1 | 169.8 (2) | C23—C24—C25—C26 | 176.6 (2) |
| C2—N1—C1—N2 | -7.5 (3) | C23—C24—C29—C28 | -178.5 (2) |
| C2—N1—C4—C5 | 62.0 (4) | C24—C25—C26—C27 | 2.5 (4) |
| C3—N2—C1—Ru1 | -177.5 (2) | C25—O1—C30—C32 | 160.9 (7) |
| C3—N2—C1—N1 | -0.8 (3) | C25—O1—C30—C31 | -88.1 (4) |
| C3—N2—C11—C12 | -84.6 (3) | C25—O1—C30—C32A | 82.4 (4) |
| C3—N2—C11—C16 | 91.0 (3) | C25—O1—C30—C31A | -171.8 (10) |
| C4—N1—C1—Ru1 | 8.7 (3) | C25—C24—C29—C28 | 1.1 (4) |
| C4—N1—C1—N2 | -168.7 (2) | C25—C26—C27—C28 | 0.1 (4) |
| C4—N1—C2—C3 | 174.5 (3) | C26—C27—C28—C29 | -2.0 (4) |
| C4—C5—C6—C7 | -173.8 (3) | C27—C28—C29—C24 | 1.4 (4) |
| C4—C5—C10—C9 | 174.3 (3) | C29—C24—C25—O1 | 176.0 (2) |
| C5—C6—C7—C8 | -0.5 (6) | C29—C24—C25—C26 | -3.1 (3) |
| C6—C5—C10—C9 | -1.6 (5) | C30—O1—C25—C24 | -176.4 (2) |
| C6—C7—C8—C9 | -1.7 (6) | C30—O1—C25—C26 | 2.7 (4) |

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