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Heteroleptic Ruthenium(II) Complexes Featuring *N*-Heterocyclic Carbene-Based C^N Donor Sets for Solar Energy Conversion

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Electronic Supporting Information

Contents

Experimental Details

Materials and Methods

Acetonitrile and dimethylformamide were distilled over calcium hydride. Distilled solvents were collected over 3 Å molecular sieves under the flow of nitrogen gas. A standard vacuum-nitrogen double-manifold Schlenk line, Schlenk tubes, or a glove box was used to handle chemicals sensitive to air and moisture. 1-(Pyridine-2-yl)-1H-benzimidazole[1] and [(η^6-*p* cymene)-Ru(C^N$^{decyl/octyl}$)(Cl)][PF_6] ([**IV**] and [**V**]) were synthesized according to the previously reported protocols. For the syntheses of [**1**] − [**4**], the reported protocol of [Ru(tpy)$^{4'\text{-Ph-COOMe}/4'\text{-COOMe}}$(C^N)(Cl)][$PF_6$] was followed.[2b] Methyl 4′-([2, 2': 6', 2''-terpyridin]-4'-yl) carboxylate[2] and 4, 4', 4''-trimethoxy carbonyl-2, 2': 6', 2''-terpyridine[3] were synthesized according to the previous reports with slight modifications. Other reagents were used as acquired from commercial sources without any purification unless otherwise stated.

^{1}H (400 MHz), ^{13}C (100.61 MHz), and 2-D NMR (nuclear magnetic resonance) spectra were performed on a Jeol ECS 400 MHz spectrometer. The proton resonances were annotated as chemical shift (δ) relative to tetramethylsilane (δ 0.0) or by using the residual solvent signal as an internal standard. High-resolution mass spectrometry (HRMS) and liquid chromatography, LC-MS analyses were performed on a Xevo G2-S Q-Tof (Waters, USA) spectrometer. LC-MS data were acquired using Xevo G2-S Q-Tof (Waters, USA) spectrometer. Mobile phases comprised 0.1% formic acid in distilled water (Solution A). In addition, 0.1% formic acid in acetonitrile (Solution B) was also used. UV-Visible and emission spectra were recorded on a Jasco V-30 spectrophotometer and Fluoromax *4 C.L*. System, respectively. Relative quantum yields were obtained using quinine sulfate as the reference. Infrared spectra were obtained from a Bruker Fourier transform infrared spectrophotometer (FTIR) (Alpha), and ATR (attenuated total reflectance) mode was used in the collection of data. Lifetime measurements were done using the HORIBA Deltaflex TCSPC lifetime fluorometer. Due to the hygroscopic nature, elemental analyses of final photosensitizers could not be obtained within the ±0.4% permissible error limit.

Electrochemical Measurements

1 mM solution of sensitizers with 0.1 M *tetra*-butyl ammonium hexafluorophosphate in anhydrous acetonitrile was utilized for electrochemical measurements. Cyclic voltammetry and differential pulse voltammetry at different scan rates of 50 mVs^{-1}, 100 mVs^{-1}, and 200 mVs^{-1} were performed on *K-Lyte* 1.2 Potentiostat. A three-electrode setup comprising Platinum as the counter electrode, Ag/Ag^+ as the reference electrode, and glassy carbon as the working electrode was used. Before each measurement, the samples were deaerated with nitrogen for 10 minutes. The potentials obtained were referenced to an internal $[Fc]/[Fc]^+$ standard, followed by conversion to a standard calomel electrode (SCE). After each measurement, the working electrode was polished using an alumina pad and rinsed with deionized water and methanol.

Photoelectrochemical Measurements

Fluorine-doped tin oxide plates of sheet resistance 7 ohm/sq were acquired from Great Cell Solar Materials. Surlyn gasket and black vinyl sticker were obtained from Solaronix. 1-Butyl-3-methyl imidazolium iodide, TiO_2 photoanodes, and platinum electrodes were prepared according to the reported procedures.[4] Further, the photoelectrochemical measurements were done according to the previously reported protocols.[4] For dye sensitization, the sintered TiO_2-coated photoanodes were cooled to 80 °C and then dipped in 0.6 mM of dye solutions in acetonitrile: *t*-butanol (1: 1, *v*: *v*) for 36 h. The sensitized photoanodes were washed with acetonitrile to remove the weakly adsorbed dye molecules. A 50-μm Surlyn gasket sandwiched the active area of the photoanode (0.25 cm^2) and the cathodes. The electrolyte comprising a mixture of I_2 (0.06 M), LiI (0.1 M), and 1-butyl-3-methyl imidazolium iodide (0.5 M) in acetonitrile was inoculated through the prior drilled holes of the cathode. The device was sealed with a Surlyn film and a cover glass. A black vinyl mask (Solaronix) was used to cover the surroundings of the photoanodes to ensure that the light falls only on the active area. Three sets of DSSCs were prepared to ensure the reproducibility of results, and the photovoltaic data were collected from the *J*–*V* plots. Photovoltaic measurements are performed in a two-electrode configuration with dye-sensitized photoanodes as the working electrode and the platinum-coated FTO plates as the counter electrode. The simulated sunlight was obtained from the Excelitas module comprising a PE175BF Xenon-arc light source in an ILC Technology (USA) system coupled with AM 1.5G filters. The radiant power of the light was adjusted to 1000 W m^{-2} using a calibrated silicon pyranometer (AM1.5G) before every measurement.

Electrochemical Impedance Spectroscopic measurements were carried out using *K*-Lyte *-Z* impedance analyzer with a sinusoidal potential perturbation of 10 mV. Measurements were done under white light LED illumination and in dark. The applied voltage was the open-circuit potential of the measured device, and the potential perturbation was applied over a frequency range of 0.1 Hz–0.1 MHz. The resulting impedance spectra were fitted according to the transmission line model and analyzed using an EIS spectrum analyzer.

Computational Details

All dispersion-corrected density functional theory (DFT–D3)[5] calculations were performed in ORCA 5.0.3[6] using the hybrid B3LYP[7] functional and double and triple ζ-quality Ahlrich's Def2-SVP for non-metallic atoms and def2-TZVP basis set for the ruthenium center, respectively[8]. The RIJCOSX[9] approximation was used for all calculations throughout with default grids. A methyl group in [**A**] bearing a COOH anchor and [**B**] having a tricarboxylic acid anchor is used throughout all computations instead of octyl and decyl side chains to reduce the computational cost. Geometry optimizations of singlet ground (S_0) states and their singly- and doubly-oxidized forms using *restricted* and *unrestricted* Kohn-Sham formalisms, respectively, were performed without symmetry constraints. The bonding nature between the [Ru–Tpy–COOH/$(COOH)_3$]$^{2+}$ and [NCS, C^N ligand]$^-$ acceptor and donor fragments, respectively, of the ground states in acetonitrile phase were analyzed by ETS-NOCV calculations[10]. The electronic structure of the lowest-lying singlet excited state was obtained *via* Time-Dependent Density Functional Theory (TDDFT) geometry optimizations in acetonitrile using a solvation model based on density (SMD)[11]. Vibrational frequency calculations confirmed the absence of negative imaginary frequencies, N_{imag} = 0. The Gibbs free energies from the frequency analysis were used to calculate oxidation potentials using the thermodynamic *Hess-Law of constant heat summation*[12]. Fifty singlet vertical transitions in acetonitrile were obtained by TDDFT single-point calculations on the optimized solvated S_0 states. Electron difference density maps (EDDMs) of the selected charge transfer transitions were obtained *via* the orca_plot utility.

Preparation of 1-(pyridine-2-yl) -1H-benzimidazole:

(**I**)**:** A mixture of 2-bromopyridine (0.40 g, 0.24 mL, 2.53 mmole), benzimidazole (0.30 g, 2.53 mmole), K_2CO_3 (0.70 g, 5.06 mmole), CuI (0.09 g, 0.51 mmole), unsymmetrical *N*, *N*-dimethylethylenediamine (L_3) (0.11 mL, 1.01 mmole), and

dry-degassed dimethyl sulphoxide (6 mL) were added inside the glove box in a screw-capped vial. The color of the reaction mixture changed to blue after adding L_3. The reaction mixture was stirred for 30 minutes at ambient temperature and then heated over a pre-heated oil bath at 120 ℃ for 48 h. Subsequently, the reaction mixture was cooled down to ambient temperature, and 20 mL of water was added to it. The product was extracted from this mixture using dichloromethane. The organic phase was washed with water (3 × times), and then the organic phase was collected and washed with a solution of brine (3 × times) and then dried over $MgSO_4$. Dichloromethane was dried *in vacuo* to yield brown-colored solids. Brown solids were purified by silica gel (100 − 200 Mesh) column chromatography, using ethyl acetate: hexanes (1: 1, *v: v*) as the solvent mixture to afford colorless solids (0.40 g, 2.02 mmole).[1] Yield: 80%.

Preparation of 3-decyl-1-(pyridine-2-yl)-1H-benzimidazole-3-ium hexafluorophosphate (II):

(**II**): A mixture of (**I**) (1.00 g, 5.12 mmole), decyl bromide (6.36 mL, 30.73 mmole), and dry-degassed dimethylformamide (6 mL) was heated over a pre-heated oil bath at 110 ℃ for 18 h. Subsequently, the reaction mixture was cooled down to ambient temperature, and dimethylformamide was removed under reduced pressure. The residue obtained was washed with cold hexane (3 × times), and then dissolved in a minimal amount of water, and excess KPF_6 (aq.) was added to it. The resulting mixture was stirred at ambient temperature for 30 minutes. The precipitate obtained was dissolved in acetonitrile, dried over $MgSO_4$, and the solvent was removed *in vacuo* to yield tan-colored solids (1.83 g, 3.81 mmole). Yield: 73.01%.

Preparation of 3-octyl-1-(pyridine-2-yl)-1H-benzimidazole-3-ium hexafluorophosphate:

(**III**): A mixture of (**I**) (1.00 g, 5.12 mmole), octyl bromide (5.03 mL, 30.7 mmole), and dry-degassed dimethylformamide (6 mL) was heated over a pre-heated oil bath at 110 ℃ for 18 h. Subsequently, the reaction mixture was cooled down to ambient temperature, and dimethylformamide was removed under reduced pressure. The residue obtained was washed with cold hexane (3 × times) and then dissolved in a minimal amount of water, and excess KPF_6 (aq.) was added to it. The resulting mixture was stirred at ambient temperature for 30 minutes. The precipitate obtained was dissolved in acetonitrile, dried over $MgSO_4$, and the solvent was removed *in vacuo* to yield tan-colored solids (1.93 g, 4.26 mmole). Yield: 83.11%.

Preparation of [(η^6-*p* cymene)-Ru(C^N^{decyl}) (Cl)](PF_6) [IV]:

(**II**) (0.15 g, 0.33 mmole), Ag_2O (0.04 g, 0.17 mmole), and dry-degassed acetonitrile (15 mL) were added to a Schlenk flask. The resulting mixture was heated over a pre-heated oil bath at 60 ℃ in the absence of light for 48 h. Subsequently, the reaction mixture was cooled to ambient temperature, filtered over celite, and [(η^6-*p* cymene)-Ru(Cl)$_2$]$_2$ (0.102 mg, 0.17 mmole) was added to the filtrate obtained. The resulting mixture was further heated over a pre-heated oil bath at 60 ℃ in the absence of light for 24 h. Subsequently, the reaction mixture was cooled to ambient temperature and filtered over celite. The solvent was removed *in vacuo* to yield orange-colored solids. Orange solids were purified by silica gel (100 − 200 Mesh) column chromatography using dichloromethane: acetone (9: 1, *v: v*) as the solvent mixture to afford yellow-colored solids (0.19 g, 0.25 mmole).[13] Yield: 81.1%.

Preparation of [(η^6-*p* cymene)-Ru(C^N^{octyl}) (Cl)](PF_6) [V]:

(**III**) (0.15 g, 0.33 mmole), Ag_2O (0.04 g, 0.17 mmole), and dry-degassed acetonitrile (15 mL) were added to a Schlenk flask. The resulting mixture was heated over a pre-heated oil bath at 60 ℃ in the absence of light for 48 h. Subsequently, the reaction mixture was cooled to ambient temperature, filtered over celite, and [(η^6-*p* cymene)-Ru(Cl)$_2$]$_2$ (0.102 mg, 0.17 mmole) was added to the filtrate obtained. The resulting mixture was further heated over a pre-heated oil bath at 60 ℃ in the absence of light for 24 h. Subsequently, the reaction mixture was cooled to ambient temperature and filtered over celite. The solvent was removed *in vacuo* to yield orange-colored solids. Orange solids were purified by silica gel (100 − 200 Mesh) column chromatography using dichloromethane: acetone (9: 1, *v: v*) as the solvent mixture to afford yellow-colored solids (0.197 g, 0.27 mmole).[13] Yield: 80.8%.

Preparation of 4-carboxylate terpyridine:

(**V**): 4-carboxylate terpyridine was isolated by following the reported protocol[2] with slight modifications. Here, we removed dimethylformamide under reduced pressure to improve the yield of (**V**) before performing extraction with ethyl acetate.

Preparation of 4, 4', 4"-tricarboxy terpyridine:

(**VI**): Initially, ethyl-2-isonicotinate was isolated as yellow solids by refluxing the mixture of paraldehyde (8.2 g, 62 mmol) and ethyl isonicotinate (1.92g, 12.7 mmol), $FeSO_4.7H_2O$ (60 mg, 0.22 mmol), trifluoroacetic acid (1.4.9 g, 13 mmol) and 70% t-BuOOH (3.2 g, 252mmol) in acetonitrile (26 mL) for 4 h. Subsequently, acetonitrile was removed *in vacuo*, and the residue was taken up in a 20 mL of sodium carbonate (aq.). The aqueous layer was extracted with benzene. The combined organic fractions were dried over (Na_2SO_4, filtered, and then the solvent was removed *in vacuo*.

The reaction mixture containing ethyl-2-isonicotinate (2 g, 10.7 mmol) was reacted with freshly distilled furfural (0.49 g, 5.18 mmol) potassium hydroxide (1.33 g, 2.44 mmol), and 10 mL of 25 % NH_3 (aq.) in 12 mL of absolute ethanol under inert atmosphere at ambient temperature for 24 h. After the completion of the reaction, the reaction mixture was filtered, washed with cold ethanol (3 × times), and then suspended in acetonitrile. The supernatant was decanted, and the precipitate was dried *in vacuo* to yield light-brown solids. Note: ethyl-2-isonicotinate melts spontaneously at ambient temperature. The above reaction should be performed at 10 ℃. Further, potassium 4′-furyl-2,2′:6′,2"-terpyridine-4,4"-dicarboxylate (2.46 g, 5.3 mmol) was reacted with $KMnO_4$ (4 g, 25.3 mmol) in water (100 mL). The solution was adjusted to pH = 10 by adding potassium hydroxide (0.04 g). The resulting mixture was stirred at room temperature for 24 h. The resulting mixture was filtered and then acidified with 37 % HCl (1.15 g). The precipitate was filtered and thoroughly washed with cold ethanol and H_2O. The esterification was done in methanol by following the procedure reported in the literature.[3]

General Procedure for the syntheses of [1] – [4]

For the syntheses of [**1**] – [**4**], the previously reported procedure for the preparation of [**1**] and [**2**] was followed.[4a] A 100 mL Schlenk flask was charged with [**IV**] or [**V**] and tpy$^{4'\text{-COOMe}}$ (**VI**) or tpy$^{4,\ 4',\ 4''\text{-(COOMe)}_3}$ (**VII**) and dry-degassed acetonitrile. The resulting mixture was heated over a pre-heated oil bath at 110 °C for 15 h under an inert atmosphere of nitrogen gas. The reaction mixture turned red, indicating the completion of the reaction. Further, the removal of acetonitrile in the rotary evaporator yielded crude red solids. Crude solids were washed with hexanes (3 × times). Silica gel column chromatography was used to purify crude solids. Dichloromethane: Acetone (9: 1, *v*: *v*) was used as the solvent mixture to isolate red to orange solids.

Synthesis of [Ru(tpy$^{4'\text{-COOMe}}$)(C^N^{decyl})(Cl)][PF$_6$] [1]:

[**1**] was synthesized following the general procedure starting from [**IV**] (0.13 g, 0.17 mmole), tpy$^{4'\text{-COOMe}}$ (**VI**) (0.05 g, 0.17 mmole), and 15 mL dry-degassed acetonitrile. The product was isolated as hygroscopic orange solids (0.07 g, 0.08 mmole). Yield: 44.5%. ^{1}H NMR (CD$_3$CN, 400 MHz, ppm) δ 8.80 (s, 2H, C*H*^{aromatic}), 8.30 (d, $^3J_{C-H}$ = 9.6 Hz, 2H, C*H*^{aromatic}), 7.95 (t, $^3J_{C-H}$ = 11.6 Hz, 2H, C*H*^{aromatic}), 7.71 (t, $^3J_{C-H}$ = 13.3 Hz, 2H, C*H*^{aromatic}), 7.62 (dd, $^3J_{C-H}$ = 9.1, $^3J_{C-H}$ = 5.4 Hz, 3H, C*H*^{aromatic}), 7.37 (t, $^3J_{C-H}$ = 9.7 Hz, 1H, C*H*^{aromatic}), 7.31 (t, $^3J_{C-H}$ = 7.7 Hz, 1H, C*H*^{aromatic}), 6.97 (t, $^3J_{C-H}$ = 6.3 Hz, 3H, C*H*^{aromatic}), 6.60 (t, $^3J_{C-H}$ = 13.1 Hz, 1H, C*H*^{aromatic}), 4.58 (t, $^3J_{C-H}$ = 6.7 Hz, 2H, decyl–*H*), 3.87 (s, 3H, COO*C*H$_3$), 1.71 (s, 3H, decyl–*H*), 1.65 (m, 5H, decyl–*H*), 0.97 (s, 8H, decyl–*H*), 0.94 (s, 3H, decyl–*H*). ^{13}C NMR (CD$_3$CN, 100.61 MHz, ppm) δ 209.6 (Ru–*C*^{NHC}), 165.7 (*C*OOCH$_3$), 159.0 (*C*^{q}), 158.6 (*C*H^{aromatic}), 157.8 (*C*H^{aromatic}), 156.9 (*C*H^{aromatic}), 152.2 (*C*^{q}), 141.0 (*C*^{q}), 140.3 (*C*H^{aromatic}), 138.7 (*C*H^{aromatic}), 133.4 (*C*H^{aromatic}), 129.6 (*C*H^{aromatic}), 126.6 (*C*H^{aromatic}), 125.7 (*C*^{q}), 124.4 (*C*^{q}), 123.1 (*C*^{q}), 114.1 (*C*H^{aromatic}), 113.6 (*C*H^{aromatic}), 112.7 (*C*H^{aromatic}), 54.7 (COO*C*H$_3$), 48.9 (decyl–*C*), 37.0 (decyl–*C*), 32.9 (decyl–*C*), 31.7 (decyl–*C*), 30.7 (decyl–*C*), 30.2 (decyl–*C*), 28.2 (decyl–*C*), 23.8 (decyl–*C*), 14.7 (decyl–*C*). HRMS: m/*z* 886.2929 (calculated for [M]$^+$), 886.2907.

Synthesis of [Ru(tpy$^{4'\text{-COOMe}}$)(C^N^{octyl})(Cl)][PF$_6$] [2]:

[**2**] was synthesized following the general procedure starting from [**V**] (0.08 g, 0.10 mmole), tpy$^{4'\text{-COOMe}}$ (**VI**) (0.03 g, 0.10 mmole), and 15 mL dry-degassed acetonitrile. The product was isolated as hygroscopic orange solids (0.05 g, 0.05 mmole). Yield: 51.1%. ^{1}H NMR (CD$_3$CN, 400 MHz, ppm) δ 9.10 (s, 2H, C*H*^{aromatic}), 8.59 (d, $^3J_{C-H}$ = 9.4 Hz, 2H, C*H*^{aromatic}), 8.24 (t, $^3J_{C-H}$ = 11.1 Hz, 2H, C*H*^{aromatic}), 8.00 (t, $^3J_{C-H}$ = 13.6 Hz, 2H, C*H*^{aromatic}), 7.93 (m, 4H, C*H*^{aromatic}), 7.65 (t, $^3J_{C-H}$ = 9.4 Hz, 1H, C*H*^{aromatic}), 7.59 (t, $^3J_{C-H}$ = 7.3 Hz, 1H, C*H*^{aromatic}), 7.25 (m, 3H, C*H*^{aromatic}), 6.90 (t, $^3J_{C-H}$ = 6.0 Hz, 1H, C*H*^{aromatic}), 4.88 (t, $^3J_{C-H}$ = 6.5 Hz, 2H, octyl–*H*), 4.15 (s, 3H, COO*C*H$_3$), 2.12 (s, 3H, octyl–*H*), 1.35 (s, 3H, octyl–*H*), 0.83 (m, 6H, octyl–*H*). ^{13}C NMR (CD$_3$CN, 100.61 MHz, ppm) δ 209.0 (Ru–*C*^{NHC}), 165.1 (*C*OOCH$_3$), 158.4 (*C*^{q}), 157.9 (*C*H^{aromatic}), 156.3 (*C*H^{aromatic}), 151.5 (*C*H^{aromatic}), 140.4 (*C*H^{aromatic}), 138.0 (*C*^{q}), 132.7 (*C*^{q}), 129.0 (*C*H^{aromatic}), 126.0 (*C*H^{aromatic}), 125.6 (*C*H^{aromatic}), 123.7 (*C*^{q}), 122.5 (*C*^{q}), 113.5 (*C*^{q}), 112.9 (*C*H^{aromatic}), 111.9 (*C*^{q}), 55.0 (COO*C*H$_3$), 48.4 (octyl–*C*), 32.1 (octyl–*C*), 31.2 (octyl–*C*), 30.0 (octyl–*C*), 29.5 (octyl–*C*), 27.6 (octyl–*C*), 23.1 (octyl–*C*), 14.2 (octyl–*C*). HRMS: m/*z* 736.1804 (calculated for [M]$^+$), 736.1873.

Synthesis of [Ru(tpy$^{4,4',4''\text{-(COOMe)}_3}$)(C^N^{decyl})(Cl)][PF$_6$] [3]:

[**3**] was synthesized following the general procedure starting from [**IV**] (0.10 g, 0.13 mmole), tpy$^{4,4',4''\text{-(COOMe)}_3}$ (**VII**) (0.06 g, 0.13 mmole), and 15 mL dry-degassed acetonitrile. The product was isolated as hygroscopic red solids (0.05 g, 0.04 mmole). Yield: 33.1%. ^{1}H NMR (CD$_3$CN, 400 MHz, ppm) δ 9.27 (s, 2H, C*H*^{aromatic}), 8.98 (d, $^3J_{C-H}$ = 9.8 Hz, 2H, C*H*^{aromatic}), 8.26 (d, $^3J_{C-H}$ = 12.6 Hz, 3H, C*H*^{aromatic}), 8.11 (d, $^3J_{C-H}$ = 11.3 Hz, 2H, C*H*^{aromatic}), 7.67 (m, 4H, C*H*^{aromatic}), 7.26 (d, $^3J_{C-H}$ = 9.1 Hz, 1H, C*H*^{aromatic}), 6.89 (m, 2H, C*H*^{aromatic}), 4.86 (t, $^3J_{C-H}$ = 6.9 Hz, 2H, decyl–*H*), 4.18 (s, 3H, COO*C*H$_3$), 3.96 (s, 6H, COO*C*H$_3$), 1.36 (s, 9H, decyl–*H*), 0.88 (s, 6H, decyl–*H*), 0.83 (s, 4H, decyl–*H*). ^{13}C NMR (CD$_3$CN, 100.61 MHz, ppm) δ 207.4 (Ru–*C*^{NHC}), 164.7 (*C*OOCH$_3$), 164.2 (*C*OOCH$_3$), 159.3 (*C*^{q}), 158.7 (*C*H^{aromatic}), 156.5 (*C*^{q}), 156.0 (*C*^{q}), 153.5 (*C*H^{aromatic}), 151.5 (*C*H^{aromatic}), 140.6 (*C*H^{aromatic}), 140.2 (*C*^{q}), 137.8 (*C*^{q}), 132.6 (*C*H^{aromatic}), 127.5 (*C*H^{aromatic}), 125.6 (*C*H^{aromatic}), 125.1 (*C*^{q}), 124.6 (*C*^{q}), 122.4 (*C*H^{aromatic}), 116.2 (*C*H^{aromatic}), 114.3 (*C*^{q}), 113.4 (*C*H^{aromatic}), 112.9 (*C*^{q}), 111.8 (*C*^{q}), 54.7 (COO*C*H$_3$), 53.6 (COO*C*H$_3$), 48.3 (decyl–*C*), 32.2 (decyl–*C*), 31.4 (decyl–*C*), 29.9 (decyl–*C*), 29.3 (decyl–*C*), 27.3 (decyl–*C*), 26.2 (decyl–*C*), 23.0 (decyl–*C*), 13.9 (decyl–*C*). HRMS: m/*z* 879.2252 (calculated for [M]$^+$), 879.2220.

Synthesis of [Ru(tpy$^{4,4',4''\text{-(COOMe)}_3}$)(C^N^{octyl})(Cl)][PF$_6$] [4]:

[**4**] was synthesized following the general procedure starting from [**V**] (0.10 g, 0.10 mmole), tpy$^{4,4',4''\text{-(COOMe)}_3}$ (**VII**) (0.12 g, 0.10 mmole), and 15 mL dry-degassed acetonitrile. The product was isolated as hygroscopic red solids (0.055 g, 0.055 mmole). Yield: 55.1%. ^{1}H NMR (CD$_3$CN, 400 MHz, ppm) δ 9.02 (d, $^3J_{C-H}$ = 10.4 Hz, 3H, C*H*^{aromatic}), 8.25 (t, $^3J_{C-H}$ = 9.8 Hz, 2H, C*H*^{aromatic}), 8.10 (d, $^3J_{C-H}$ = 10.7 Hz, 2H, C*H*^{aromatic}), 7.97 (t, $^3J_{C-H}$ = 13.2 Hz, 1H, C*H*^{aromatic}), 7.71 (d, $^3J_{C-H}$ = 9.2 Hz, 1H, C*H*^{aromatic}), 7.63 (m, 2H, C*H*^{aromatic}), 7.39 (d, $^3J_{C-H}$ = 7.1 Hz, 1H, C*H*^{aromatic}), 6.94 (d, $^3J_{C-H}$ = 6.4 Hz, 1H, C*H*^{aromatic}), 6.88 (d, $^3J_{C-H}$ = 6.3 Hz, 1H, C*H*^{aromatic}), 4.88 (t, $^3J_{C-H}$ = 6.5 Hz, 2H, octyl–*H*), 4.19 (s, 3H, COO*C*H$_3$), 3.96 (s, 6H, COO*C*H$_3$), 2.11 (m, 3H, octyl–*H*), 1.52 (m, 3H, octyl–*H*), 1.39 (d, $^3J_{C-H}$ = 4.5 Hz, 2H, octyl–*H*), 0.86 (m, 4H, octyl–*H*). ^{13}C NMR (CD$_3$CN, 100.61 MHz, ppm) δ 208.4 (Ru–*C*^{NHC}), 164.6 (*C*OOCH$_3$), 164.3 (*C*OOCH$_3$), 160.2 (*C*^{q}), 159.0 (*C*H^{aromatic}), 156.5 (*C*^{q}), 156.0 (*C*^{q}), 153.8 (*C*H^{aromatic}), 151.7 (*C*H^{aromatic}), 147.4 (*C*^{q}), 141.1 (*C*H^{aromatic}), 140.7 (*C*H^{aromatic}), 138.1 (*C*^{q}), 132.8 (*C*H^{aromatic}), 127.4 (*C*H^{aromatic}), 125.7 (*C*^{q}), 125.3 (*C*^{q}), 124.3 (*C*^{q}), 122.6 (*C*H^{aromatic}), 119.1 (*C*H^{aromatic}), 114.2 (*C*^{q}), 113.5 (*C*H^{aromatic}), 112.9 (*C*H^{aromatic}), 112.1 (*C*^{q}), 54.6 (COO*C*H$_3$), 54.0 (COO*C*H$_3$), 48.6 (octyl–*C*), 32.3 (octyl–*C*), 31.7 (octyl–*C*), 30.2 (octyl–*C*), 29.7 (octyl–*C*), 27.7 (octyl–*C*), 23.3 (octyl–*C*), 14.3 (octyl–*C*). HRMS: m/*z* 858.2505 (calculated for [M]$^+$), 858.2566.

NMR Spectra of representative compounds

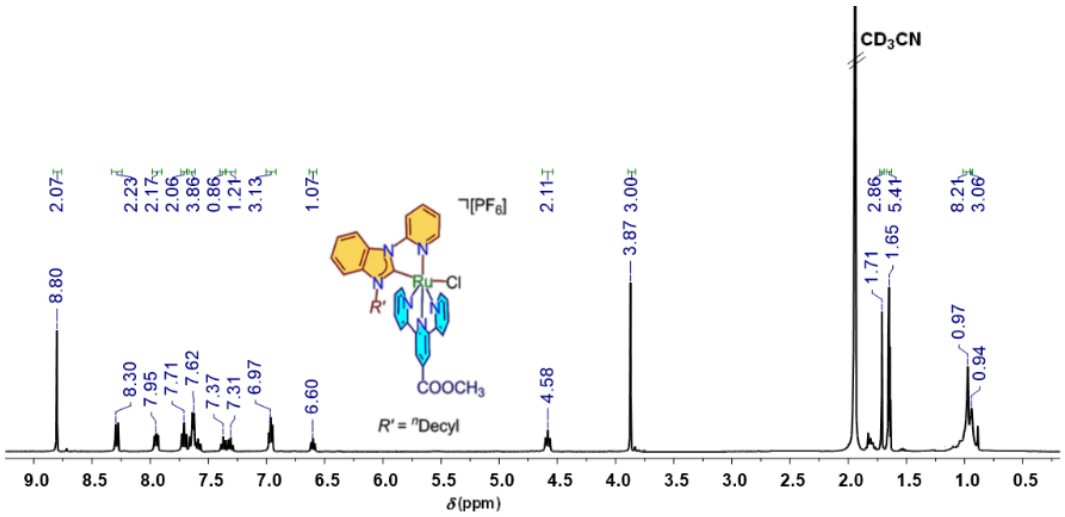


Fig. S1. ^{1}H NMR spectrum of [**1**] in CD_3CN at 400 MHz.

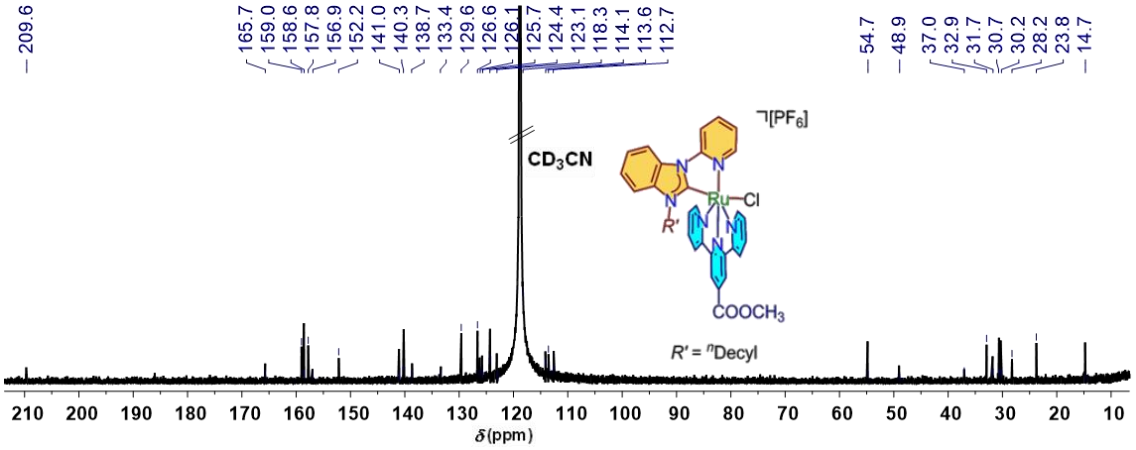


Fig. S2. ^{13}C NMR spectrum of [**1**] in CD_3CN at 100.61 MHz.

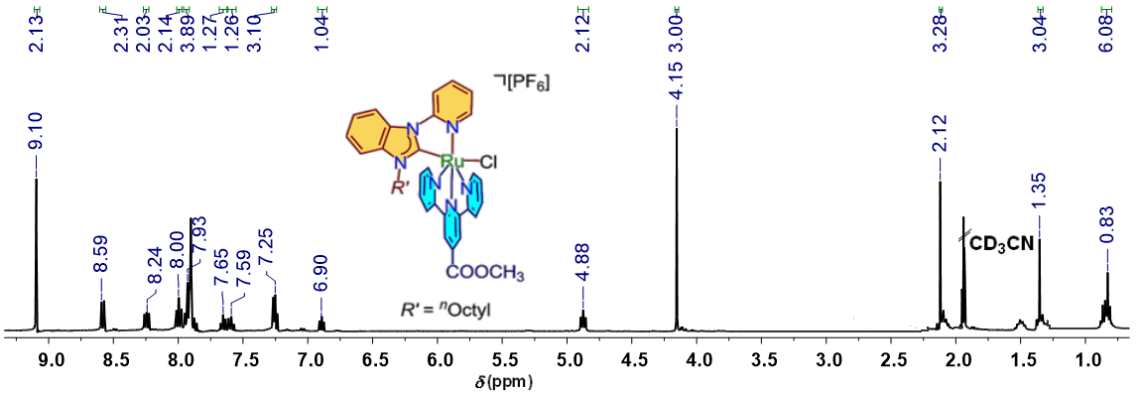


Fig. S3. ^{1}H NMR spectrum of [**2**] in CD_3CN at 400 MHz.

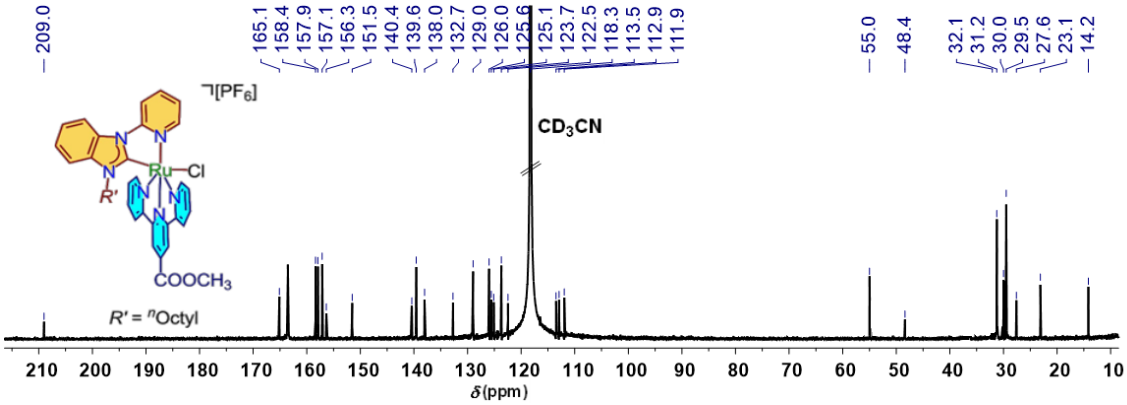


Fig. S4. ^{13}C NMR spectrum of [**2**] in CD_3CN at 100.61 MHz.

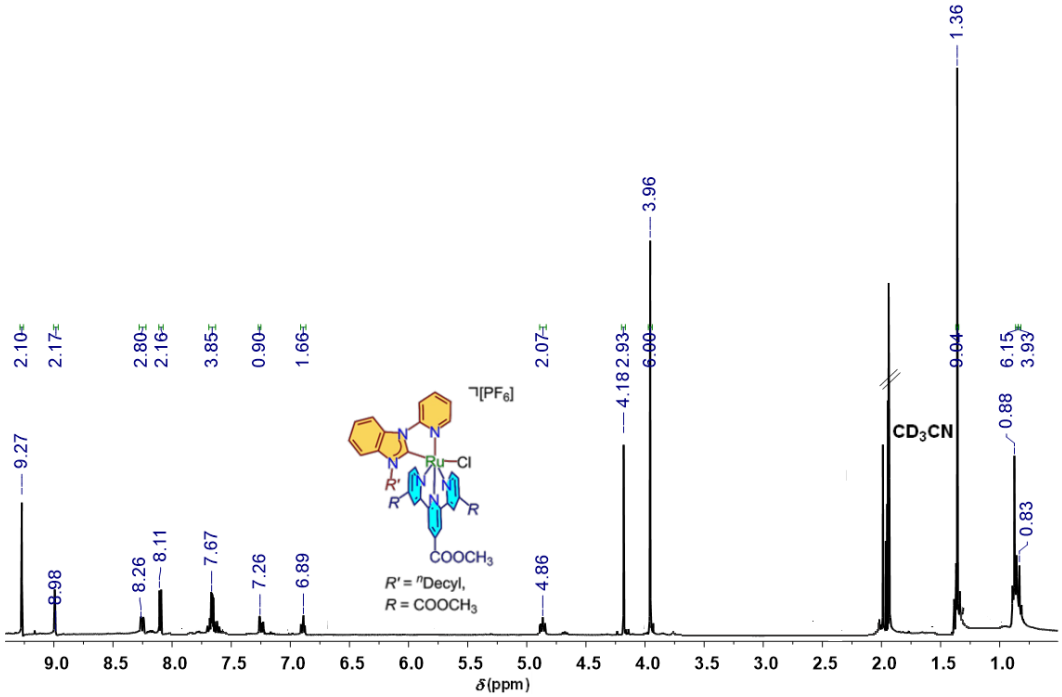


Fig. S5. ^{1}H NMR spectrum of [**3**] in CD_3CN at 400 MHz.

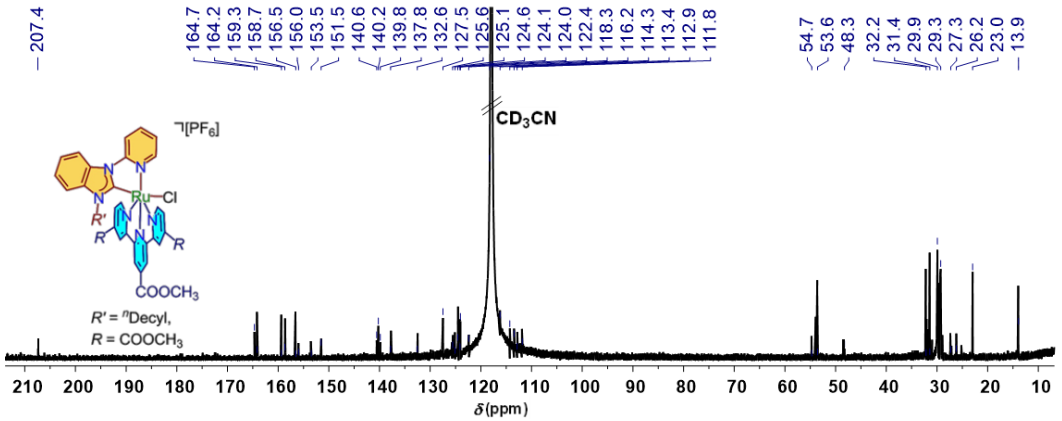


Fig. S6. ^{13}C NMR spectrum of [**3**] in CD_3CN at 100.61 MHz.

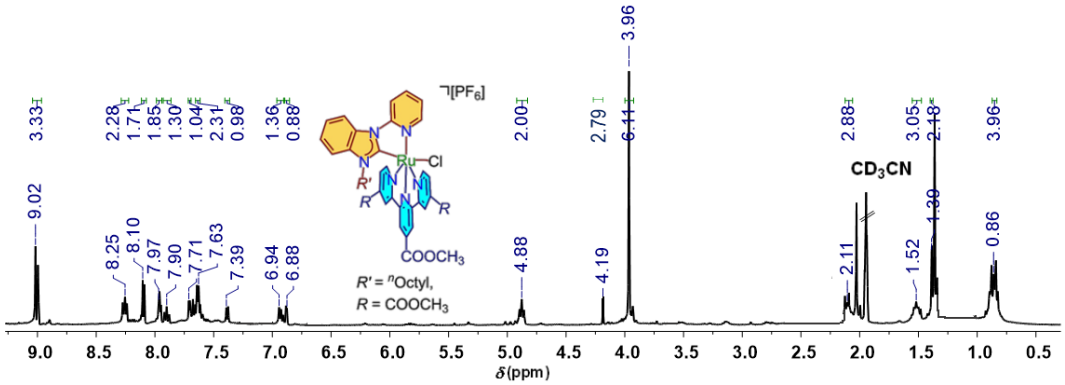


Fig. S7. ^{1}H NMR spectrum of [**4**] in CD_3CN at 400 MHz.

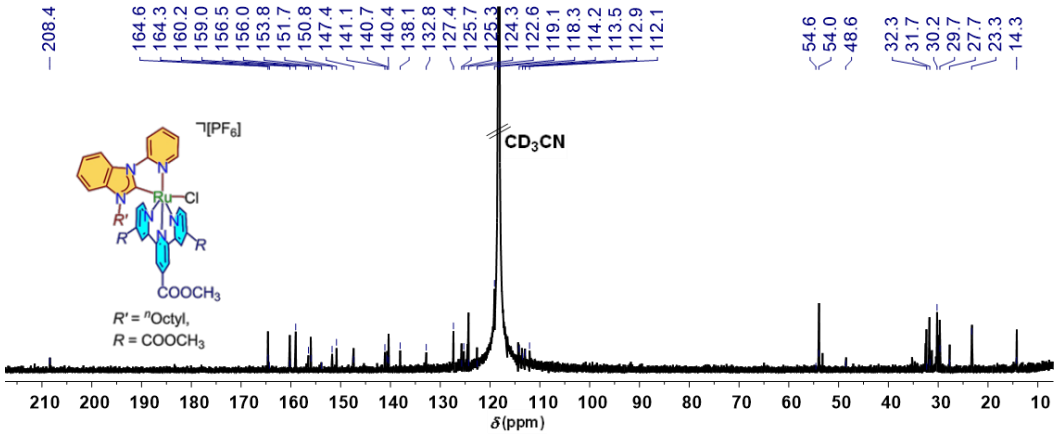


Fig. S8. ^{13}C NMR spectrum of [**4**] in CD_3CN at 100.61 MHz.

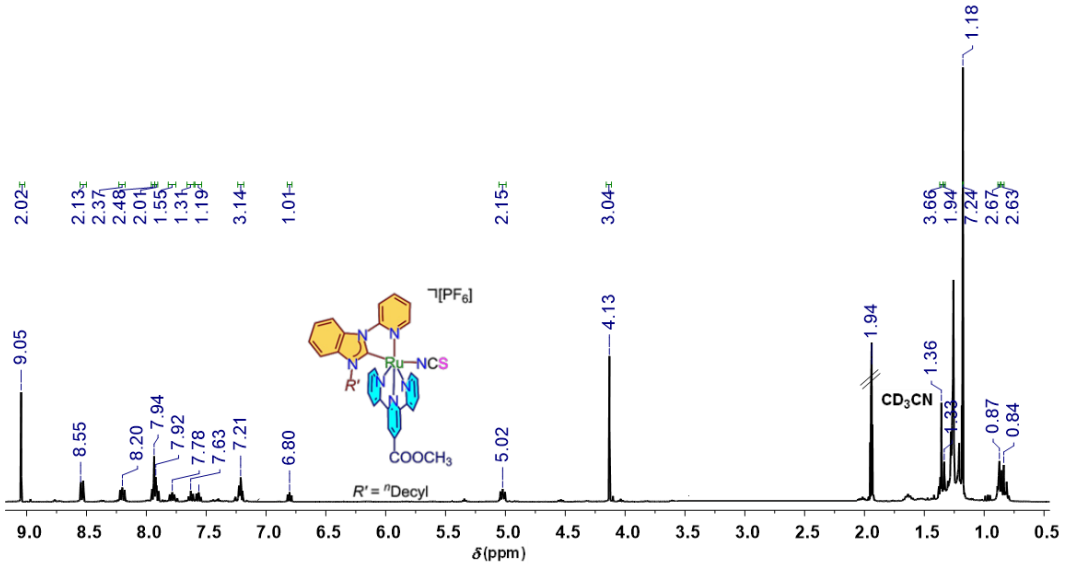


Fig. S9. ^{1}H NMR spectrum of [**5**] in CD_3CN at 400 MHz.

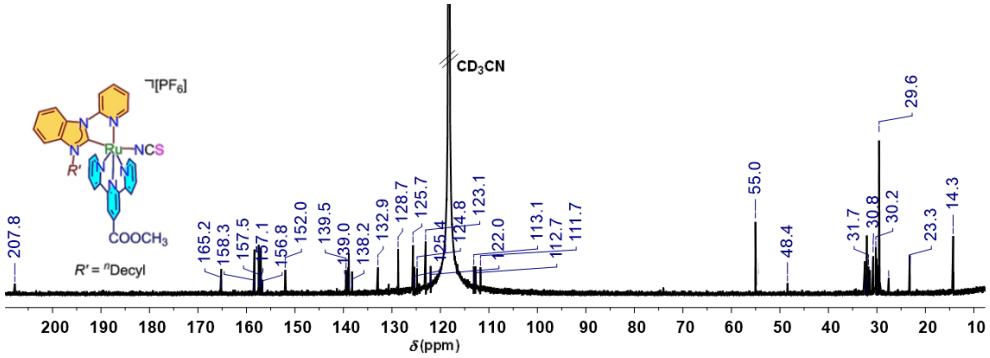


Fig. S10. ^{13}C NMR spectrum of [**5**] in CD_3CN at 100.61 MHz.

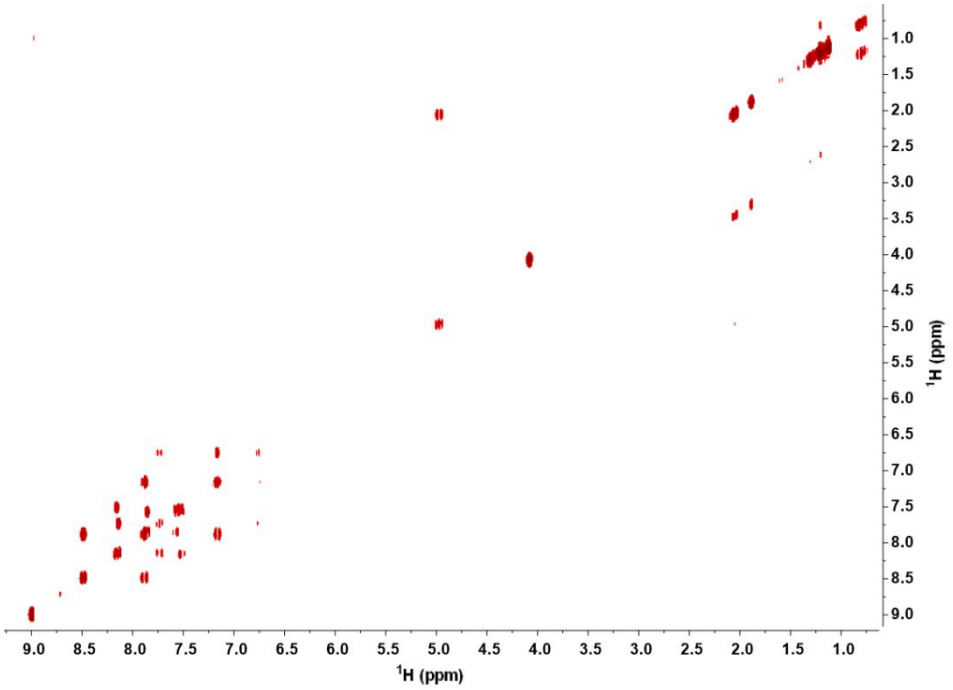


Fig. S11. $^{1}H-^{1}H$ COSY NMR spectrum of [**5**] in CD_3CN.

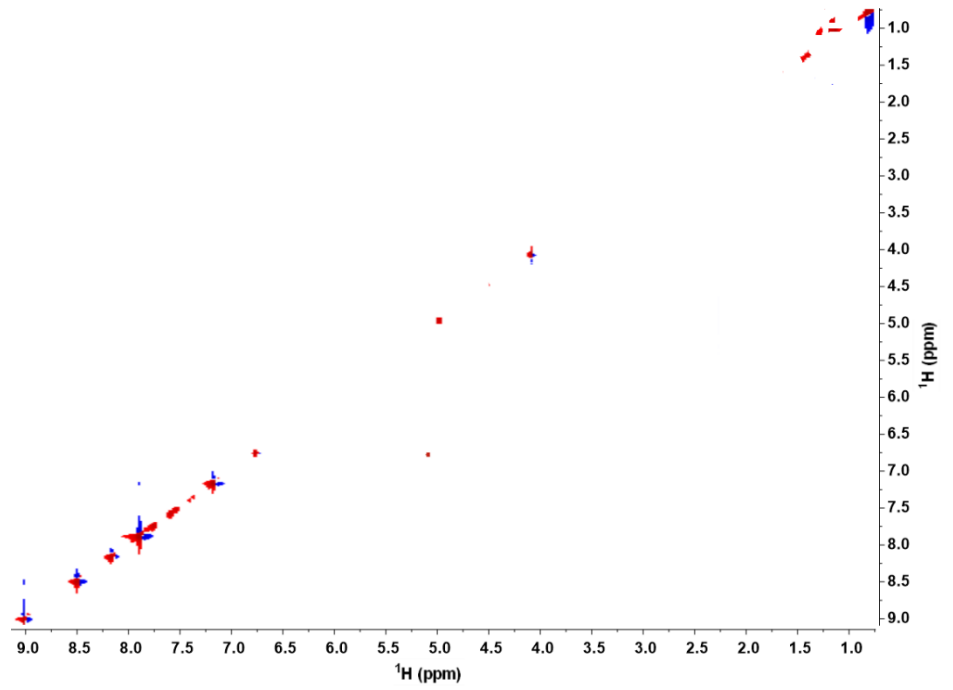


Fig. S12. $^{1}H-^{1}H$ NOESY NMR spectrum of [**5**] in CD_3CN.

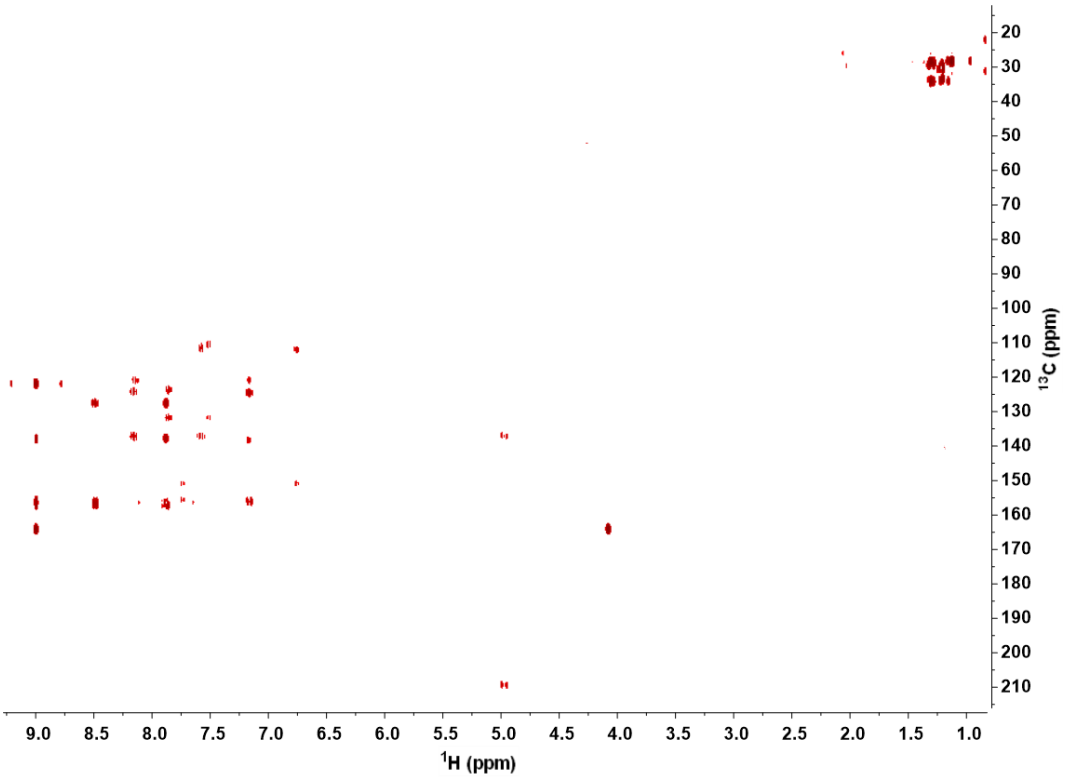


Fig. S13. ^{1}H–^{13}C HMBC NMR spectrum of [**5**] in CD_3CN.

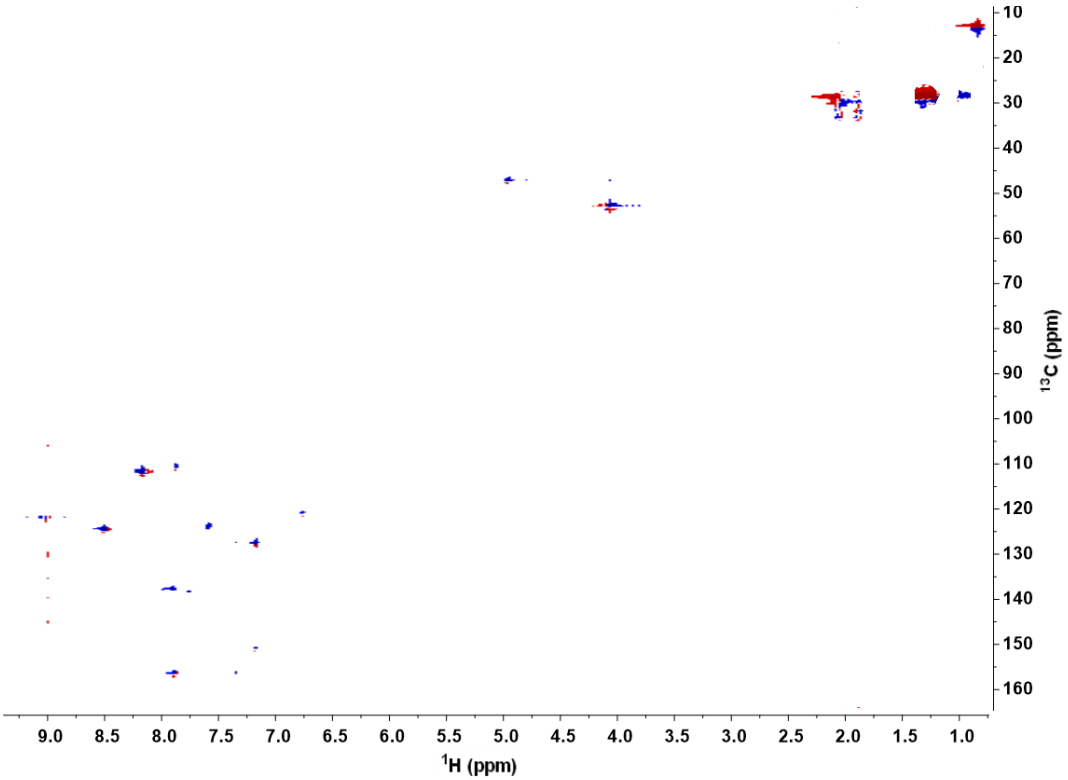


Fig. S14. ^{1}H–^{13}C HSQC NMR spectrum of [**5**] in CD_3CN.

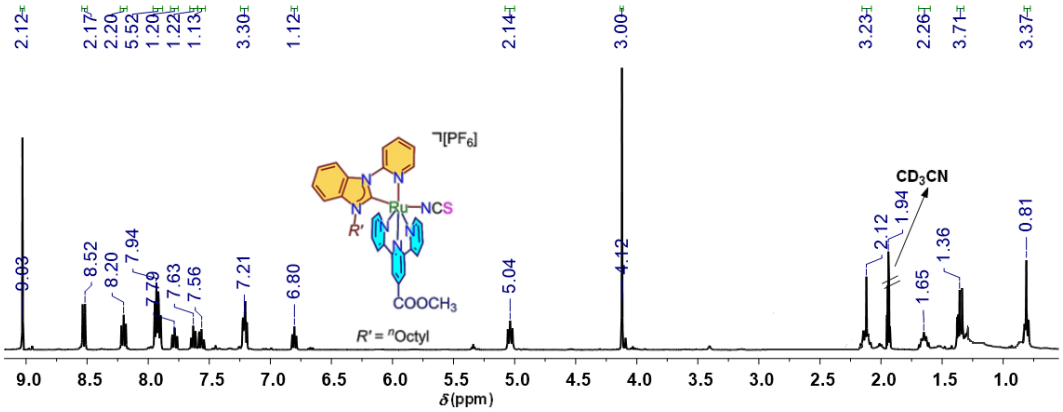


Fig. S15. ^{1}H NMR spectrum of [**6**] in CD_3CN at 400 MHz.

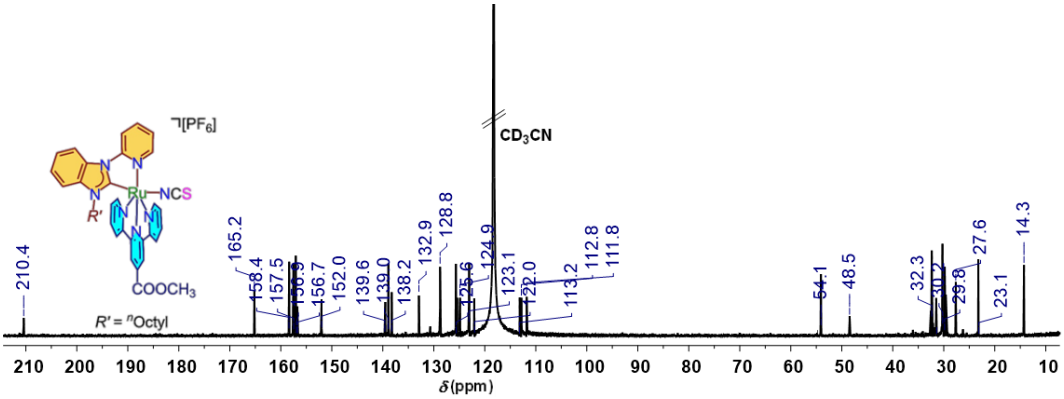


Fig. S16. ^{13}C NMR spectrum of [**6**] in CD_3CN at 100.61 MHz.

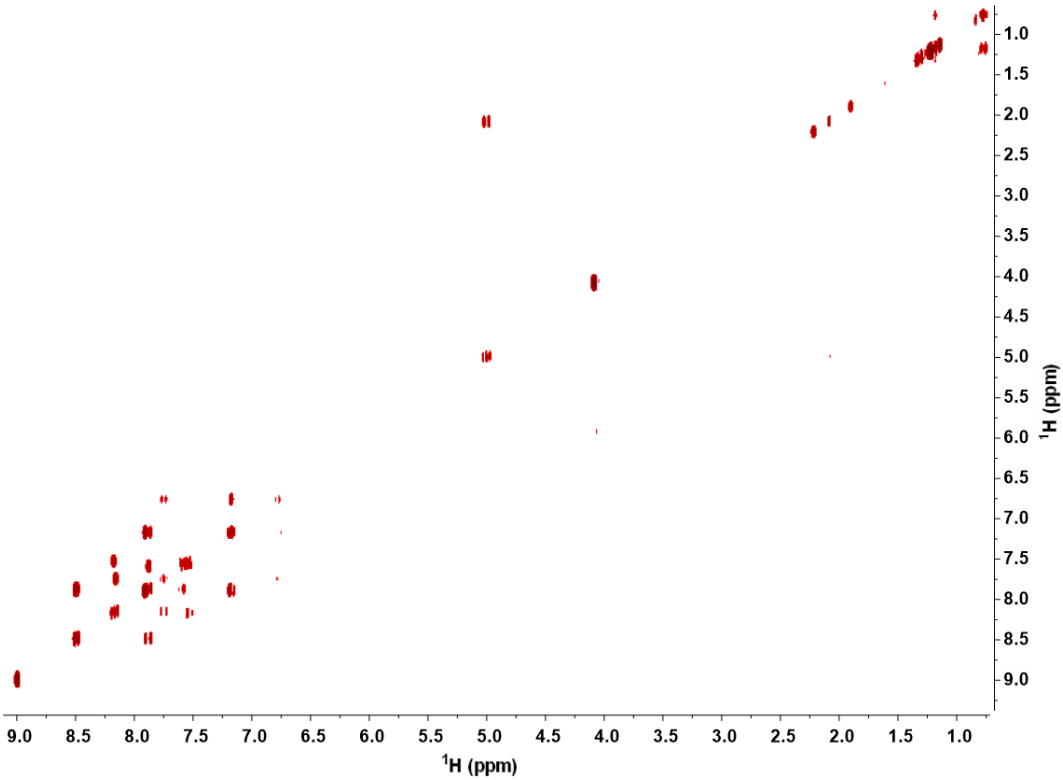


Fig. S17. $^{1}H-^{1}H$ COSY NMR spectrum of [**6**] in CD_3CN.

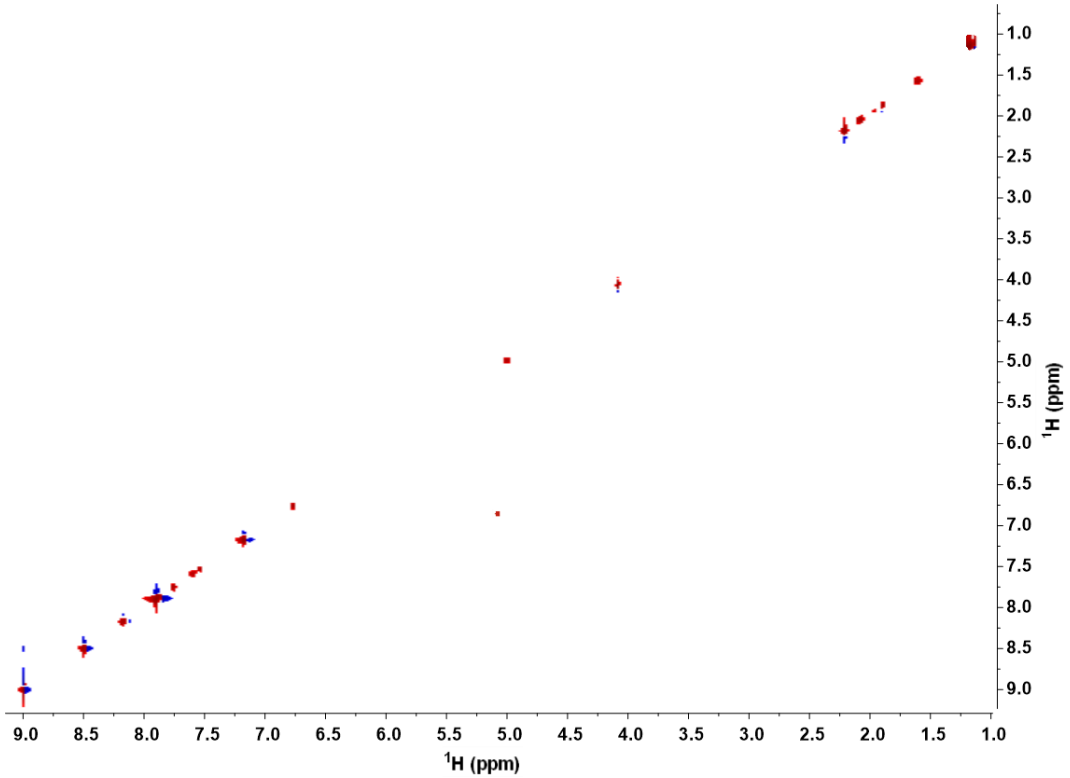


Fig. S18. ^{1}H–^{1}H NOESY NMR spectrum of [**6**] in CD_3CN.

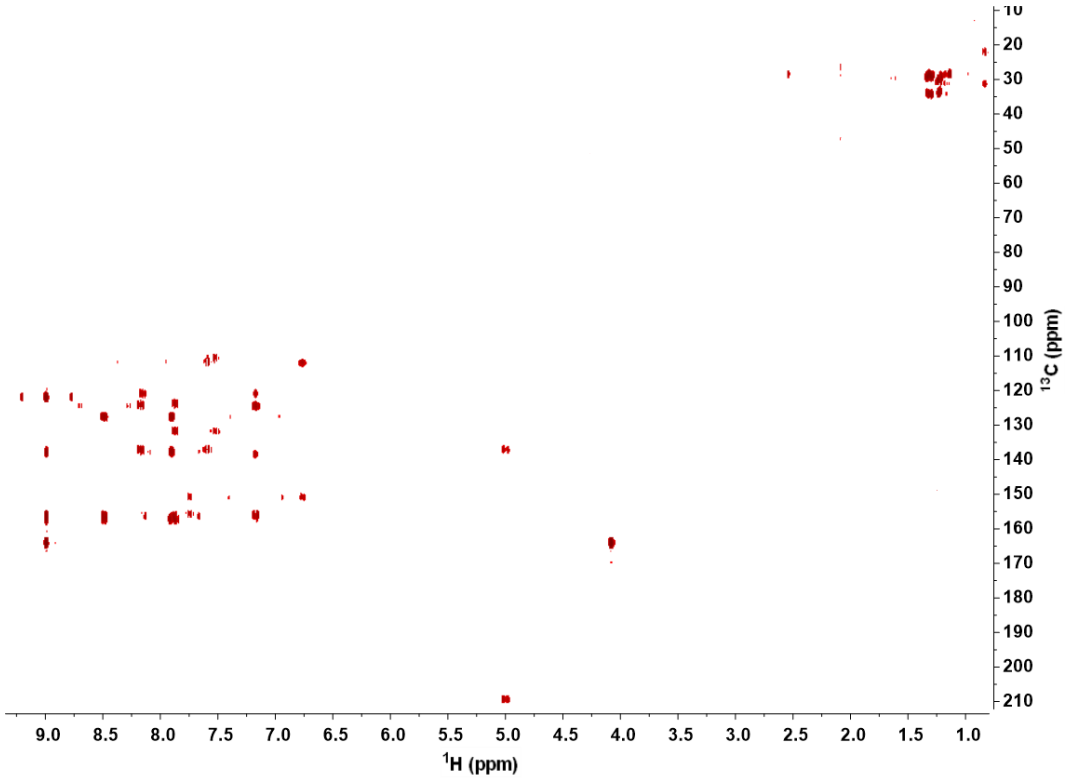


Fig. S19. ^{1}H–^{13}C HMBC NMR spectrum of [**6**] in CD_3CN.

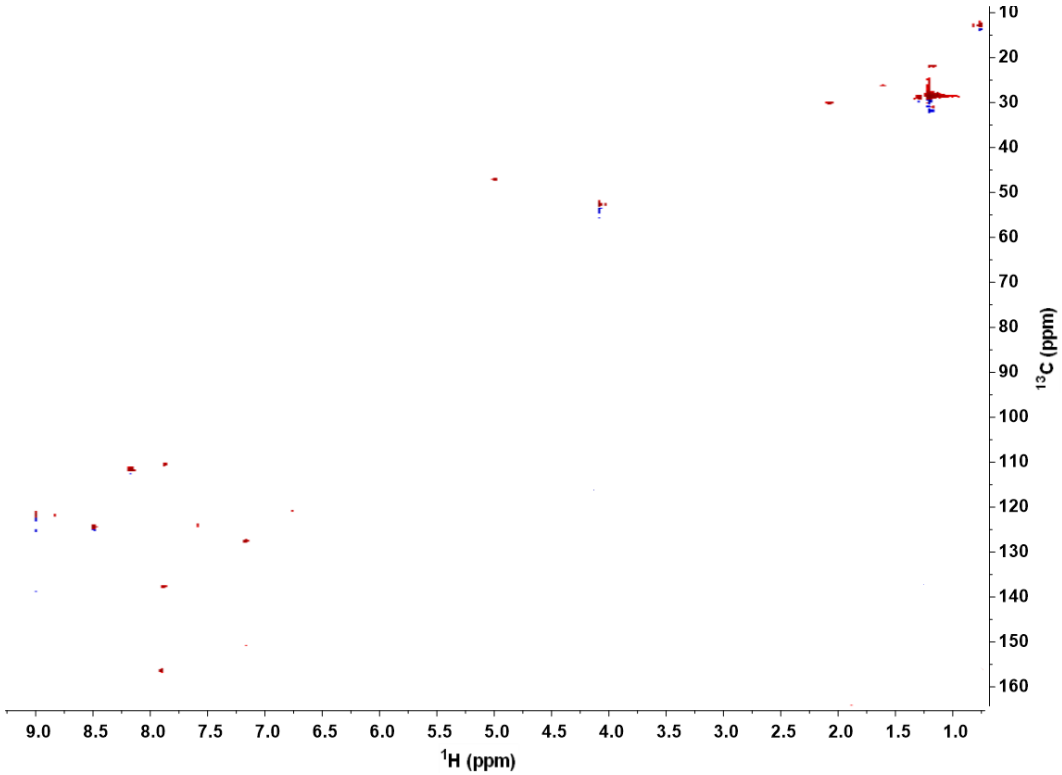


Fig. S20. ^{1}H–^{13}C HSQC NMR spectrum of [**6**] in CD_3CN.

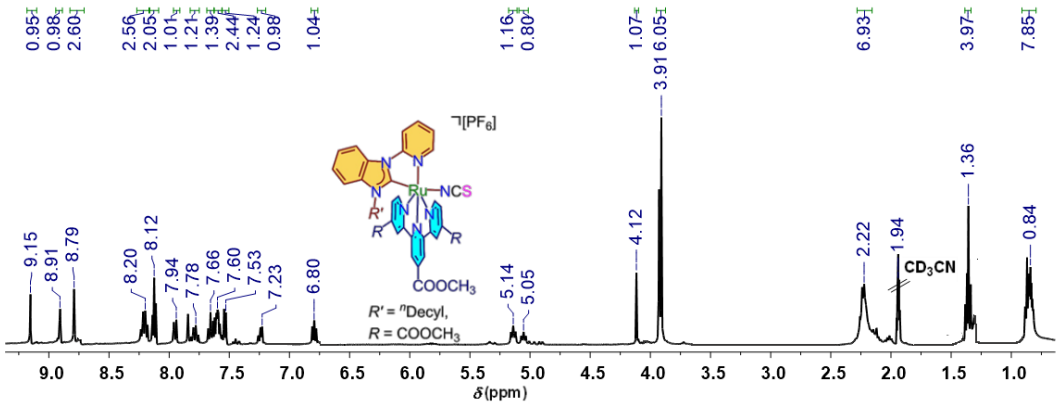


Fig. S21. ^{1}H NMR spectrum of [**7**] in CD_3CN at 400 MHz.

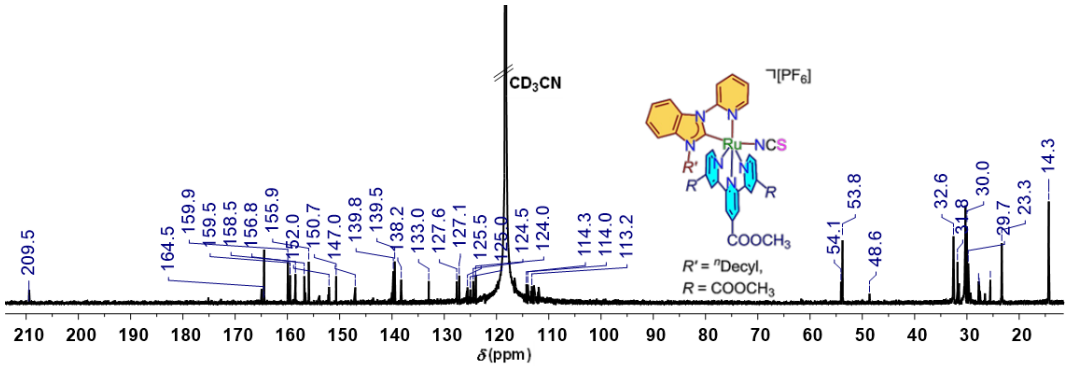


Fig. S22. ^{13}C NMR spectrum of [**7**] in CD_3CN at 100.61 MHz.

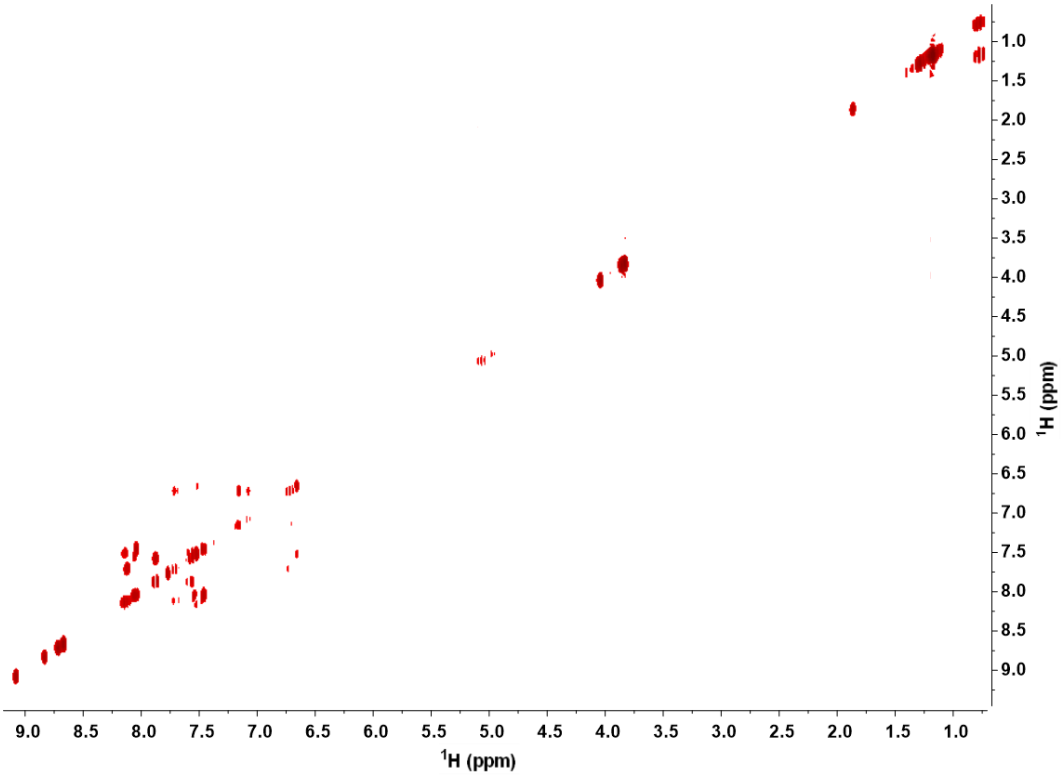


Fig. S23. ^{1}H–^{1}H COSY NMR spectrum of [**7**] in CD_3CN.

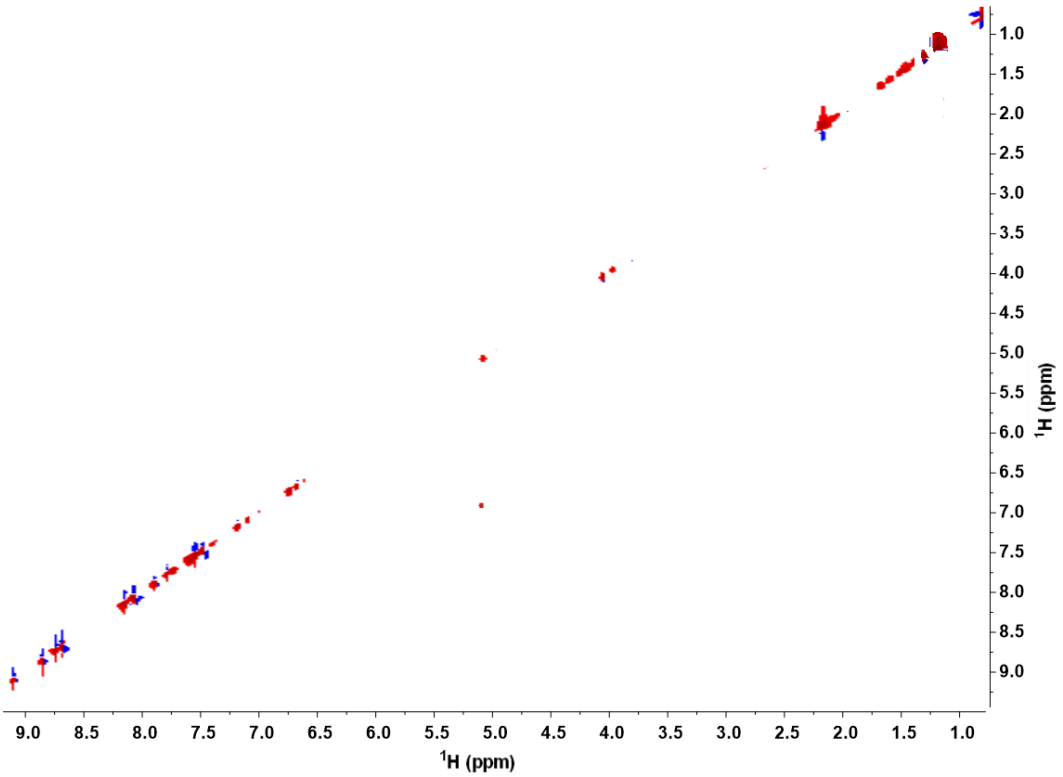


Fig. S24. ^{1}H–^{1}H NOESY NMR spectrum of [**7**] in CD_3CN.

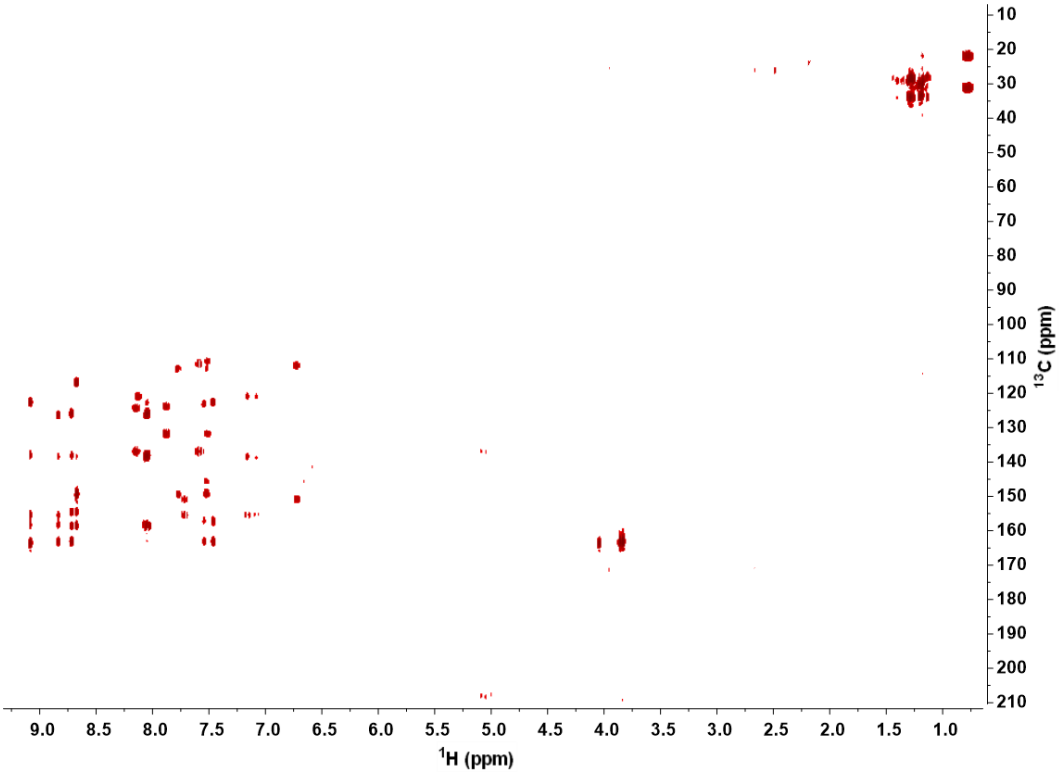


Fig. S25. ^{1}H–^{13}C HMBC NMR spectrum of [**7**] in CD_3CN.

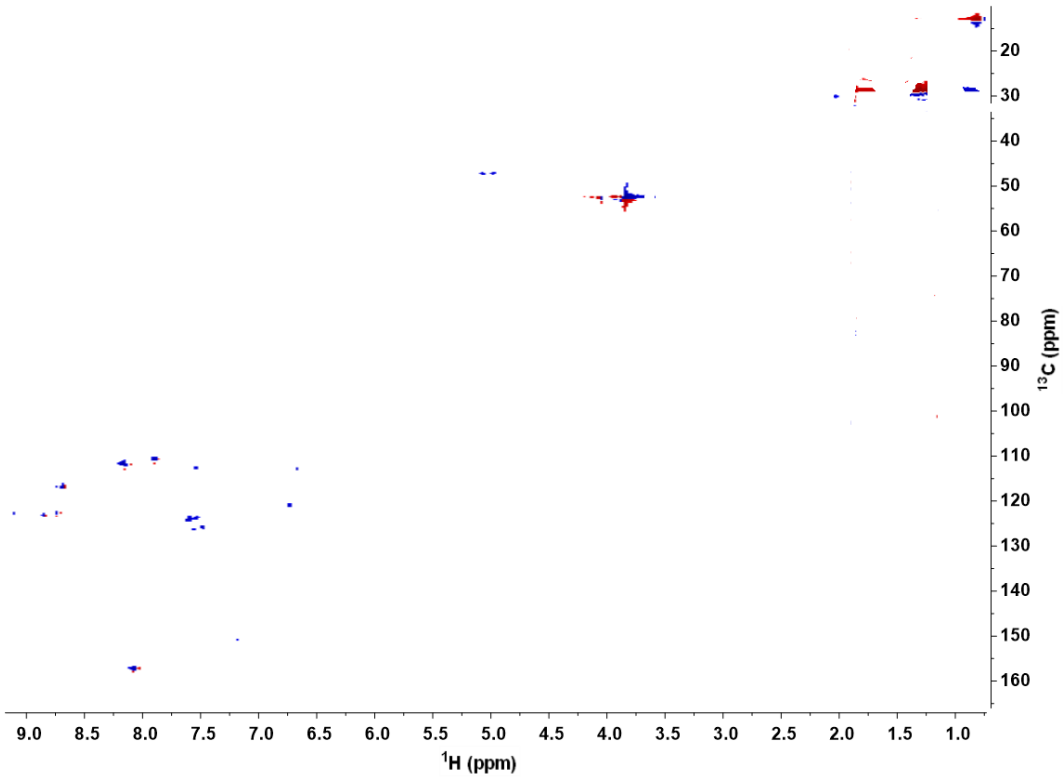


Fig. S26. ^{1}H–^{13}C HSQC NMR spectrum of [**7**] in CD_3CN.

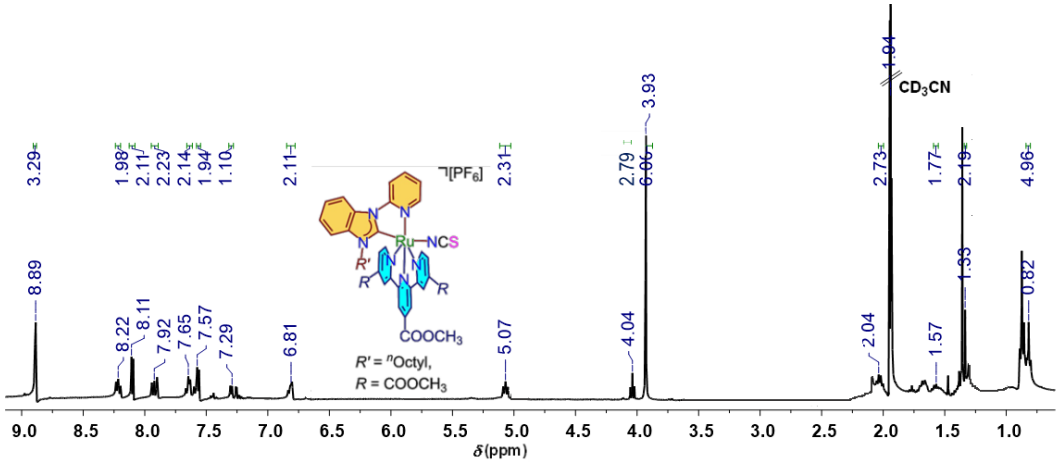


Fig. S27. ^{1}H NMR spectrum of [**8**] in CD_3CN at 400 MHz.

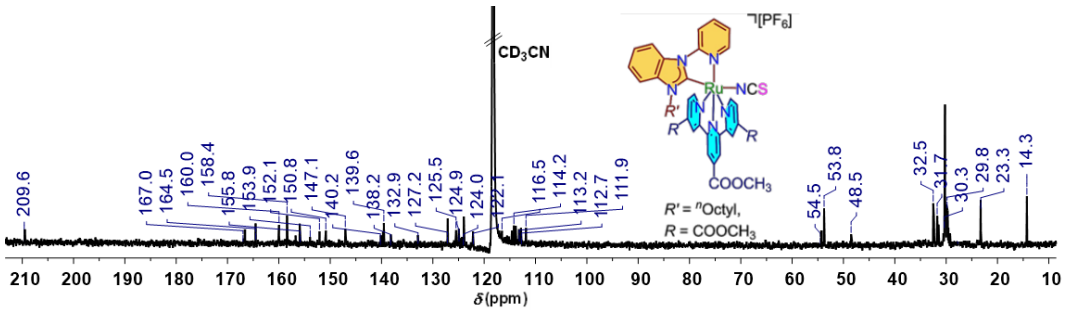


Fig. S28. ^{13}C NMR spectrum of [**8**] in CD_3CN at 100.61 MHz.

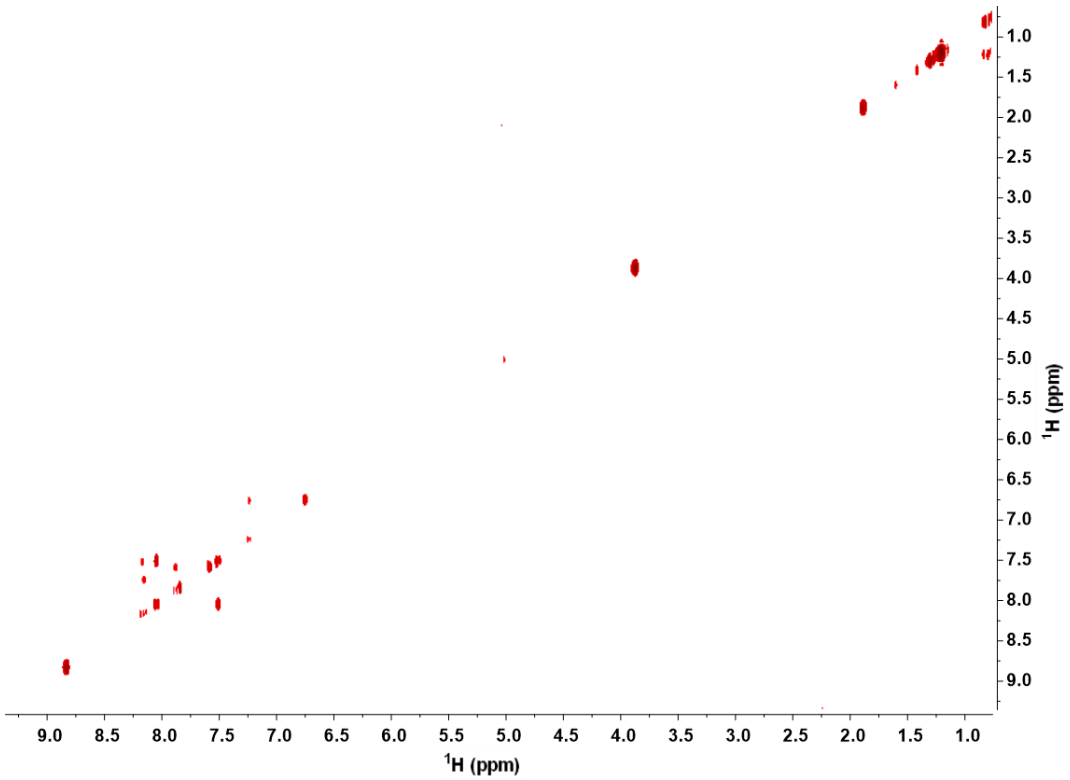


Fig. S29. $^{1}H-^{1}H$ COSY NMR spectrum of [**8**] in CD_3CN.

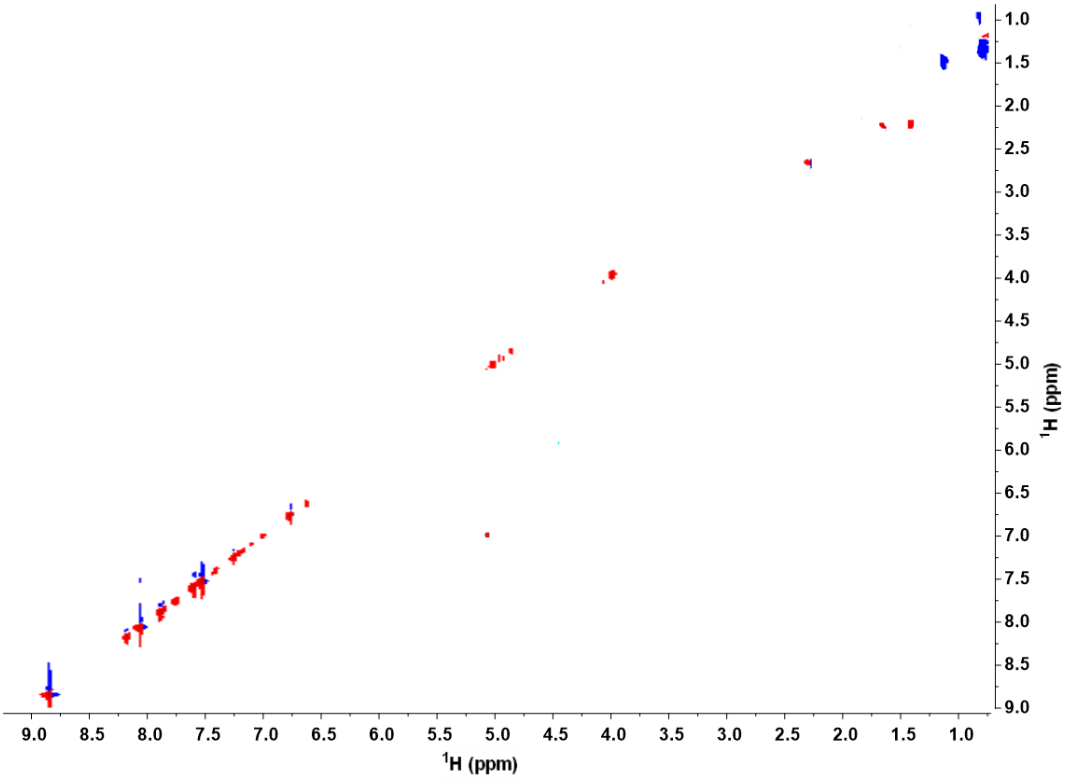


Fig. S30. ^{1}H–^{1}H NOESY NMR spectrum of [**8**] in CD_3CN.

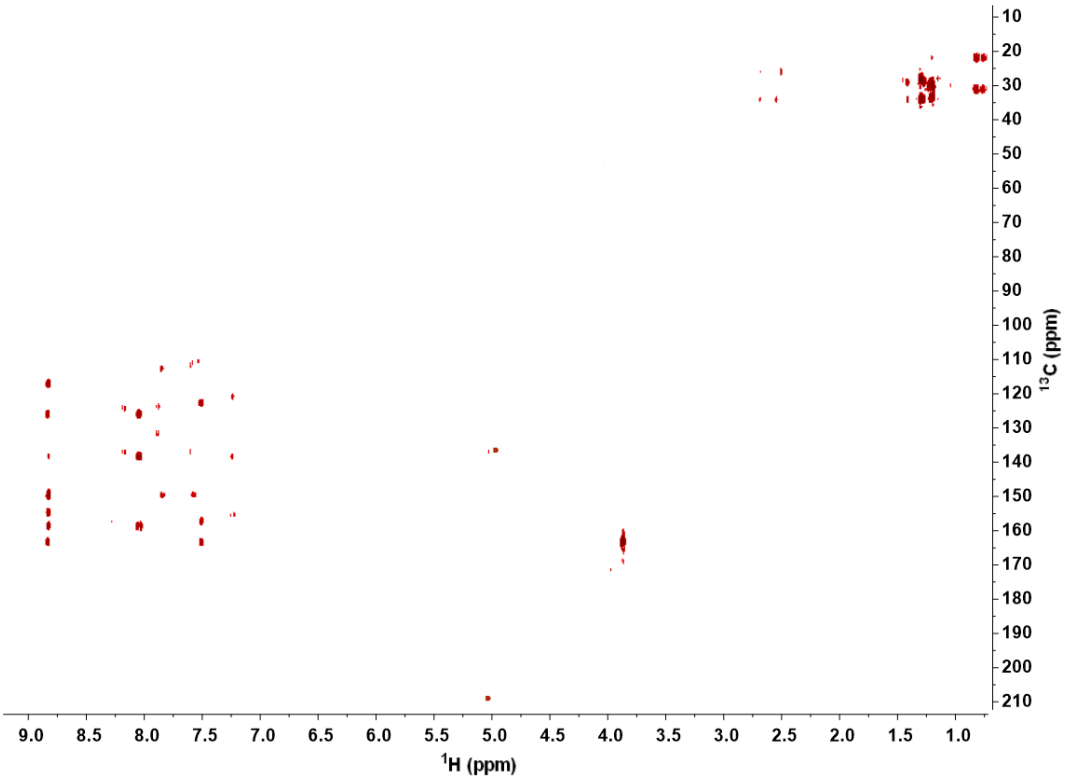


Fig. S31. ^{1}H–^{13}C HMBC NMR spectrum of [**8**] in CD_3CN.

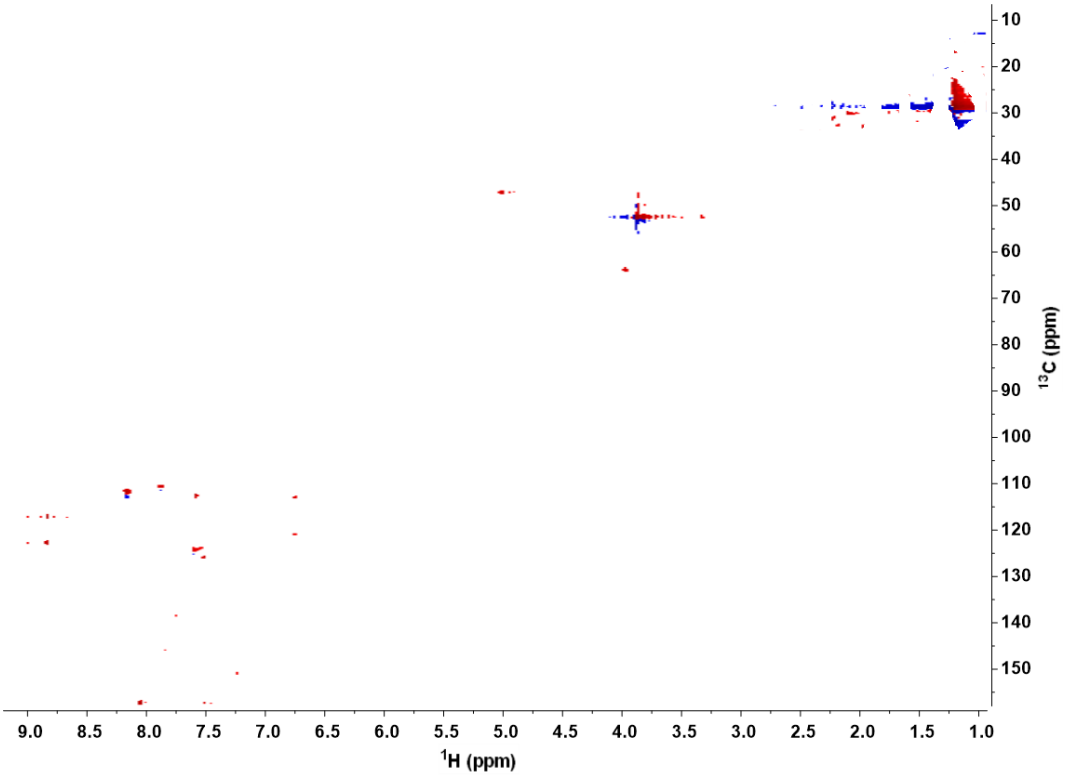


Fig. S32. ^{1}H–^{13}C HSQC NMR spectrum of [**8**] in CD_3CN.

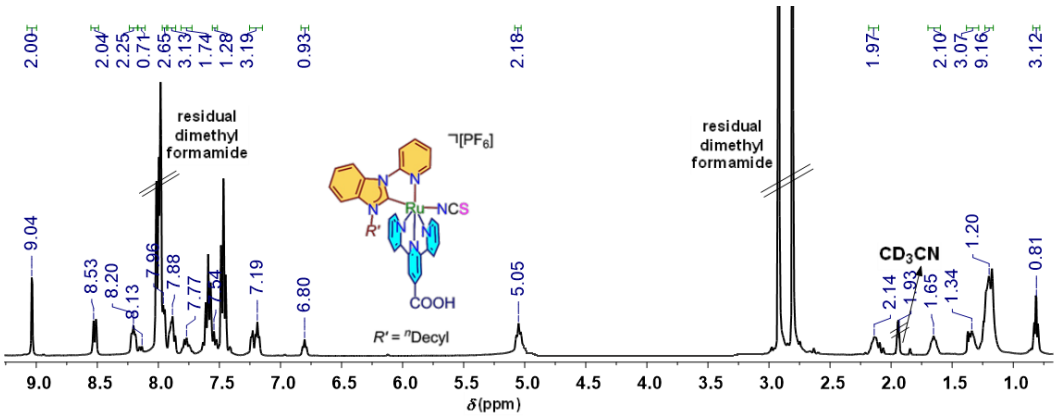


Fig. S33. ^{1}H NMR spectrum of [**S1**] in CD_3CN at 400 MHz.

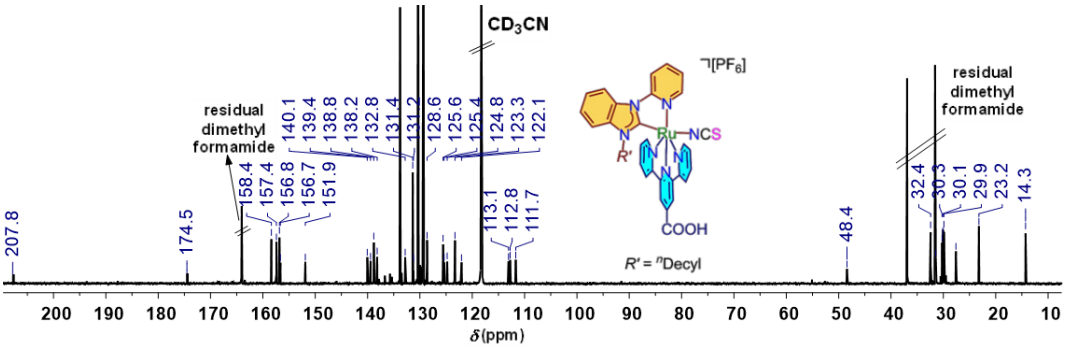


Fig. S34. ^{13}C NMR spectrum of [**S1**] in CD_3CN at 100.61 MHz.

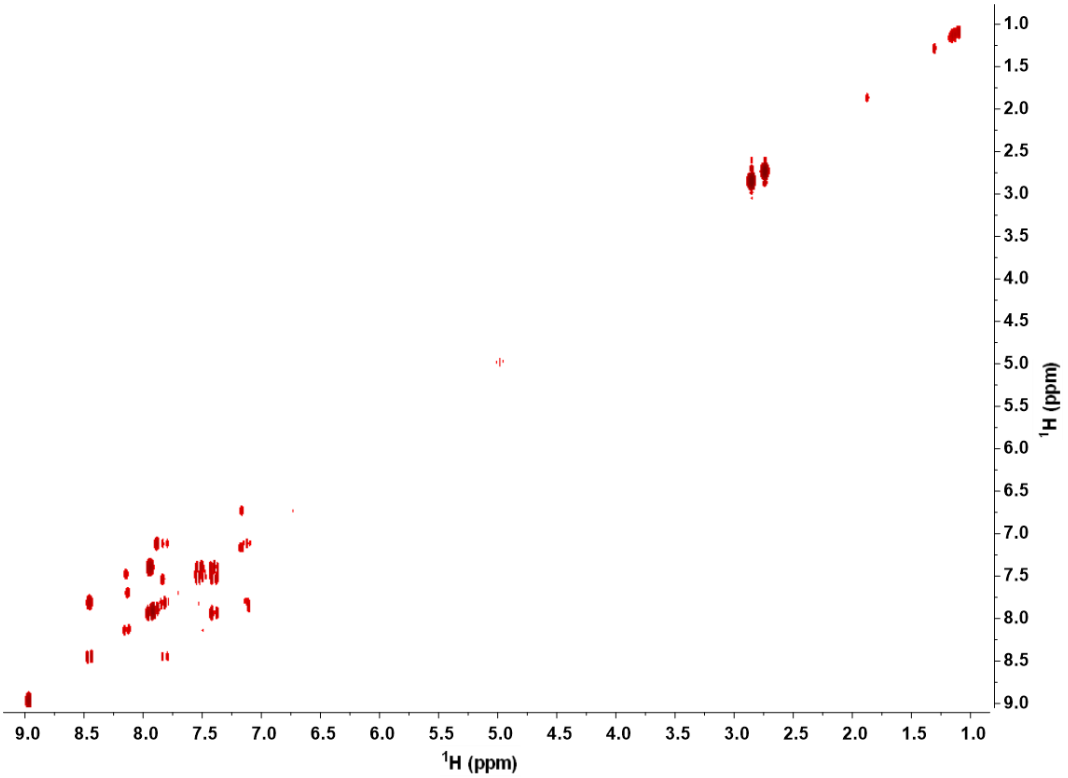


Fig. S35. ^{1}H–^{1}H COSY NMR spectrum of [**S1**] in CD_3CN.

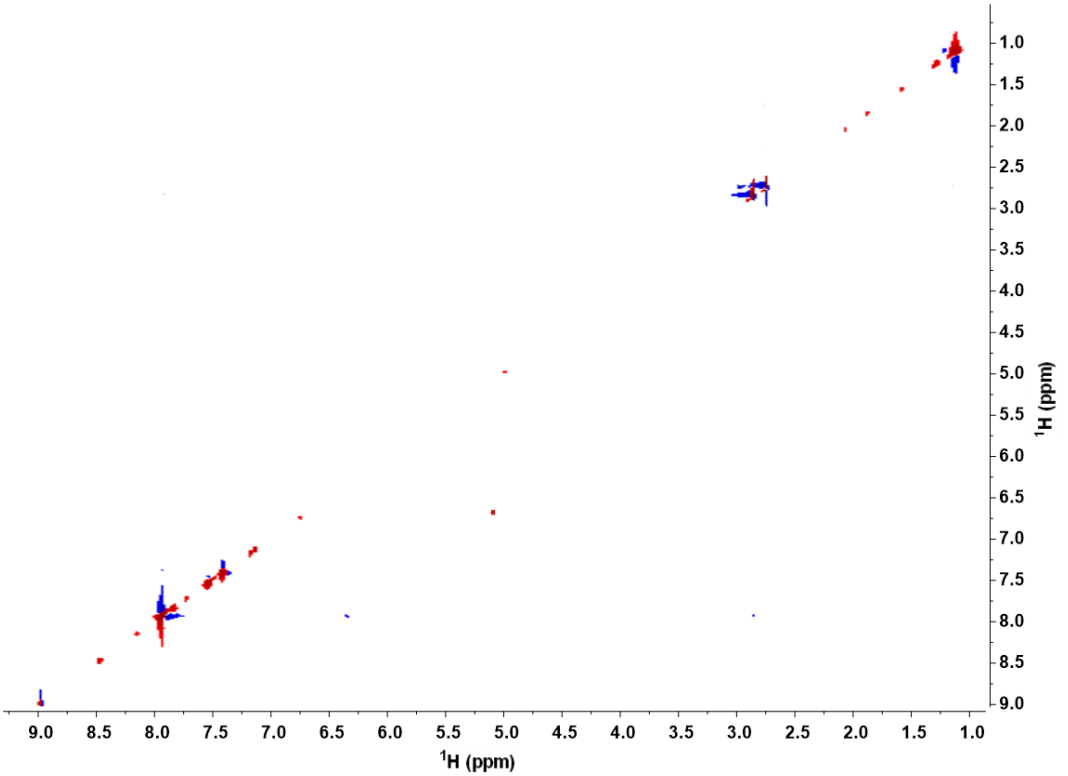


Fig. S36. ^{1}H–^{1}H NOESY NMR spectrum of [**S1**] in CD_3CN.

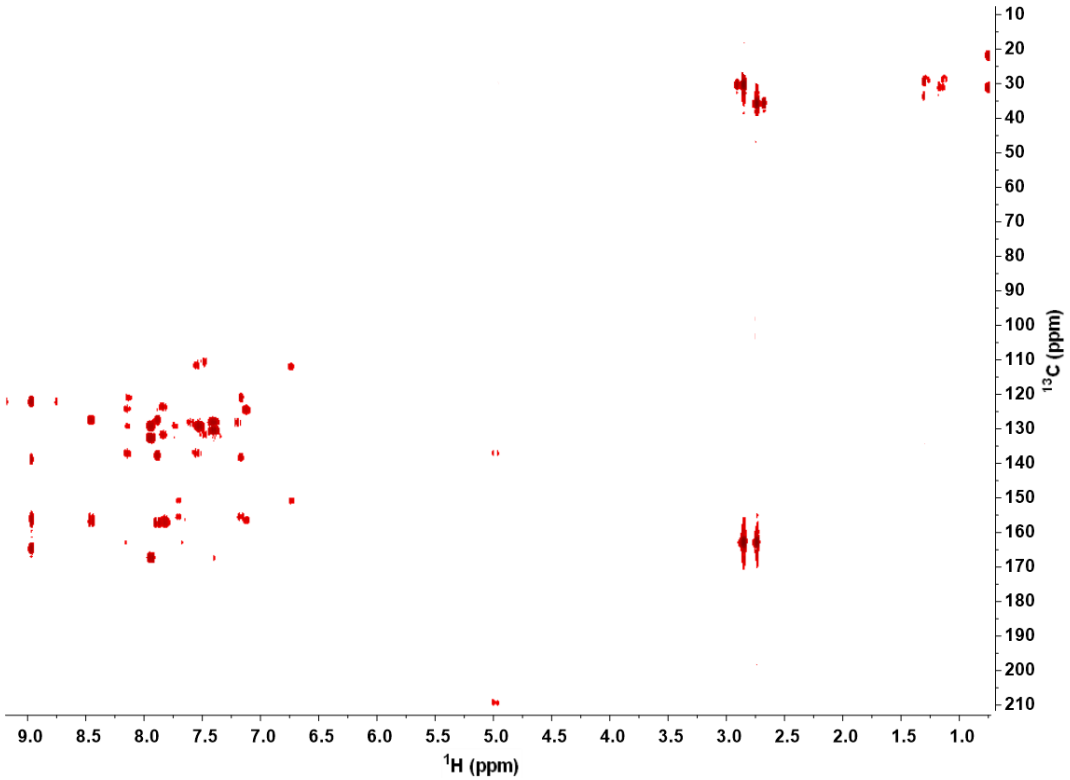


Fig. S37. ^{1}H–^{13}C HMBC NMR spectrum of [**S1**] in CD_3CN.

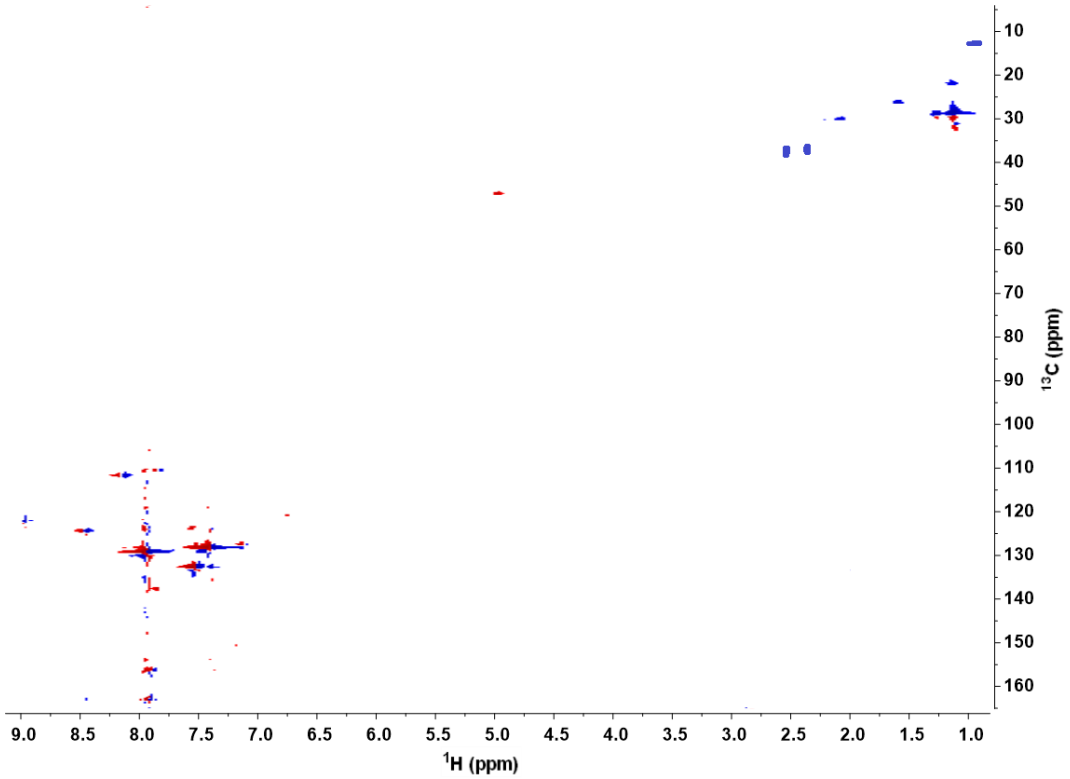


Fig. S38. ^{1}H–^{13}C HSQC NMR spectrum of [**S1**] in CD_3CN at 100.61 MHz.

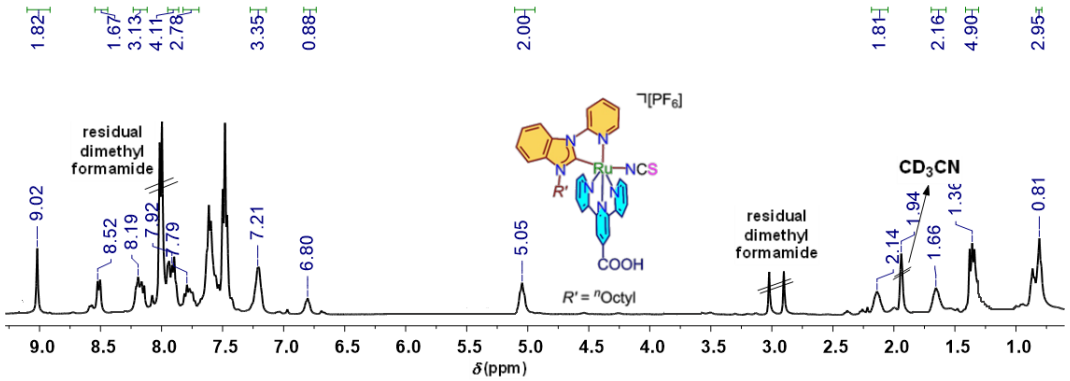


Fig. S39. ^{1}H NMR spectrum of [**S2**] in CD_3CN at 400 MHz.

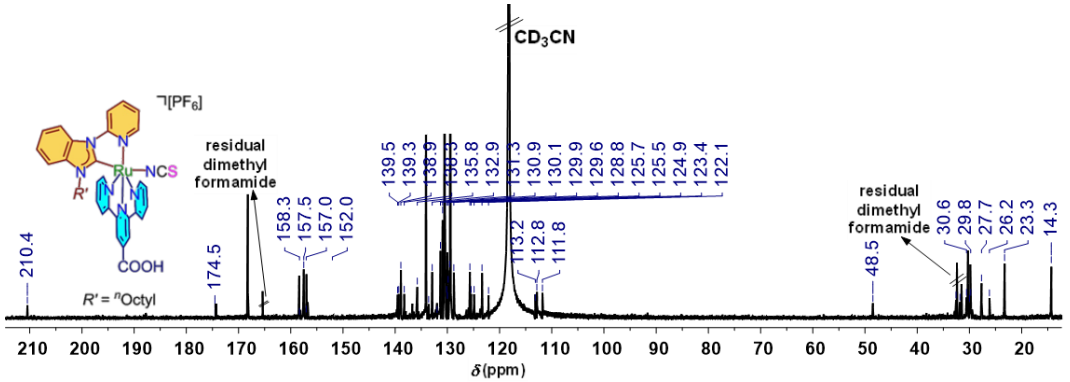


Fig. S40. ^{13}C NMR spectrum of [**S2**] in CD_3CN at 100.61 MHz.

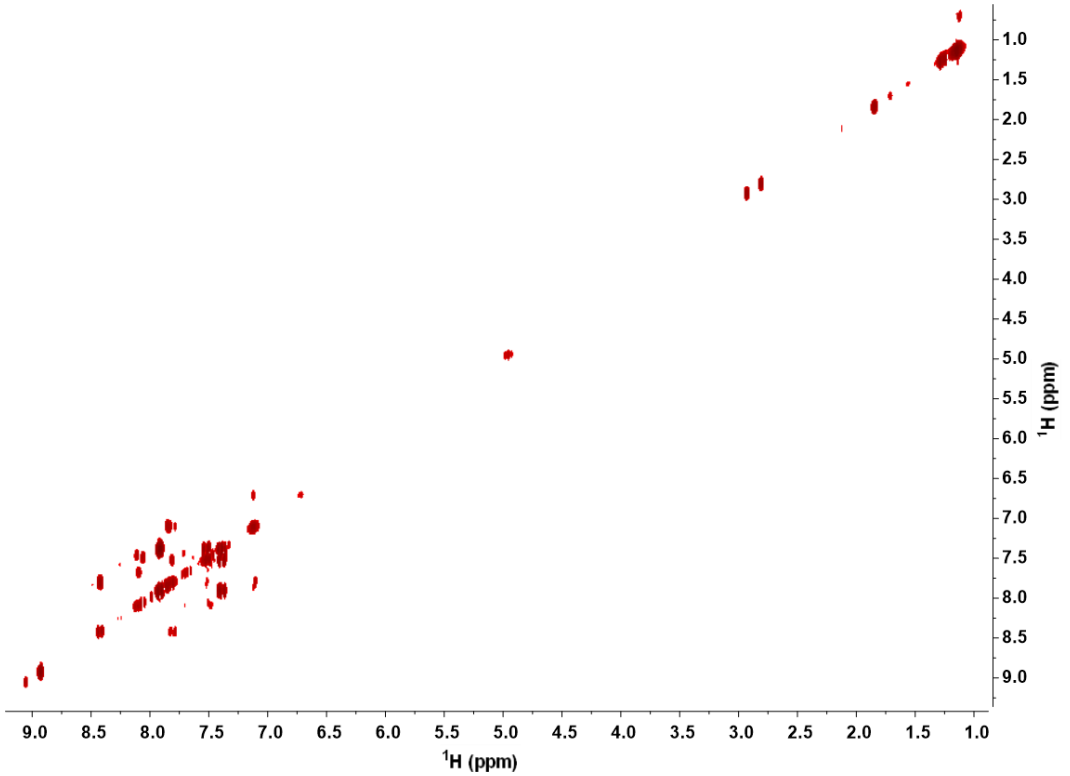


Fig. S41. $^{1}H-^{1}H$ COSY NMR spectrum of [**S2**] in CD_3CN.

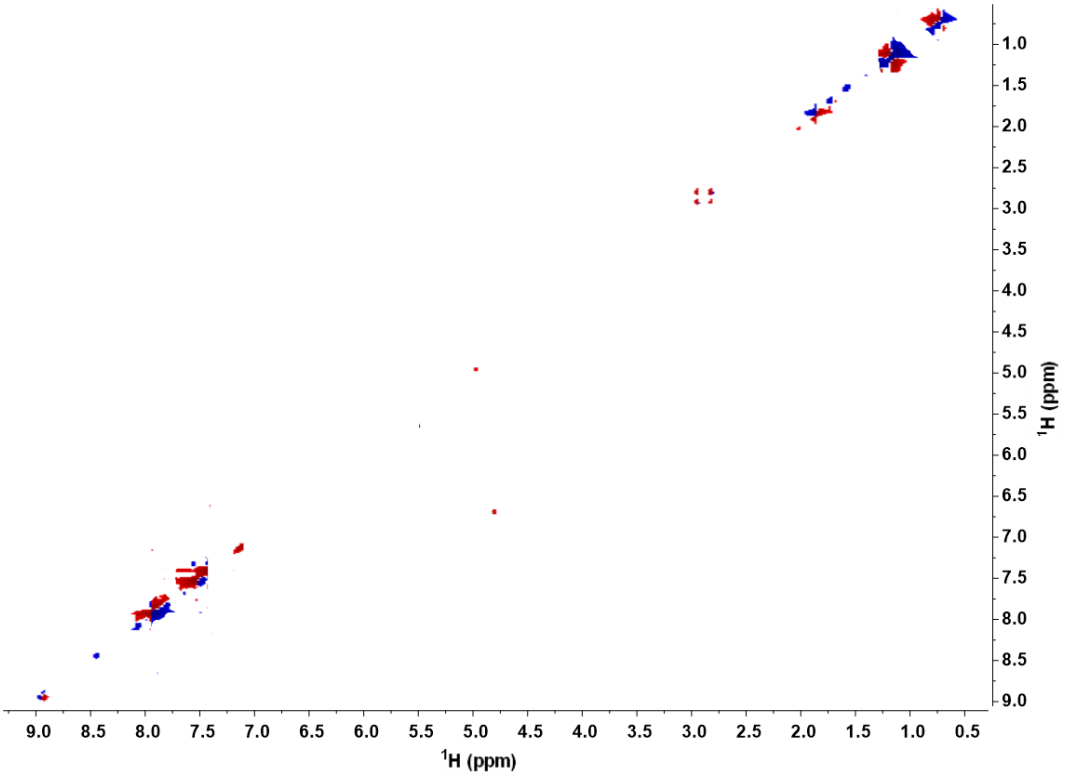


Fig. S42. ^{1}H–^{1}H NOESY NMR spectrum of [**S2**] in CD_3CN.

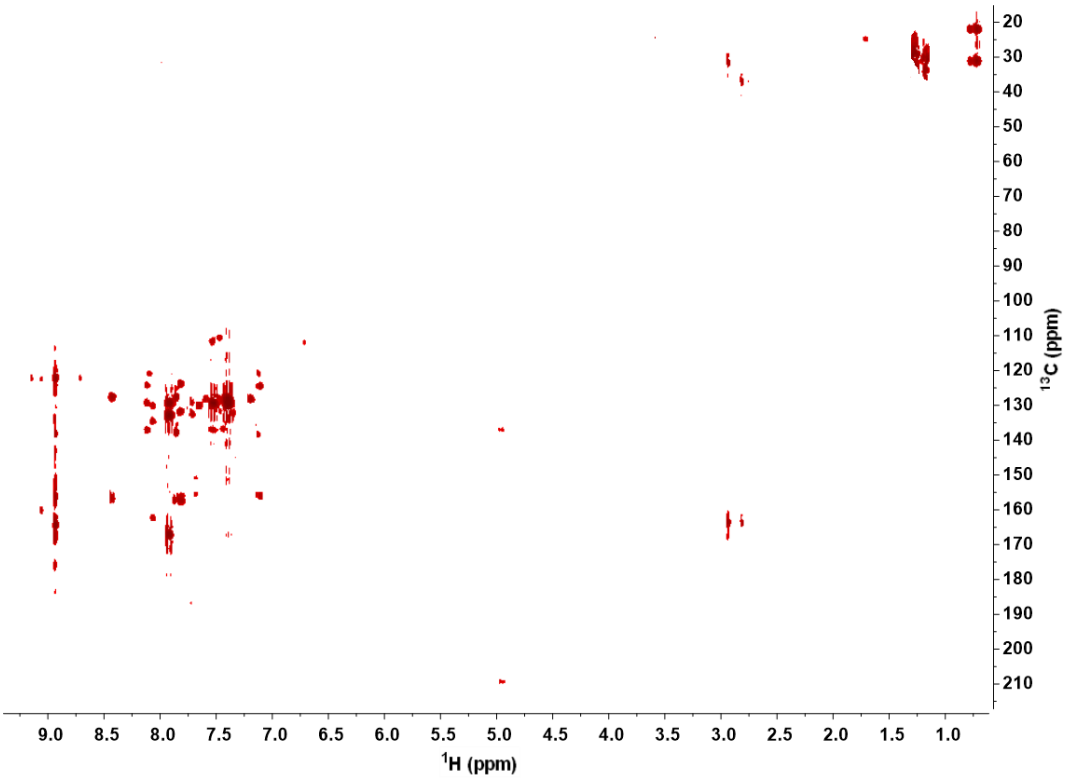


Fig. S43. ^{1}H–^{13}C HMBC NMR spectrum of [**S2**] in CD_3CN.

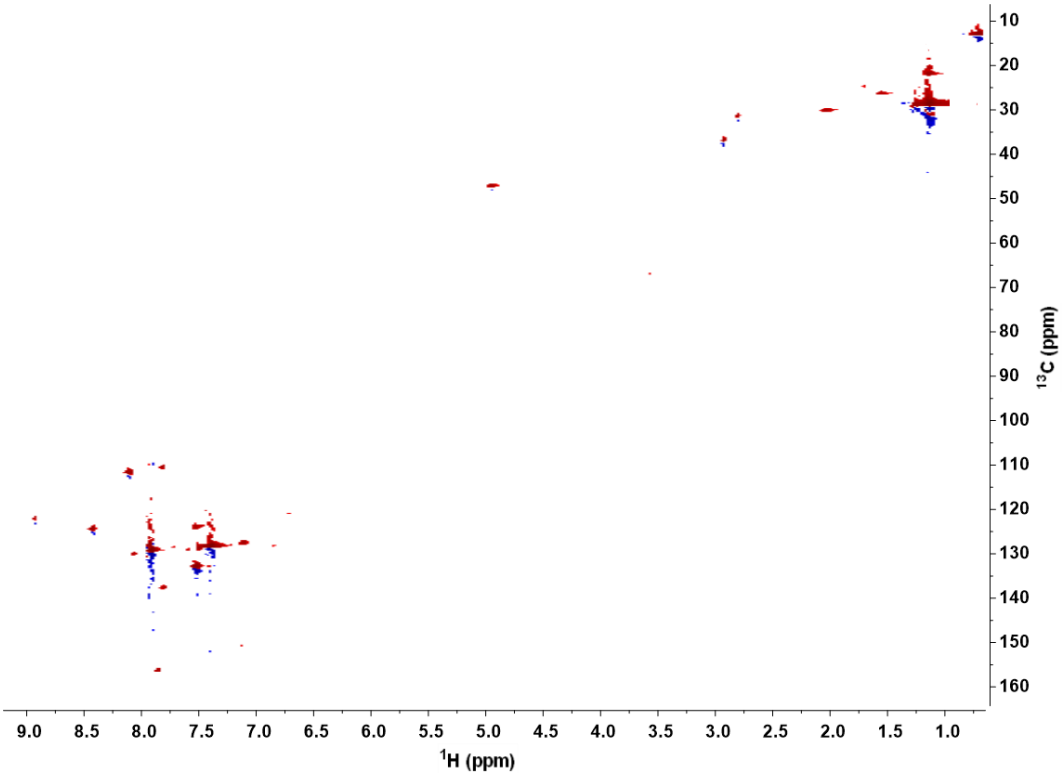


Fig. S44. ^{1}H–^{13}C HSQC NMR spectrum of [**S2**] in CD_3CN.

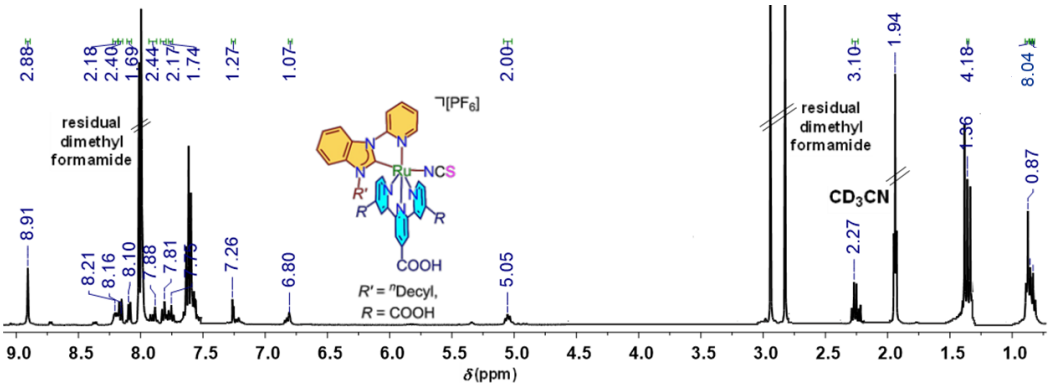


Fig. S45. ^{1}H NMR spectrum of [**S3**] in CD_3CN at 400 MHz.

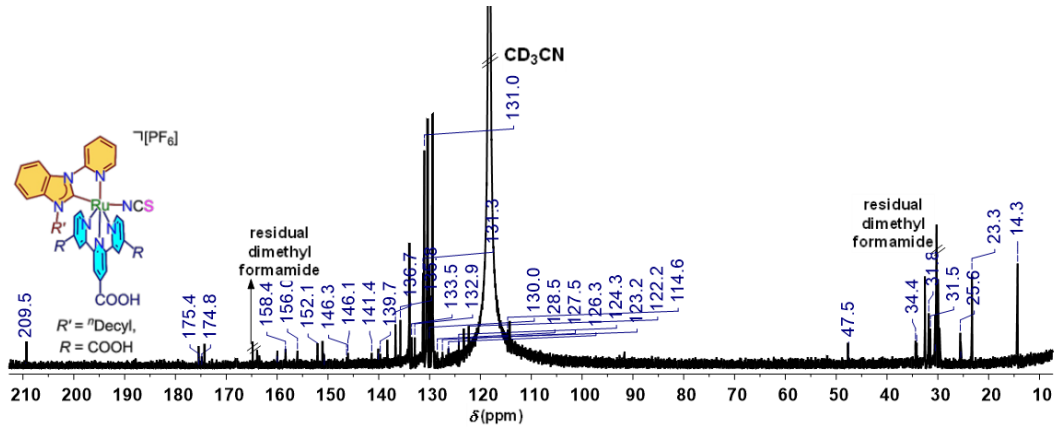


Fig. S46. ^{13}C NMR spectrum of [**S3**] in CD_3CN at 100.61 MHz.

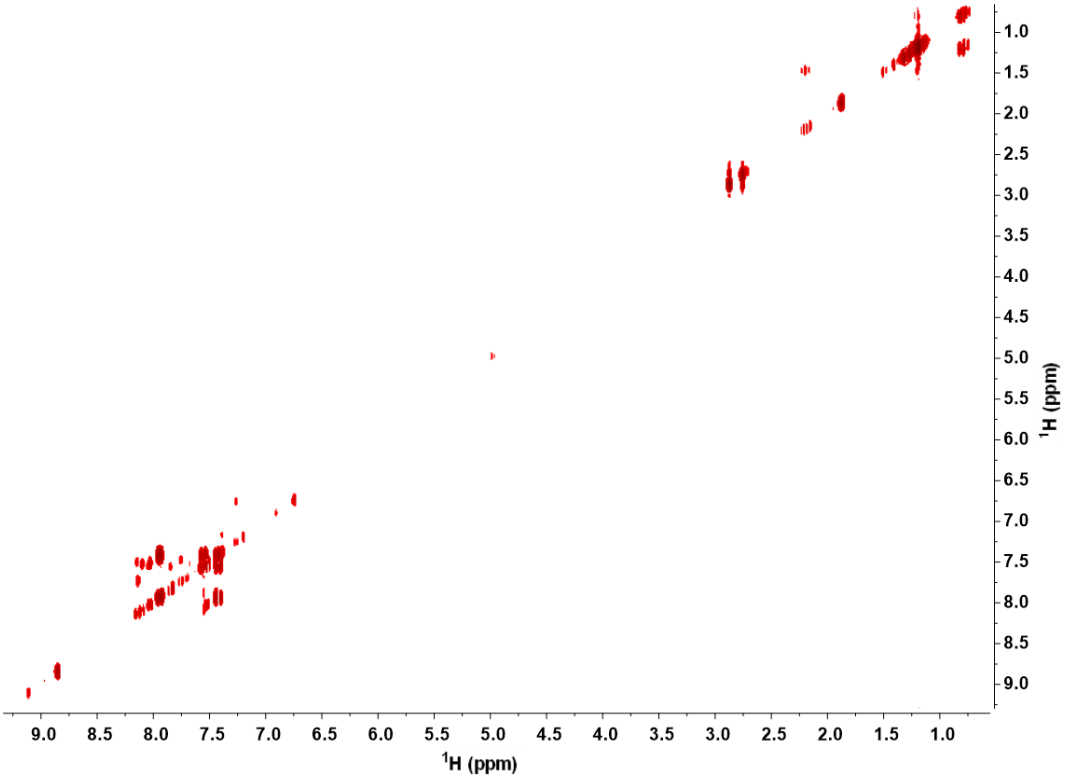


Fig. S47. ^{1}H–^{1}H COSY NMR spectrum of [**S3**] in CD_3CN.

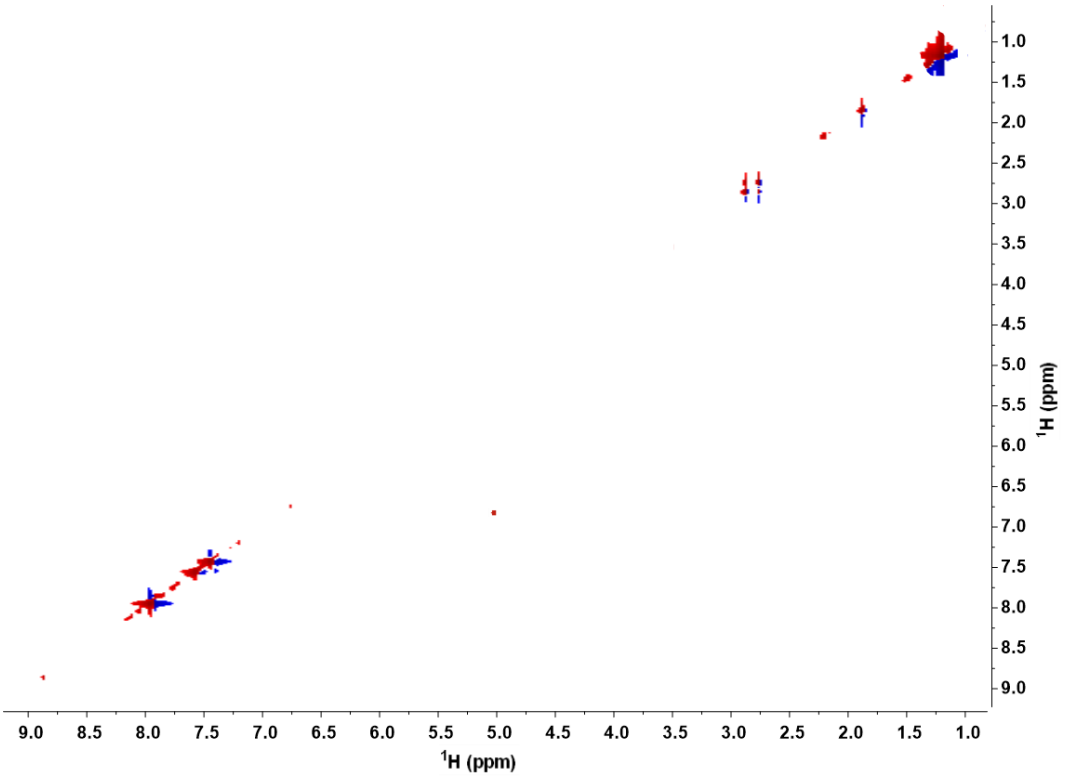


Fig. S48. ^{1}H–^{1}H NOESY NMR spectrum of [**S3**] in CD_3CN.

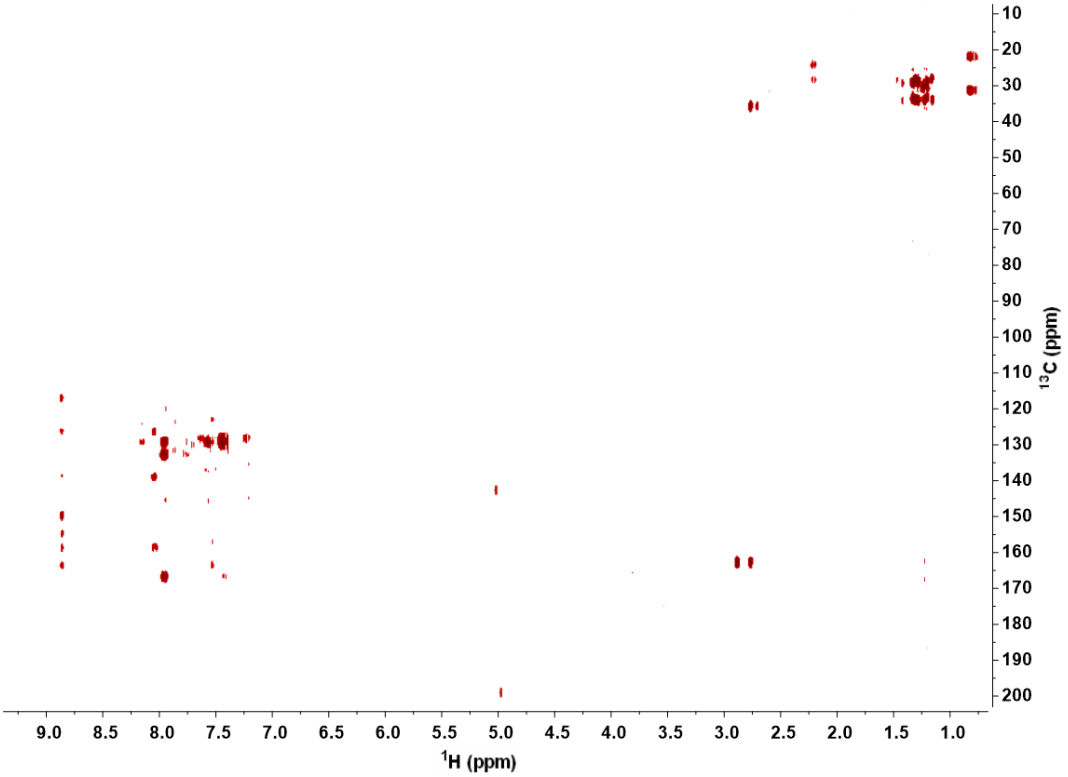


Fig. S49. ^{1}H–^{13}C HMBC NMR spectrum of [**S3**] in CD_3CN.

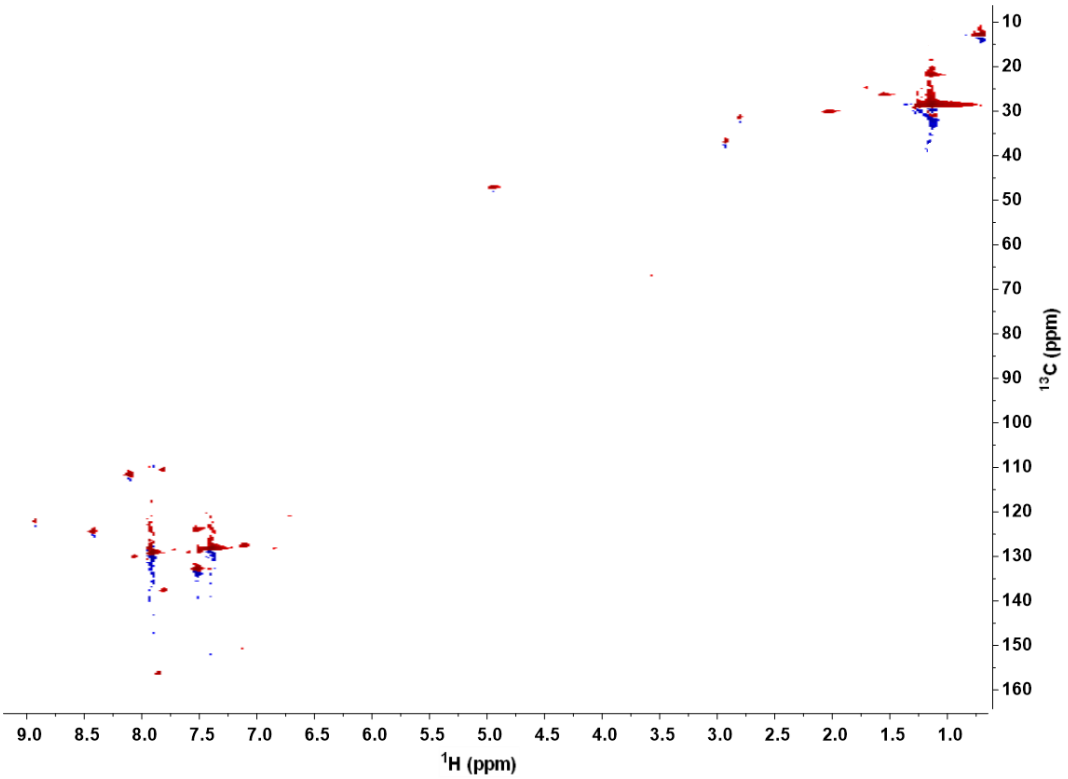


Fig. S50. ^{1}H–^{13}C HSQC NMR spectrum of [**S3**] in CD_3CN.

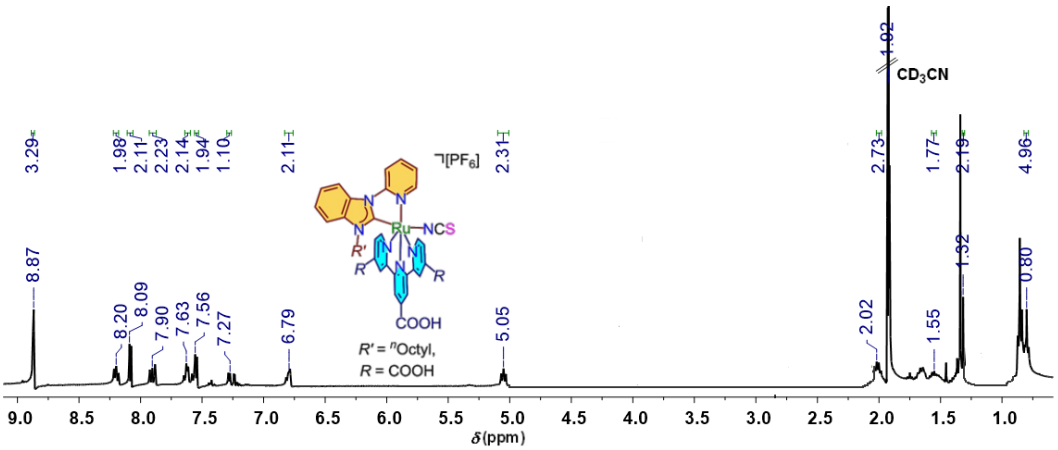


Fig. S51. ^{1}H NMR spectrum of [**S4**] in CD_3CN at 400 MHz.

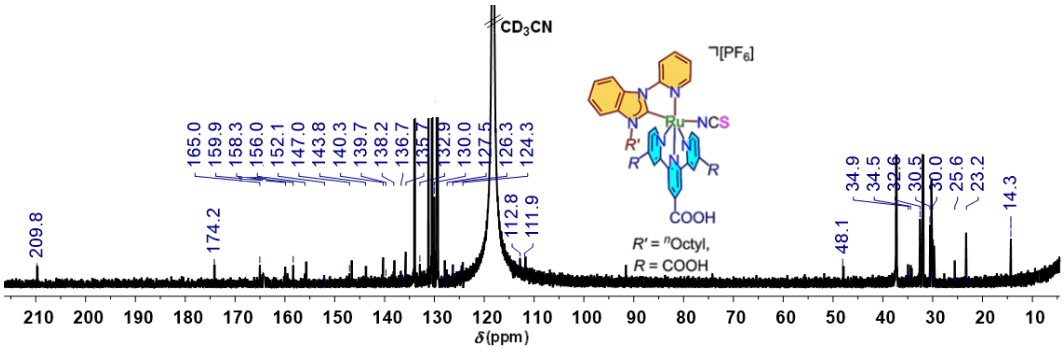


Fig. S52. ^{13}C NMR spectrum of [**S4**] in CD_3CN at 100.61 MHz.

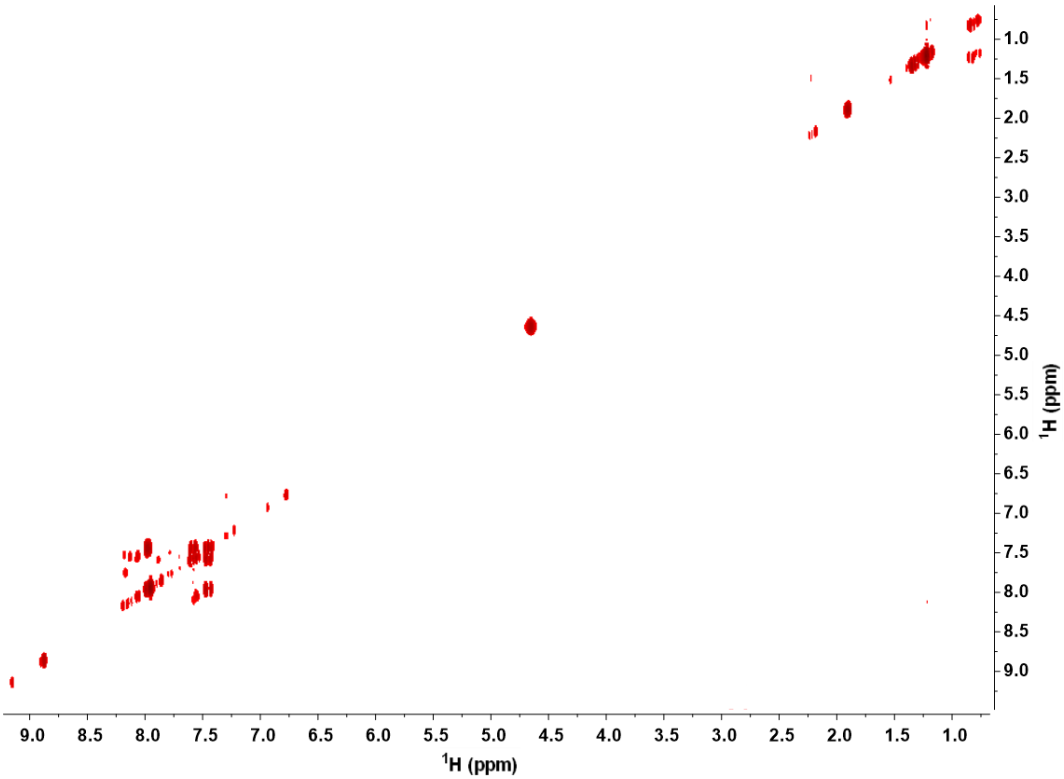


Fig. S53. ^{1}H–^{1}H COSY NMR spectrum of [**S4**] in CD_3CN.

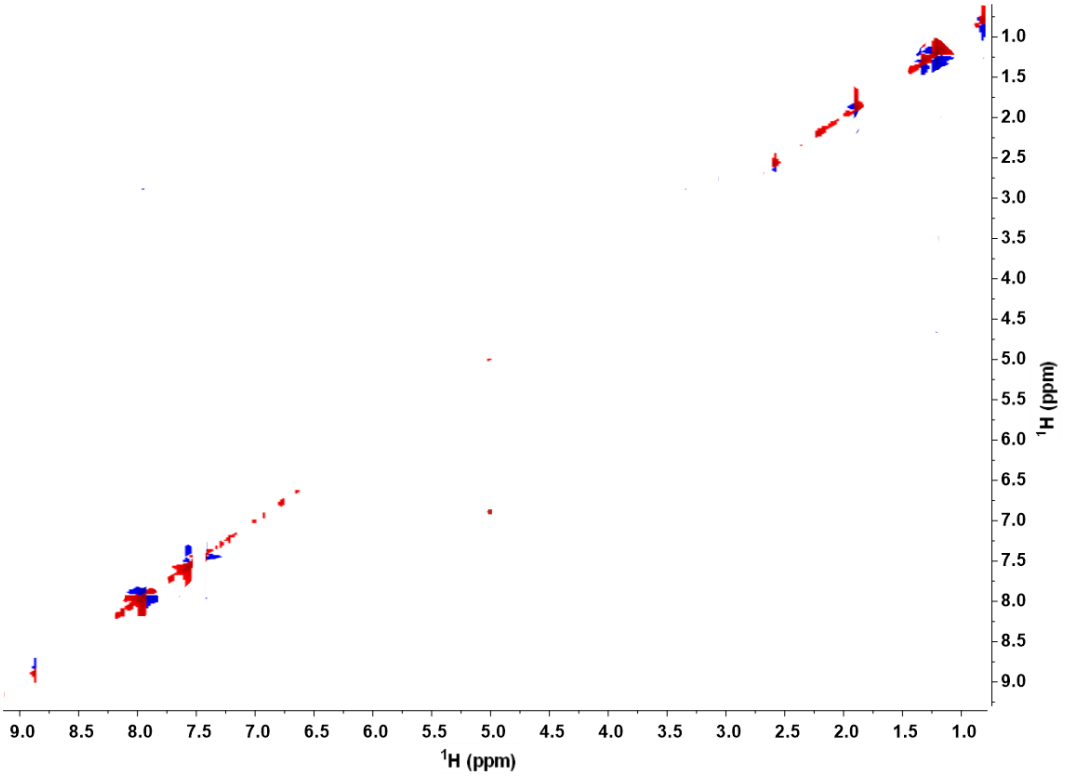


Fig. S54. ^{1}H–^{1}H NOESY NMR spectrum of [**S4**] in CD_3CN.

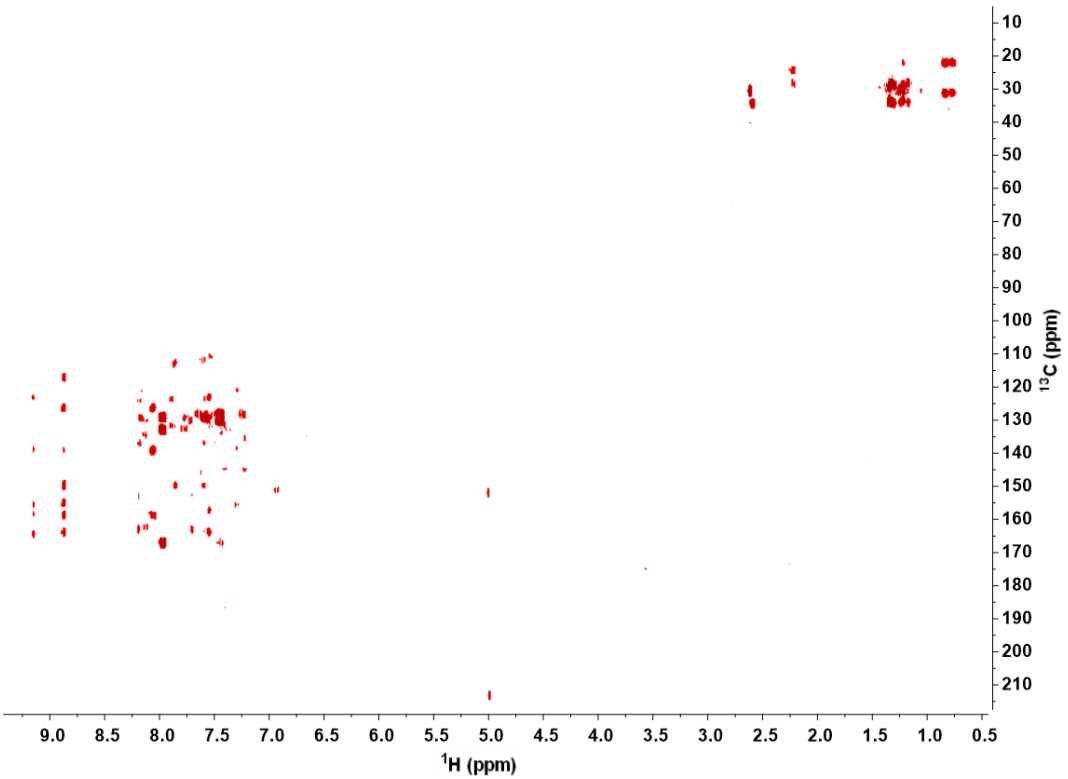


Fig. S55. ^{1}H–^{13}C HMBC NMR spectrum of [**S4**] in CD_3CN.

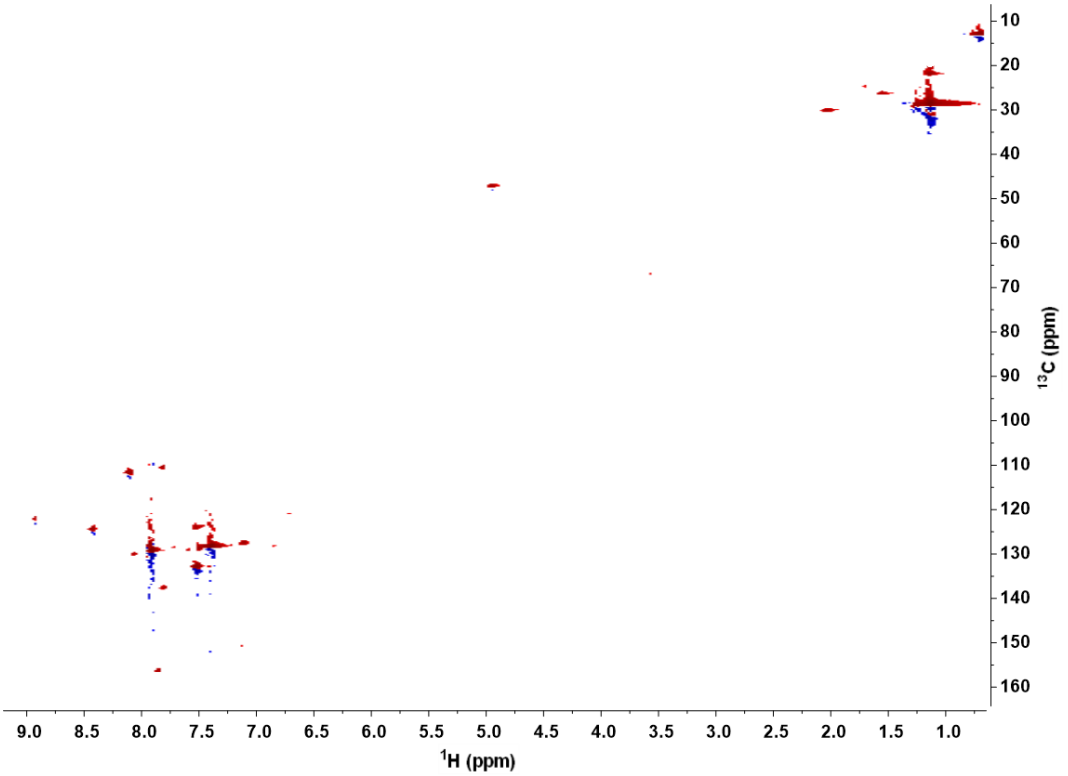
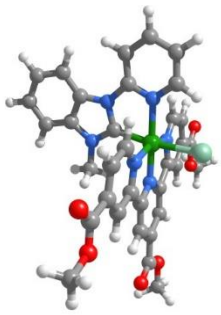
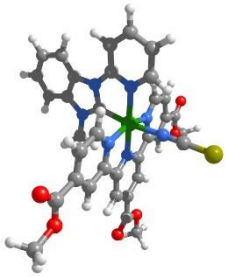
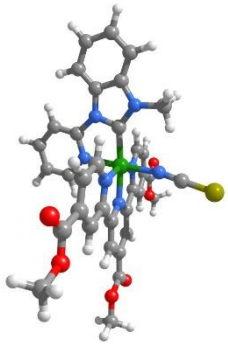


Fig. S56. ^{1}H–^{13}C HSQC NMR spectrum of [**S4**] in CD_3CN.

Table S1

Gibbs free energy calculation for Scheme 1.

[**3**]/[**4**]	[**7**]/[**8**]	Isomer-[**7**]/[**8**]
		

*Optimized geometries

The geometries of reactants [**3**]/[**4**] with KSCN and by-product KCl were optimized in the dimethyl formamide/water mixture[4a] together with their frequency calculations at 373.15 K. These calculations suggest that the formation of product [**7**]/[**8**] + KCl is energetically more favorable than the formation of Isomer-[**7**]/[**8**] by *ca.* 12.0 kJ mol^{-1}.

Gibbs free energy of reactant (E_h)	
KSCN	–1090.64095821
[**3**]/[**4**] + KSCN	–3735.02631586
Gibbs free energy of product (E_h)	
KCl	–1059.91987272
Isomer-[**7**]/[**8**] + KCl	–3735.03717928
[**7**]/[**8**] + KCl	–3735.04117602
Gibbs free energy for reaction (kJ/mol)	
[**3**]/[**4**] + KSCN → Isomer-[**7**]/[**8**] + KCl	–28.5219113827
[**3**]/[**4**] + KSCN → [**7**]/[**8**] + KCl	–39.015353052

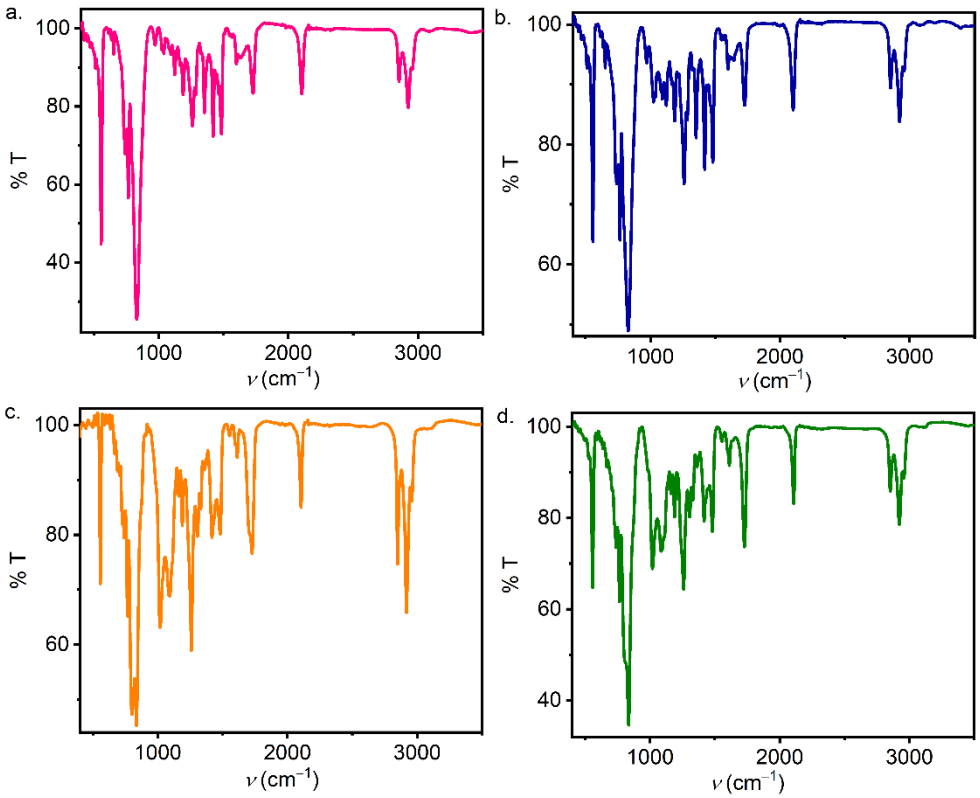


Fig. S57. Fourier Transform Infrared (FTIR) spectra of [**5**] – [**8**]. (a. [**5**], b. [**6**], c. [**7**], and [**8**]).

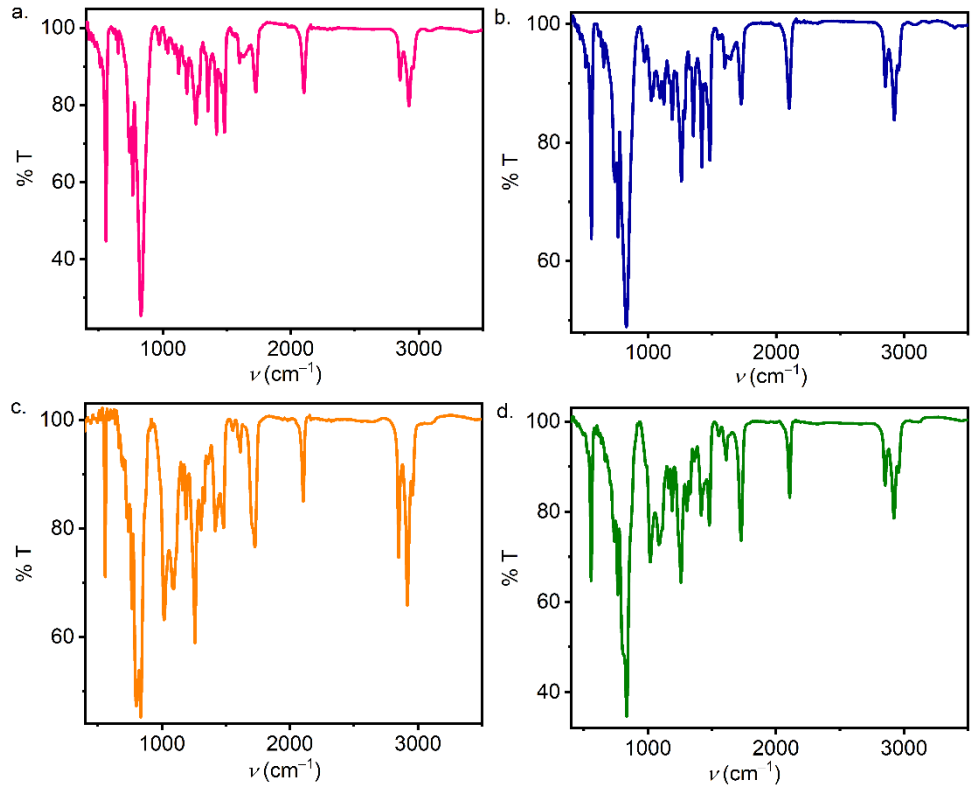


Fig. S58. Fourier Transform Infrared (FTIR) spectra of [**S1**] – [**S4**]. (a. [**S1**], b. [**S2**], c. [**S3**], and [**S4**]).

Table S2 Selected Attenuated Total Reflectance (ATR)-FTIR data (cm^{-1}) of [**5**] – [**8**], and [**S1**] – [**S4**].

	[5]	[6]	[7]	[8]	[S1]	[S2]	[S3]	[S4]
–CH stretch of CH_3 group	2927.2	2921.0	2915.9	2927.2	2927.7	2922.1	2922.1	2939.5
–CH stretch of CH_2 group	2856.4, 2950.8	2856.4, 2974.4	2856.4, 2968.2	2850.2, 2968.2	2851.9	2851.9	2851.9	2845.1
–N=CS stretch	2106.4	2101.2	2108.4	2106.4	2104.1	2099.5	2099.5	2106.4
C=O stretch of ester/acid	1721.6	1735.0	1723.7	1728.8	1717.1	1685.3	1717.1	1728.8
C–O stretch of ester/acid	1050.6	1027.0	1014.7	1014.7	1029.1	1023.5	1029.1	1074.2
Ru–N (peripheral pyridine)	761.3	767.4	796.2	755.1	765.5	716.9	711.3	707.9
Ru–C (carbene)	838.2	838.2	832.1	832.1	833.7	835.6	840.3	843.4
N–C–N	1486.7	1492.8	1492.8	1481.5	1491.8	1480.6	1480.6	1481.5
–OH stretch of COOH group	-	-	-	-	3293.2	3314.7	3443.7	3186.7

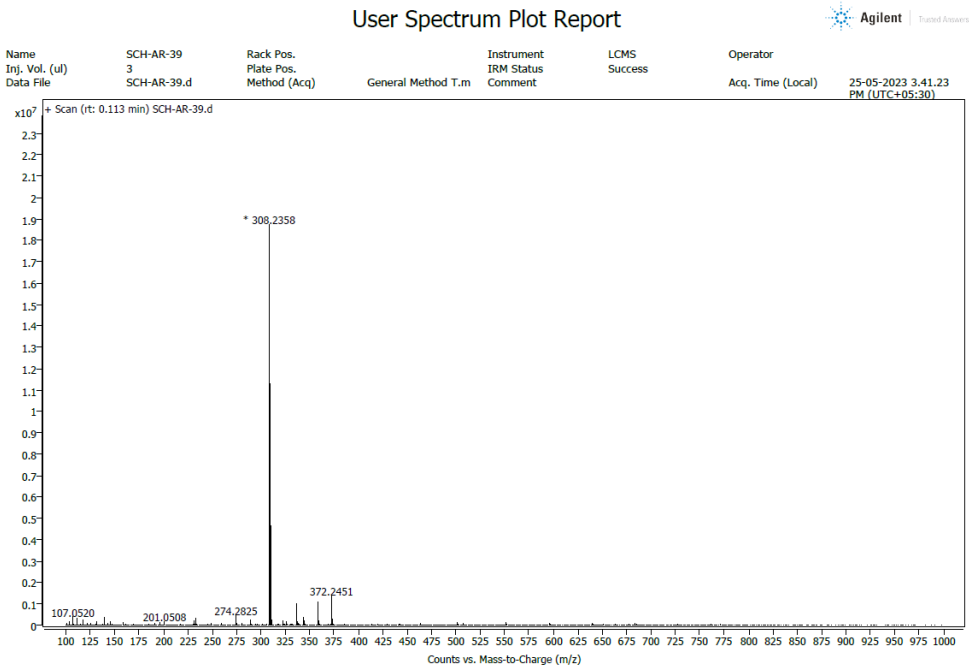


Fig. S59(a). High resolution mass spectrum (HRMS) of (**II**).

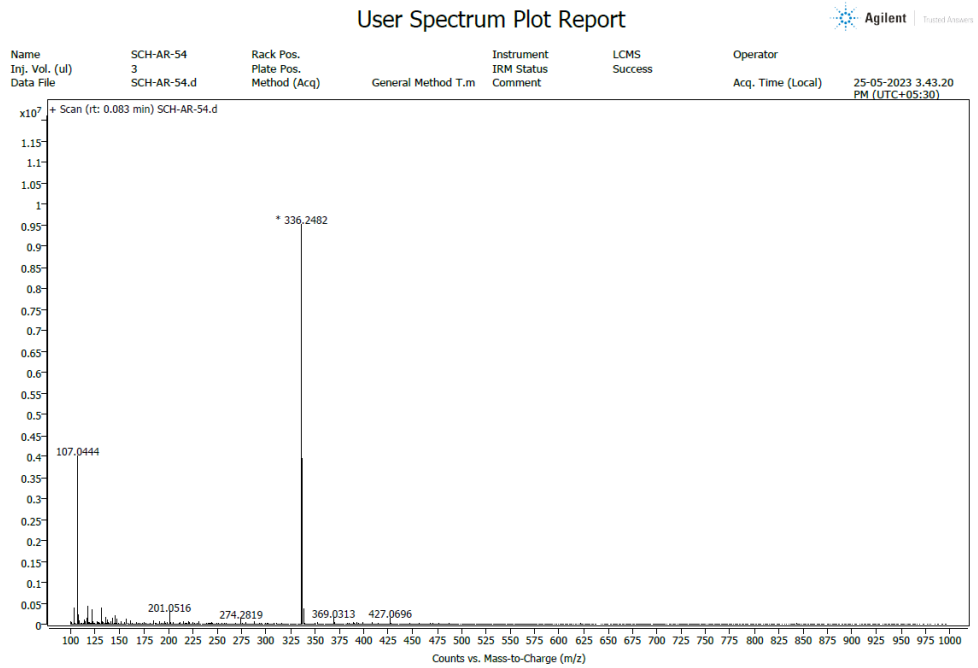


Fig. S59(b). High resolution mass spectrum (HRMS) of (**III**).

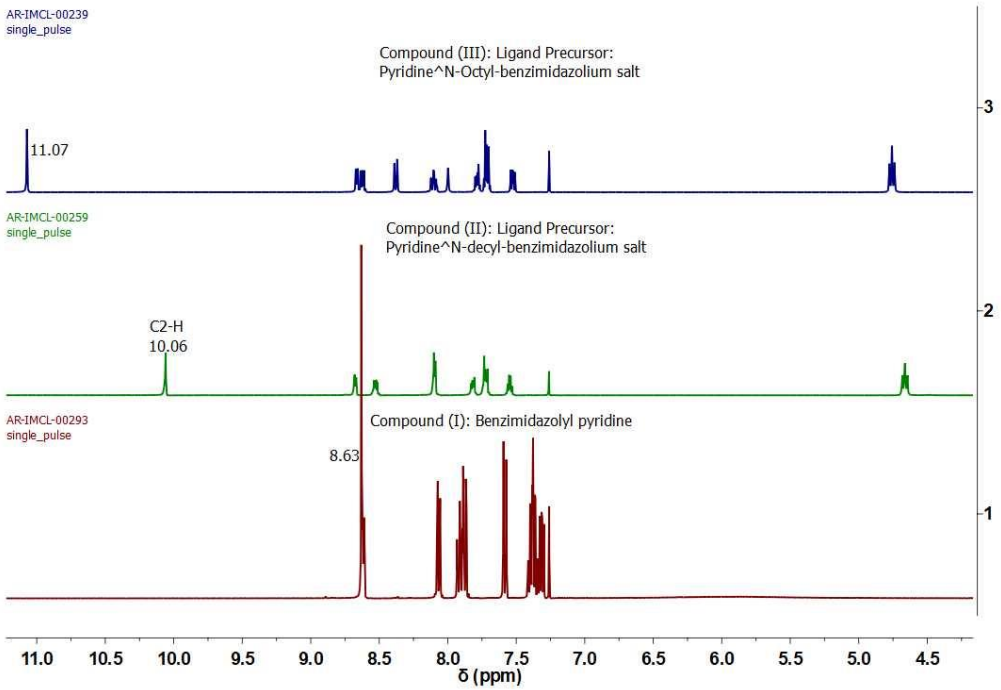


Fig. S59(c). Stacked ^{1}H NMR spectra of (**I**), (**II**), and (**III**).

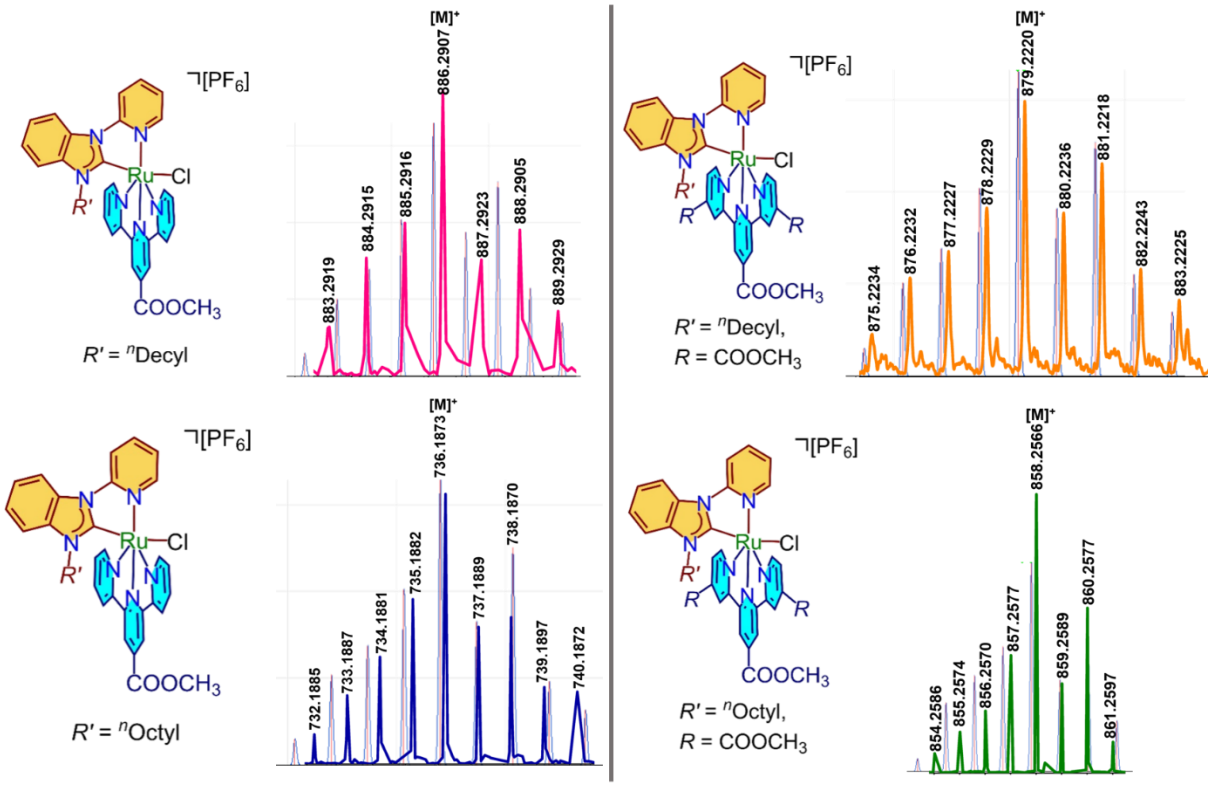


Fig. S60. HRMS of [**1**] – [**4**]. a. [**1**], b. [**2**], c. [**3**], and [**4**].

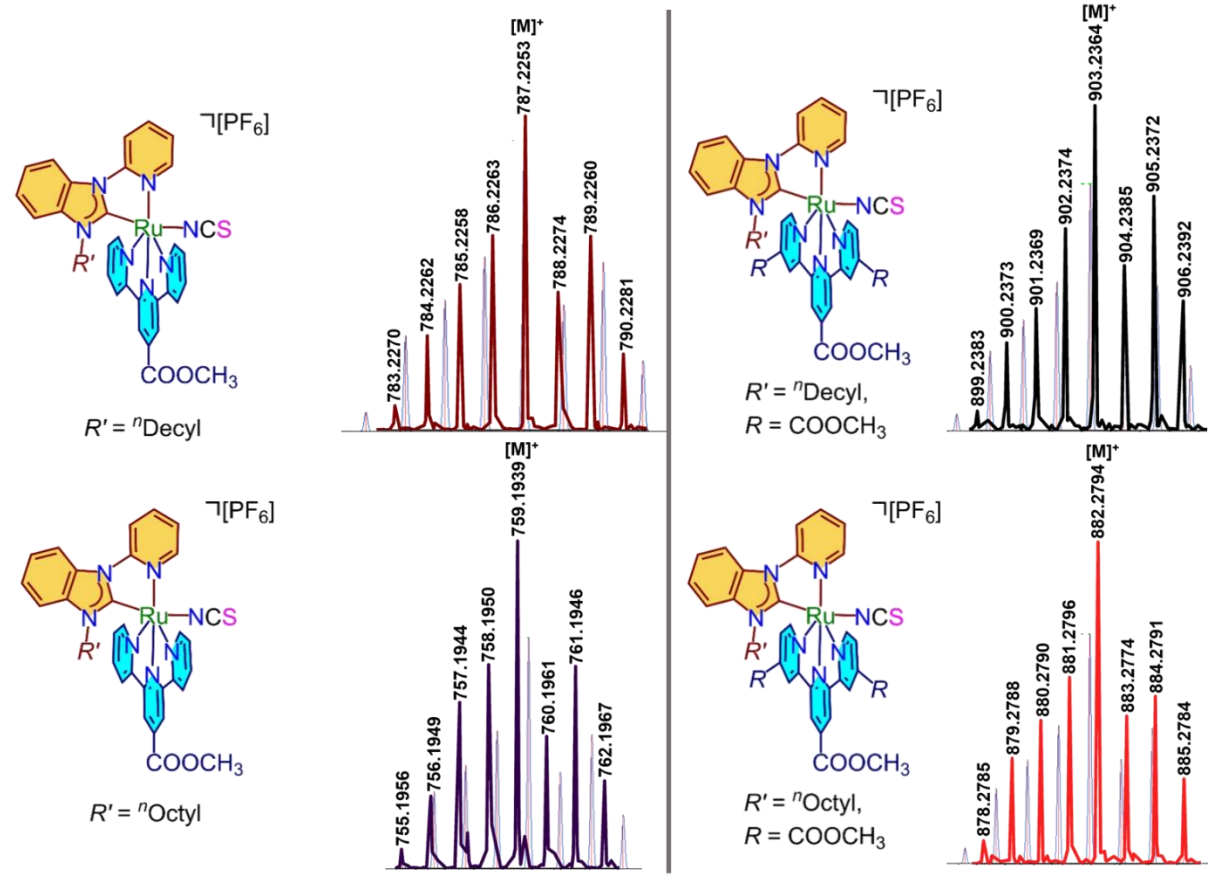


Fig. S61. HRMS of [**5**] – [**8**]. a. [**5**], b. [**6**], c. [**7**], and [**8**].

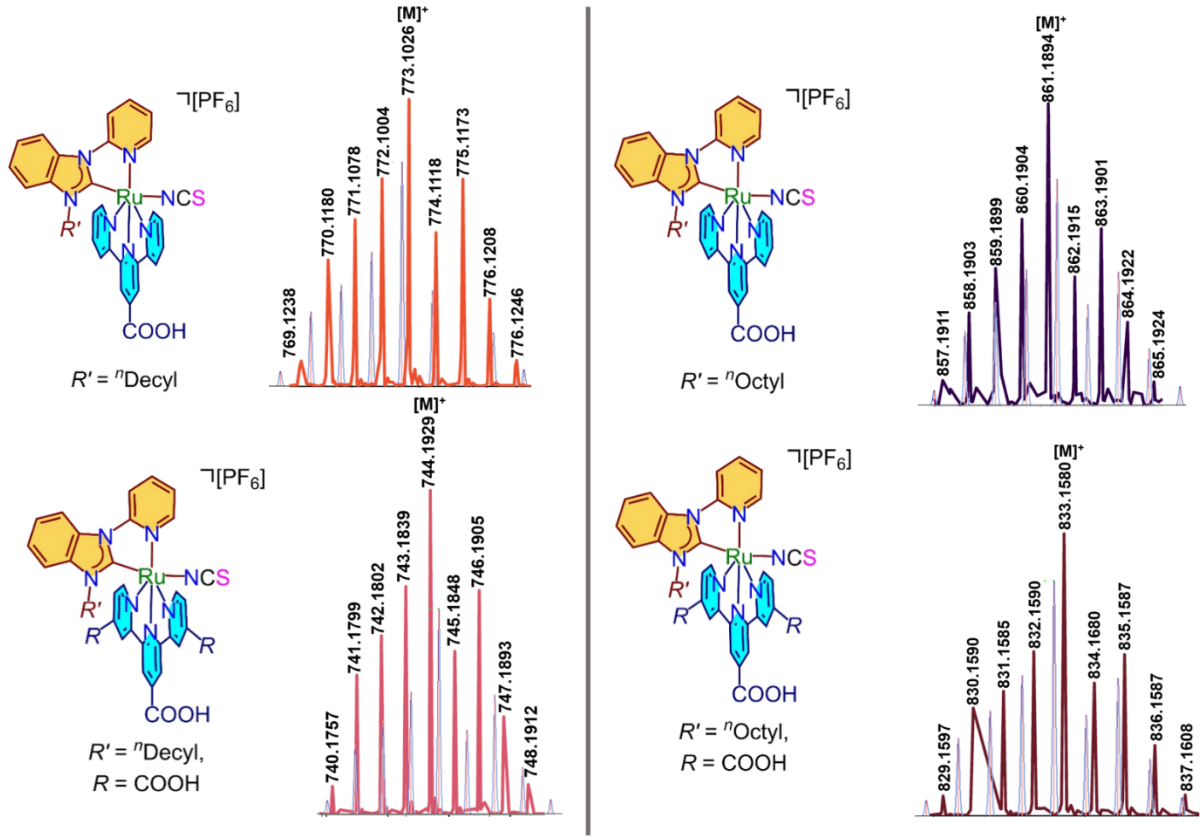


Fig. S62. HRMS of [**S1**] – [**S4**]. a. [**S1**], b. [**S2**], c. [**S3**], and [**S4**].

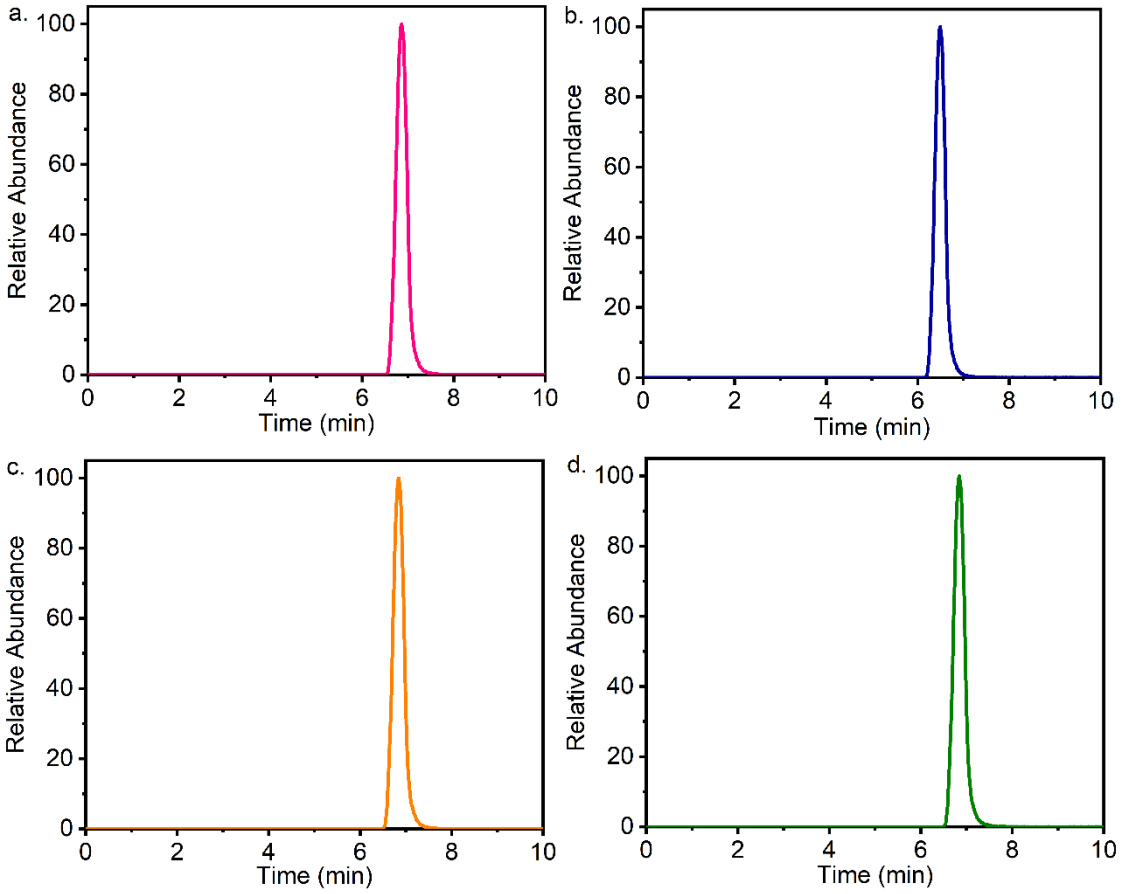


Fig. S63. LC-MS of [**5**] – [**8**]. a. [**5**], b. [**6**], c. [**7**], and [**8**].

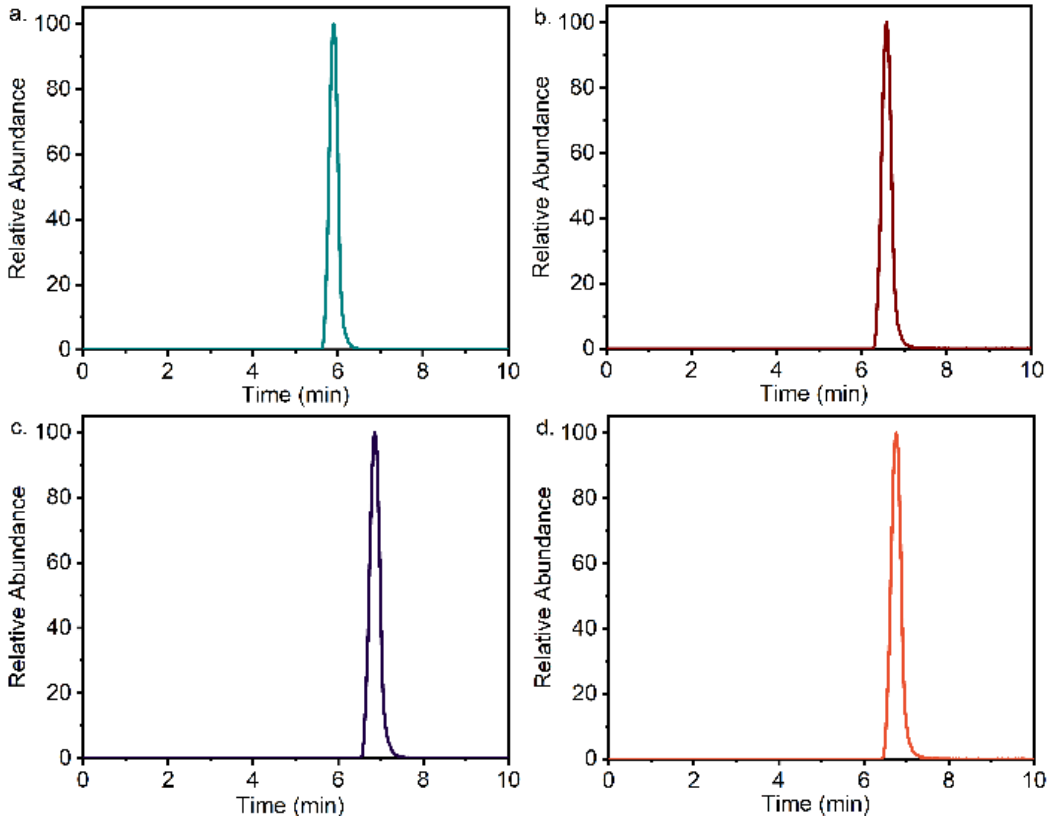


Fig. S64. LC-MS of [**S1**] – [**S4**]. a. [**S1**], b. [**S2**], c. [**S3**], and [**S4**].

Table S3

Selected geometrical parameters (bond distances, in Å and angles, in degrees) of complexes [**A**] and [**B**] in ground and lowest-lying singlet excited state in acetonitrile phase.

Electronic States	Ru–N^a		Ru–N^b		Ru–N^c	
	[**A**]	[**B**]	[**A**]	[**B**]	[**A**]	[**B**]
$S_0^{Ru^{2+}}$	1.962	1.962	2.083	2.077	2.086	2.077
^{1}MLLCT	1.994	1.994	2.088	2.084	2.087	2.083
$S_0^{Ru^{3+}}$	1.996	1.994	2.083	2.083	2.082	2.083
	Ru–N^{NCS}		Ru–C^{NHC}		Ru–N^{Py}	
	[**A**]	[**B**]	[**A**]	[**B**]	[**A**]	[**B**]
$S_0^{Ru^{2+}}$	2.087	2.084	1.990	1.997	2.105	2.107
^{1}MLLCT	2.028	2.025	2.009	2.011	2.101	2.099
$S_0^{Ru^{3+}}$	2.018	2.013	2.031	2.033	2.096	2.097
	∠^{b}N–Ru–N^c		∠^{NHC}C–Ru–N^{Py}		∠N–C^{NHC}–N (NHC ligand)	
	[**A**]	[**B**]	[**A**]	[**B**]	[**A**]	[**B**]
$S_0^{Ru^{2+}}$	159.52	159.68	77.76	77.69	105.82	105.93
^{1}MLLCT	157.47	157.89	77.85	77.89	106.51	106.50
$S_0^{Ru^{3+}}$	157.96	158.06	77.47	77.47	106.96	106.99

*Coordinating N atoms of central and terminal pyridyl (py) rings tpy are written as-N^a, N^b and N^c.

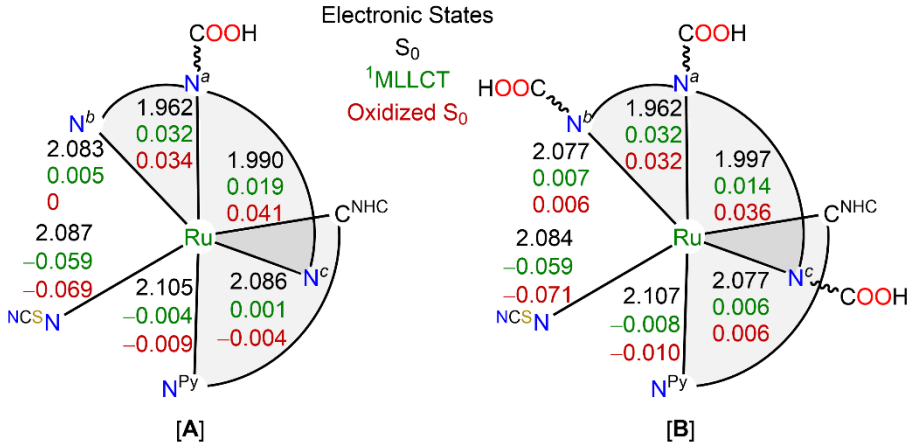
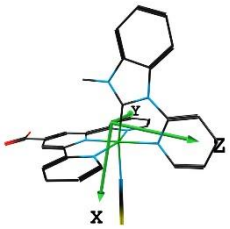
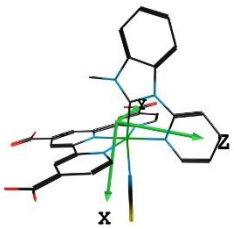
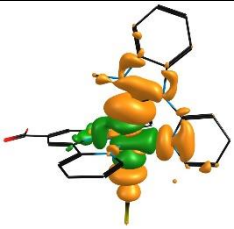
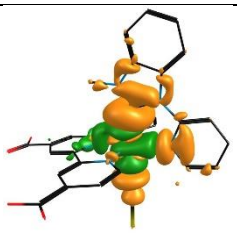
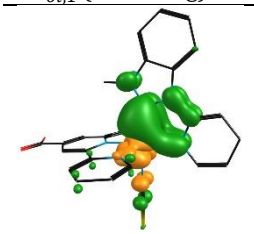
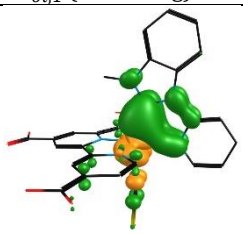
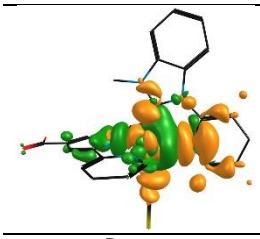
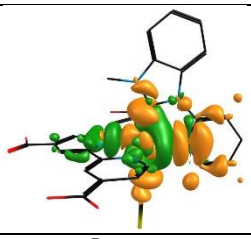


Fig. S65. Changes in geometries of [**A**] and [**B**] in their lowest-lying singlet excited state of ^{1}MLLCT character and singly oxidized doublets with respect to their corresponding S_0 ground states in acetonitrile phase.

Table S4

ETS–NOCV total (ΔE_{oi}) and important pairwise orbital stabilization energies ($\Delta E_{oi,i}$) for the interaction between acceptor fragment [Ru–Tpy–COOH]$^{2+}$ and donor fragment [NCS, NHC–Py]$^-$ of [**A**] and acceptor fragment [Ru–Tpy–(COOH)$_3$]$^{2+}$ and donor fragment [NCS, NHC–Py]$^-$ of [**B**]. Isosurfaces of deformation density flow channels of contour value 0.001 depict the flow of charge from orange (negative eigenvalue) to green (positive eigenvalue) region. The schematic diagram shows the coordination axes of ligands around the ruthenium center.

[A]				[B]		
						
	Fragments	Outflow	Inflow		Fragments	Outflow	Inflow
	Ru	05	86		Ru	06	86
	NHC	63	–		NHC	62	–01
	NCS	17	–01		NCS	17	–01
	Py	14	04		Py	14	03
	Tpy–COOH	02	12		Tpy–(COOH)$_3$	02	12
$C^{NHC}_{sp_xp_z}, N^{Py}_{sp_zp_x}, N^{NCS}_{sp_x} \rightarrow Ru_{d_{x^2-y^2}, d_{z^2}}$				$C^{NHC}_{sp_xp_z}, N^{Py}_{sp_zp_x}, N^{NCS}_{sp_x} \rightarrow Ru_{d_{x^2-y^2}, d_{z^2}}$			
$\Delta E_{oi,1}$ (σ-bonding) = –87.150 kcal mol^{-1} (45.3%)				$\Delta E_{oi,1}$ (σ-bonding) = –87.545 kcal mol^{-1} (45.4%)			
	Fragments	Outflow	Inflow		Fragments	Outflow	Inflow
	Ru	68	32		Ru	68	32
	NHC	20	48		NHC	20	46
	NCS	02	03		NCS	02	03
	Py	06	13		Py	06	12
	Tpy–COOH	04	05		Tpy–(COOH)$_3$	04	07
$Ru_{d_{xy}} \rightarrow C^{NHC}_{p_y}, N^{Py}_{p_y}$				$Ru_{d_{xy}} \rightarrow C^{NHC}_{p_y}, N^{Py}_{p_y}$			
$\Delta E_{oi,2}$ (π back-bonding) = –21.596 kcal mol^{-1} (11.2%)				$\Delta E_{oi,2}$ (π back-bonding) = –20.516 kcal mol^{-1} (10.6%)			
	Fragments	Outflow	Inflow		Fragments	Outflow	Inflow
	Ru	10	75		Ru	10	77
	NHC	22	–08		NHC	22	–09
	NCS	14	–05		NCS	14	–05
	Py	50	12		Py	50	13

	Tpy–COOH	04	25		Tpy–$(COOH)_3$	04	24
$C^{NHC}_{sp_xp_z}, N^{Py}_{sp_zp_x}, N^{NCS}_{sp_x} \rightarrow Ru_{d_{x^2-y^2}, d_{z^2}}$				$C^{NHC}_{sp_xp_z}, N^{Py}_{sp_zp_x}, N^{NCS}_{sp_x} \rightarrow Ru_{d_{x^2-y^2}, d_{z^2}}$			
$\Delta E_{oi,4}$ (σ-bonding) = –31.024 kcal mol^{-1} (16.1%)				$\Delta E_{oi,4}$ (σ-bonding) = –31.913 kcal mol^{-1} (16.5%)			
ΔE_{oi} (Total) = –192.508				ΔE_{oi} (Total) = –192.964			

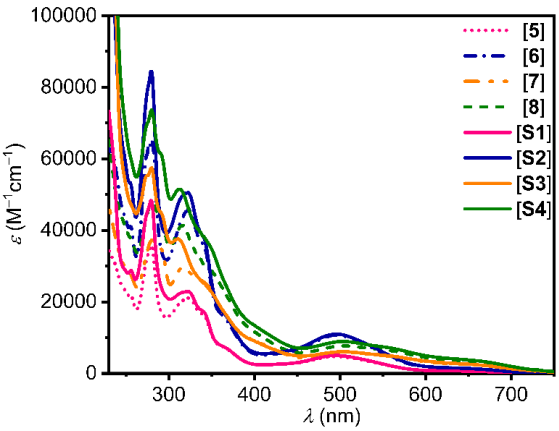


Fig. S66(a). Comparison of UV-Visible spectra of [**5**] – [**8**], and [**S1**] – [**S4**] in their 2.5 × 10^{-5} M acetonitrile solutions.

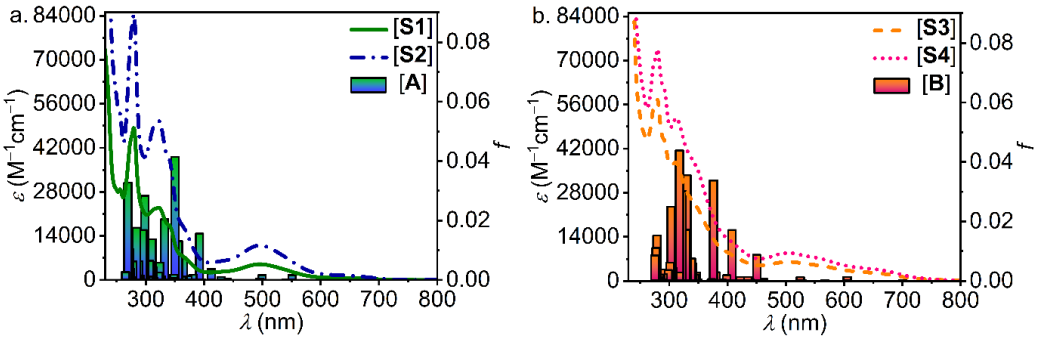


Fig. S66(b). UV-Visible spectra of [**S1**] – [**S4**] with computed vertical transitions shown as bars. [**A**] and [**B**] denote computational structures of photosensitizers bearing $tpy^{4'\text{-}COOH}$ and $tpy^{4,4',4''\text{-}(COOH)_3}$, respectively.

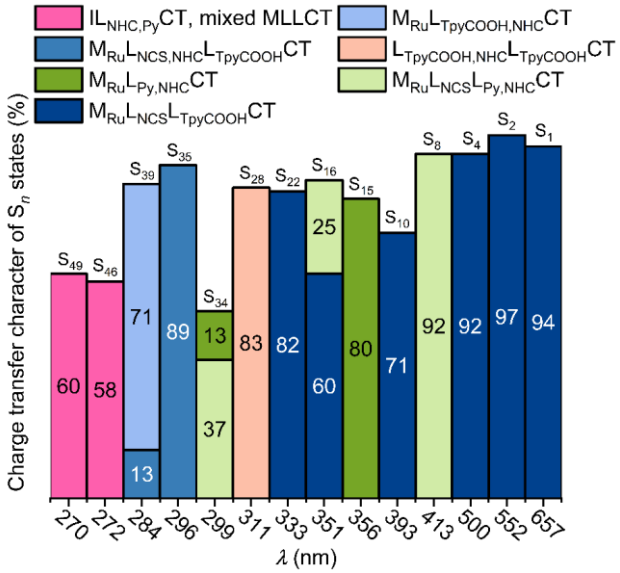


Fig. S67(a). Selected TDDFT electronic transitions with wavelengths (λ) and charge transfer character of [**A**].

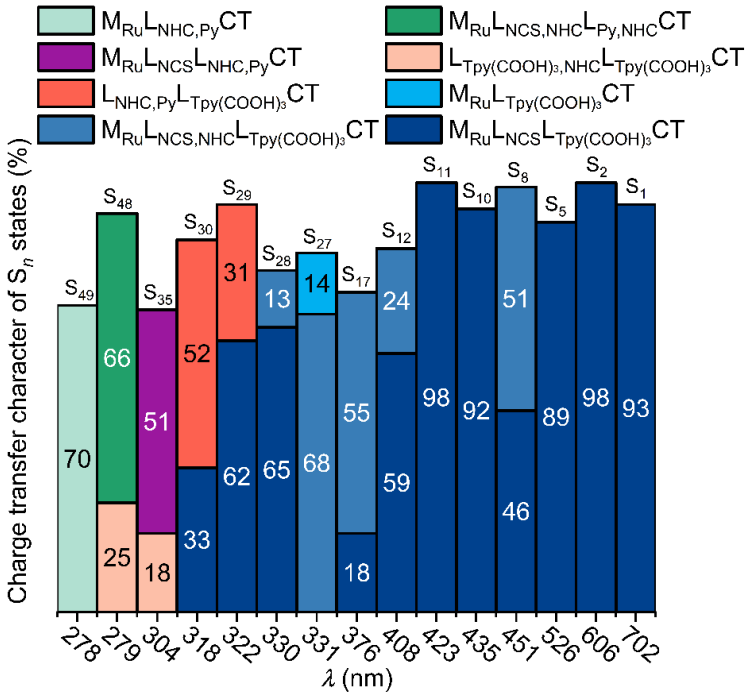


Fig. S67(b). Selected TDDFT electronic transitions with wavelengths (λ) and charge transfer character of [**B**].

Table S5

Vertical transition energies (), oscillator strengths (f) transition probabilities (%) of the major excitation configurations with the ground state occupied and unoccupied molecular orbitals and character of selected TDDFT excitations of [**A**] and [**B**].

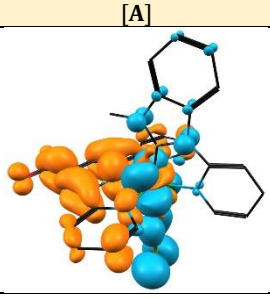
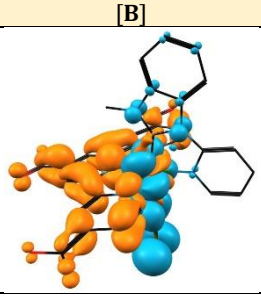
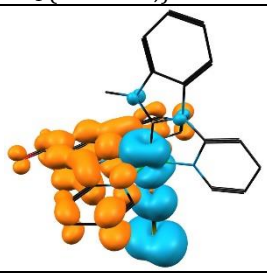
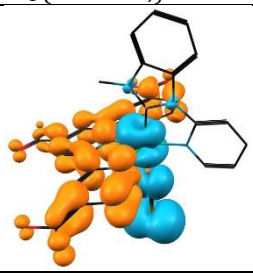
Excited State	λ (nm)	Oscillator strength (f)	Excitation (Maximum orbital contribution)	Atom/Ligand % From Anchor TpyCOOH/ Tpy(COOH)$_3$	Ru	Donor end NCS	NHC	Py	To Anchor TpyCOOH/ Tpy(COOH)$_3$	Ru	Donor end NCS	NHC	Py	Excitation character
[**A**]														
S_1	657	2.0E-04	H → L (94%)	07	39	45	09	01	88	10	01	01	–	^{1}MLLCT
S_2	552	0.001	H – 1 → L (68%)	09	32	57	01	01	88	10	01	01	–	^{1}MLLCT
			H → L+1 (29%)	07	39	45	09	01	98	01	–	–	–	^{1}MLLCT
S_4	500	0.001	H → L+1 (66%)	07	39	45	09	01	98	01	–	–	–	^{1}MLLCT
			H – 1 → L (26%)	09	32	57	01	01	88	10	01	01	–	^{1}MLLCT
S_8	413	0.004	H → L + 2 (92%)	07	39	45	09	01	07	06	–	19	68	^{1}MLLCT
S_{10}	393	0.015	H – 4 → L (71%)	15	38	44	02	01	88	10	01	01	–	^{1}MLLCT
S_{15}	356	0.013	H → L + 5 (44%)	07	39	45	09	01	01	04	01	29	66	^{1}MLLCT
			H – 2 → L + 2 (36%)	07	75	01	07	10	07	06	–	19	68	^{1}MLLCT
S_{16}	351	0.041	H → L + 4 (60%)	07	39	45	09	01	84	02	–	06	07	^{1}MLLCT
			H → L + 5 (25%)	07	39	45	09	01	01	04	01	29	66	^{1}MLLCT
S_{22}	333	0.020	H – 1 → L + 6 (82%)	09	32	57	01	01	99	01	–	–	–	^{1}MLLCT
S_{28}	311	0.014	H – 7 → L (83%)	36	12	02	49	01	88	10	01	01	–	^{1}LLCT
S_{34}	299	0.028	H → L + 7 (37%)	07	39	45	09	01	07	03	–	71	20	^{1}MLLCT
			H – 2 → L + 2 (13%)	07	75	01	07	10	07	06	–	19	68	^{1}MLLCT
S_{35}	296	0.017	H – 3 → L + 3 (89%)	08	22	53	15	02	99	01	–	–	–	^{1}MLLCT
S_{39}	284	0.017	H – 2 → L + 7 (71%)	07	75	01	07	10	07	03	–	71	20	^{1}MLLCT
			H – 3 → L + 4 (13%)	08	22	53	15	02	84	02	–	06	07	^{1}MLLCT
S_{46}	272	0.010	H – 3 → L + 5 (30%)	08	22	53	15	02	01	04	01	29	66	^{1}MLLCT
			H – 5 → L + 2 (28%)	01	02	–	70	27	07	06	–	19	68	^{1}LLCT/^{1}ILCT
S_{49}	270	0.033	H – 5 → L + 2 (50%)	01	02	–	70	27	07	06	–	19	68	^{1}LLCT/^{1}ILCT
			H – 3 → L + 5 (10%)	08	22	53	15	02	01	04	01	29	66	^{1}MLLCT

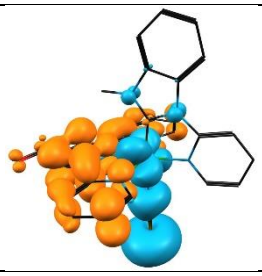
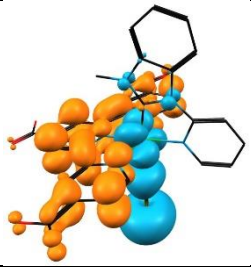
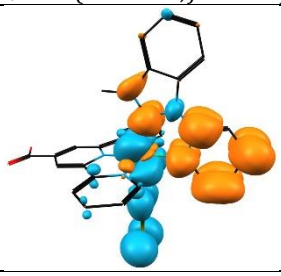
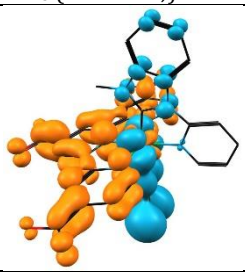
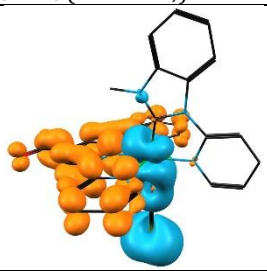
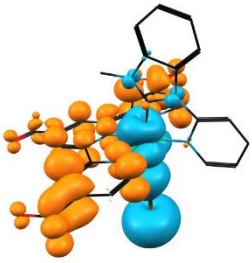
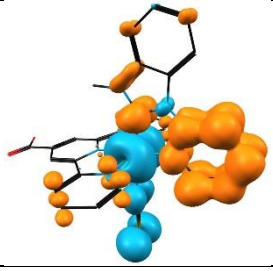
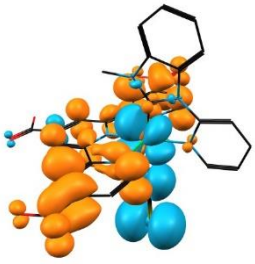
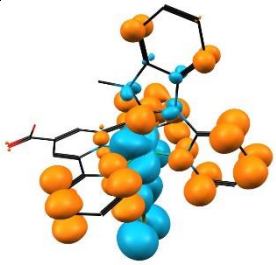
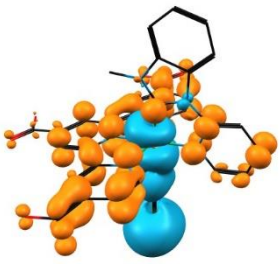
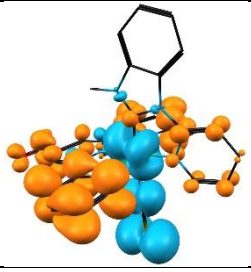
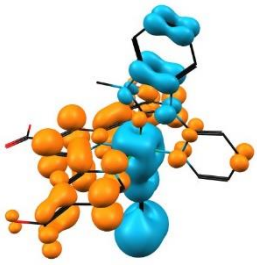
[B]														
S_1	702	2.9E-05	H → L (93%)	07	34	50	08	01	89	10	01	01	–	^{1}MLLCT
S_2	606	0.001	H – 1 → L (77%)	09	28	62	01	01	89	10	01	01	–	^{1}MLLCT
			H → L + 1 (21%)	07	34	50	08	01	95	04	–	01	–	^{1}MLLCT
S_5	526	0.001	H → L + 1 (71%)	07	34	50	08	01	95	04	–	01	–	^{1}MLLCT
			H – 1 → L (18%)	09	28	62	01	01	89	10	01	01	–	^{1}MLLCT
S_8	451	0.009	H – 3 → L (51%)	09	23	47	19	02	89	10	01	01	–	^{1}MLLCT
			H → L + 2 (46%)	07	34	50	08	01	99	01	–	–	–	^{1}MLLCT
S_{10}	435	0.001	H → L + 3 (63%)	07	34	50	08	01	96	01	–	02	01	^{1}MLLCT
			H – 1 → L + 2 (29%)	09	28	62	01	01	99	01	–	–	–	^{1}MLLCT
S_{11}	423	0.001	H – 1 → L + 3 (98%)	09	28	62	01	01	96	01	–	02	01	^{1}MLLCT
S_{12}	408	0.017	H – 4 → L (44%)	16	42	40	02	01	89	10	01	01	–	^{1}MLLCT
			H – 3 → L + 1 (24%)	09	23	47	19	02	95	04	–	01	–	^{1}MLLCT
			H → L + 4 (15%)	07	34	50	08	01	03	07	01	18	71	^{1}MLLCT
S_{17}	376	0.034	H – 3 → L + 1 (55%)	09	23	47	19	02	95	04	–	01	–	^{1}MLLCT
			H – 4 → L (18%)	16	42	40	02	01	89	10	01	01	–	^{1}MLLCT
S_{27}	331	0.035	H – 3 → L + 3 (68%)	09	23	47	19	02	96	01	–	02	01	^{1}MLLCT
			H – 2 → L + 4 (14%)	07	75	01	07	10	03	07	01	18	71	^{1}MLLCT
S_{28}	330	0.017	H – 4 → L + 2 (65%)	16	42	40	02	01	99	01	–	–	–	^{1}MLLCT
			H – 3 → L + 3 (13%)	09	23	47	19	02	96	01	–	02	01	^{1}MLLCT
S_{29}	322	0.030	H – 4 → L + 3 (62%)	16	42	40	02	01	96	01	–	02	01	^{1}MLLCT
			H – 7 → L (31%)	55	11	02	30	01	89	10	01	01	–	^{1}LLCT
S_{30}	318	0.044	H – 7 → L (52%)	55	11	02	30	01	89	10	01	01	–	^{1}LLCT
			H – 4 → L + 3 (33%)	16	42	40	02	01	96	01	–	02	01	^{1}MLLCT
S_{35}	304	0.025	H → L + 7 (51%)	07	34	50	08	01	02	02	–	73	23	^{1}MLLCT
			H – 6 → L + 1 (18%)	51	05	–	42	01	95	04	–	01	–	^{1}LLCT
S_{48}	279	0.015	H – 3 → L + 5 (66%)	09	23	47	19	02	99	01	–	–	–	^{1}MLLCT
			H – 6 → L + 2 (25%)	51	05	–	42	01	99	01	–	–	–	^{1}LLCT
S_{49}	278	0.011	H – 2 → L + 7 (70%)	07	75	01	07	10	02	02	–	73	23	^{1}MLLCT

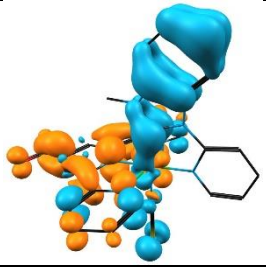
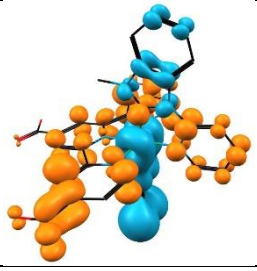
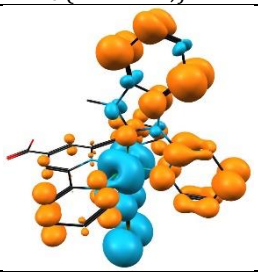
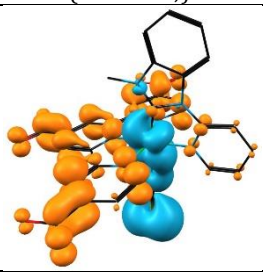
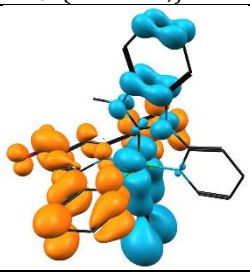
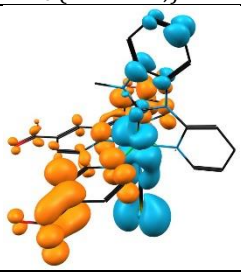
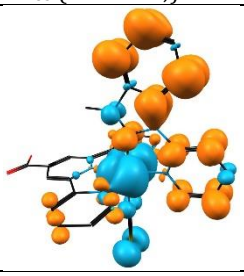
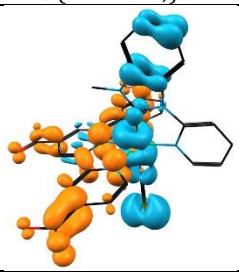
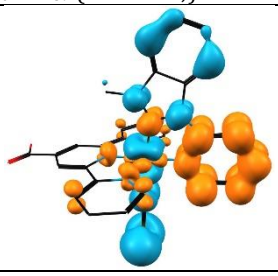
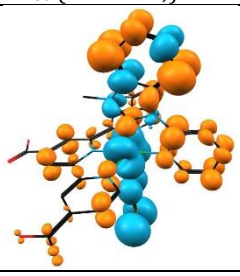
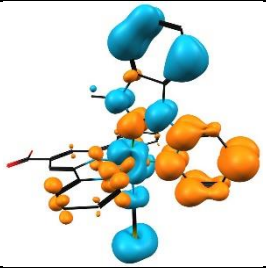
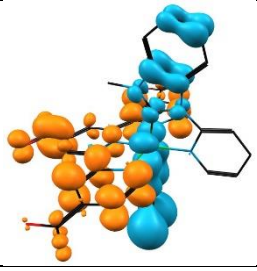
*H and L denote the HOMO and LUMO levels.

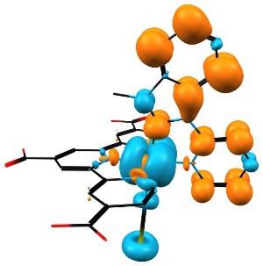
Table S6

Electron density difference maps (EDDM) of selected $S_0 \rightarrow S_n$ vertical excitations of [**A**] and [**B**] (contour value = 0.001). Hydrogen atoms are omitted for clarity.

[A]	[B]
	
$S_0 \rightarrow S_1$ (657.2 nm, f = 2.0E – 04)	$S_0 \rightarrow S_1$ (701.6 nm, f = 2.9E – 05)
	
$S_0 \rightarrow S_2$ (551.6 nm, f = 0.001)	$S_0 \rightarrow S_2$ (605.9 nm, f = 0.001)

	
$S_0 \rightarrow S_4$ (500.0 nm, f = 0.001)	$S_0 \rightarrow S_5$ (525.6 nm, f = 0.001)
	
$S_0 \rightarrow S_8$ (412.8 nm, f = 0.004)	$S_0 \rightarrow S_8$ (450.8 nm, f = 0.009)
	
$S_0 \rightarrow S_{10}$ (392.5 nm, f = 0.015)	$S_0 \rightarrow S_{10}$ (435.0 nm, f = 0.001)
	
$S_0 \rightarrow S_{15}$ (356.3 nm, f = 0.013)	$S_0 \rightarrow S_{11}$ (422.5 nm, f = 0.001)
	
$S_0 \rightarrow S_{16}$ (350.7 nm, f = 0.041)	$S_0 \rightarrow S_{12}$ (408.4 nm, f = 0.017)
	
$S_0 \rightarrow S_{22}$ (332.6 nm, f = 0.020)	$S_0 \rightarrow S_{17}$ (376.4 nm, f = 0.034)

	
$S_0 \rightarrow S_{28}$ (311.2 nm, f = 0.014)	$S_0 \rightarrow S_{27}$ (330.9 nm, f = 0.035)
	
$S_0 \rightarrow S_{34}$ (298.7 nm, f = 0.028)	$S_0 \rightarrow S_{28}$ (329.9 nm, f = 0.017)
	
$S_0 \rightarrow S_{35}$ (295.6 nm, f = 0.017)	$S_0 \rightarrow S_{29}$ (322.3 nm, f = 0.030)
	
$S_0 \rightarrow S_{39}$ (284.4 nm, f = 0.017)	$S_0 \rightarrow S_{30}$ (318.1 nm, f = 0.044)
	
$S_0 \rightarrow S_{46}$ (272.0 nm, f = 0.010)	$S_0 \rightarrow S_{35}$ (303.7 nm, f = 0.025)
	
$S_0 \rightarrow S_{49}$ (269.6 nm, f = 0.033)	$S_0 \rightarrow S_{48}$ (279.3 nm, f = 0.015)

	
	$S_0 \rightarrow S_{49}$ (277.8 nm, f = 0.011)

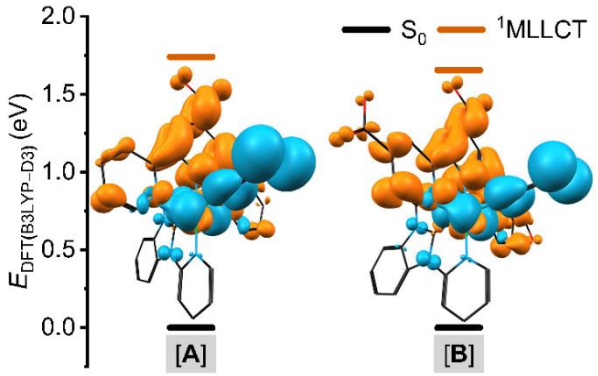


Fig. S68. Relaxed ^{1}MLLCT–S_0 states energy gap of [**A**] and [**B**] in the acetonitrile phase and their respective electron density difference maps (contour value: 0.001) depicting charge depletion from the blue region and its accumulation in the orange region.

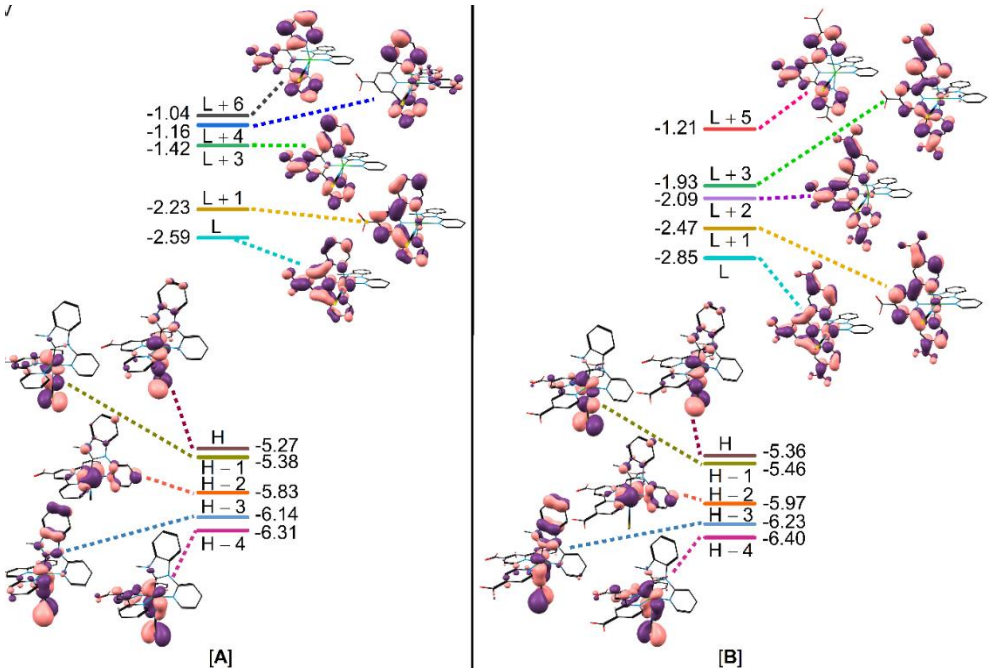


Fig. S69. Ground state *Kohn-Sham* doubly occupied and unoccupied molecular orbitals of isosurface value: 0.03 for complexes [**A**] and [**B**] in the acetonitrile phase.

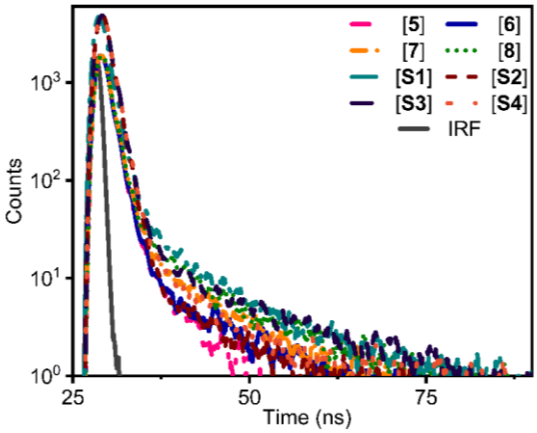


Fig. S70. Overlay of decay profiles of [**S1**] – [**S4**] over instrument response time.

Table S7

(a) Ground- and excited-state oxidation potentials and electron injection and dye regeneration driving forces for [**A**] and [**B**]. All energies displayed are in Hartree, unless specified.

Electrochemical parameters		[**A**]	[**B**]
${}^{a}G^{\circ}_{vac}$	Ru^{2+}	−2180.636	−2557.328
	Ru^{3+}	−2180.324	−2557.013
${}^{b}\Delta G^{\circ ox\,(Ru^{2+}/Ru^{3+})}_{vac}$		0.312	0.315
$E^{Ru^{2+}}_{vac}$	Ru^{2+}	−2181.051	−2557.767
	Ru^{3+}	−2180.740	−2557.452
$E^{Ru^{2+}}_{solv}$	Ru^{2+}	−2181.160	−2557.885
	Ru^{3+}	−2180.982	−2557.702
${}^{c/d}\Delta G^{\circ}_{solvation}$	Ru^{2+}	−0.109	−0.119
	Ru^{3+}	−0.242	−0.250
${}^{e}\Delta\Delta G^{\circ ox\,(Ru^{2+}/Ru^{3+})}_{solvation}$		−0.133	−0.131
${}^{f}\Delta G^{\circ ox\,(Ru^{2+}/Ru^{3+})}_{solv}$		0.179	0.184
${}^{g}{}^{DFT}E^{\circ(Ru^{2+}/Ru^{3+})}$ (V *vs* SCE)		0.691	0.815
ΔE_{calc} (eV)		1.887	1.767
${}^{DFT}E^{\circ(Ru^{2+*}/Ru^{3+})}$ (V *vs* SCE)		−1.195	−0.952
${}^{h}D_{inj}$ (V *vs* SCE)		0.495	0.252
${}^{i}D_{reg}$ (V *vs* SCE)		0.491	0.615

**solv* refers to Acetonitrile solvent modelled by SMD. Here, the *E* corresponds to the "FINAL SINGLE POINT ENERGY" printed at the end of ORCA output calculation file.

$*\Delta G^{\circ ox\,(Ru^{2+}/Ru^{3+})}_{vac} = G^{\circ Ru^{3+}}_{vac} - G^{\circ Ru^{2+}}_{vac}$.

$*\Delta G^{\circ Ru^{2+}}_{solvation} = E^{Ru^{2+}}_{solv} - E^{Ru^{2+}}_{vac}$.

$*\Delta G^{\circ Ru^{3+}}_{solvation} = E^{Ru^{3+}}_{solv} - E^{Ru^{3+}}_{vac}$.

$*\Delta\Delta G^{\circ ox\,(Ru^{2+}/Ru^{3+})}_{solvation} = \Delta G^{\circ Ru^{3+}}_{solvation} - \Delta G^{\circ Ru^{2+}}_{solvation}$.

$*\Delta G^{\circ ox\,(Ru^{2+}/Ru^{3+})}_{solv} = \Delta G^{\circ ox\,(Ru^{2+}/Ru^{3+})}_{vac} + \Delta\Delta G^{\circ ox\,(Ru^{2+}/Ru^{3+})}_{solvation}$.

$*\Delta G^{\circ ox\,(Ru^{2+}/Ru^{3+})}_{solv}$ (in *E*h) values are converted to ${}^{DFT}E^{\circ(Ru^{2+}/Ru^{3+})}$ using a conversion factor of 27.2114 V/Hartree where *n* (number of the electron) is 1 and then, subtracting 4.1888 V potential value of SCE (27.2114 ($\Delta G^{\circ ox\,(Ru^{2+}/Ru^{3+})}_{solv}$) – 4.188 V).

$*D_{reg} = |E^{I_3^-/I^-} - E^{\circ Ru^{2+}/Ru^{3+}}|$ where, potential of the redox couple ($E^{I_3^-/I^-}$) is 0.2 V *vs* SCE.

*The driving force for electron injection (D_{inj}) from the excited ^{1}MLLCT state was calculated using the equation: $D_{inj} = |{}^{b}E^{\circ(Ru^{2+*}/Ru^{3+})} - E^{TiO_2}_{CB}| = |{}^{b}E^{\circ(Ru^{2+}/Ru^{3+})} - \Delta E_{calc} - E^{TiO_2}_{CB}|$ where $E^{TiO_2}_{CB}$ is the conduction band edge of TiO_2 (–0.7 V *vs* SCE).

(b) Band gaps, HOMO and LUMO energies (in eV) of all dyes.

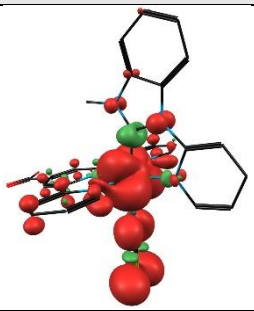
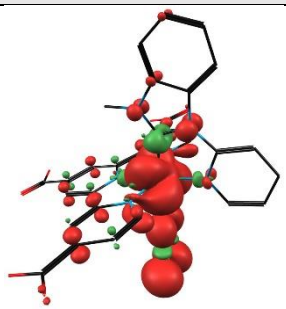
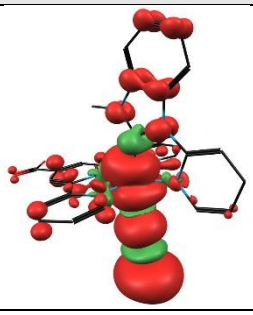
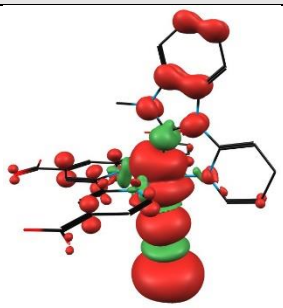
Optical and electrochemical energies						**DFT energies**			
Dye	Wingtip	$E_{0\text{-}0}{}^{a}$	$E_{HOMO}{}^{b}$	$E_{LUMO}{}^{b}$	$E_{gap}{}^{c}$ /$E_{el}{}^{c}$	Dye	E_{HOMO}	E_{LUMO}	E_{gap}
[**S1**]	^{n}Decyl	1.75	–5.76	–3.90	1.86	[**A**]	–5.27	–2.59	2.68
[**S2**]	^{n}Octyl	1.73	–5.80	–3.98	1.82				
[**S3**]	^{n}Decyl	1.72	–5.82	–3.96	1.86	[**B**]	–5.36	–2.85	2.51

[**S4**]	^{n}Octyl	1.72	–5.83	–3.97	1.86

[a]Optical band gaps, $E_{0\text{-}0}$, are obtained using onset wavelength ($1240/\lambda_{onset}$) of the absorption spectra in acetonitrile solution. Computed structures **A** is analogous to [**S1**] and [**S2**] and **B** is analogous to [**S3**] and [**S4**], however, with ^{n}Methyl wingtips.
[b]The HOMO and LUMO energies are calculated using the following equations *w.r.t.* the internal standard Ferrocene value of −4.8 eV, $E_{HOMO} = -e\,(E_{ox} + 4.8)$ (eV), $E_{LUMO} = -e\,(E_{red} + 4.8)$ (eV) where, E_{ox} and E_{red} are the first oxidation and reduction potentials, respectively.
[c]The electrochemical bandgap, E_{gap} is estimated from the HOMO − LUMO energy difference. $E_{gap} = E_{el}$ where, E_{el} is the difference between the first oxidation and reduction potentials. The order of electrochemical HOMO and LUMO energies of [**S1**] – [**S4**] correlate with those of [**A**] and [**B**].

Table S8

Mulliken spin densities of [**A**] and [**B**] after one- and two-electron oxidation (Contour value: 0.001).

[**A**]	[**B**]
Single oxidation	
	
Double oxidation	
	

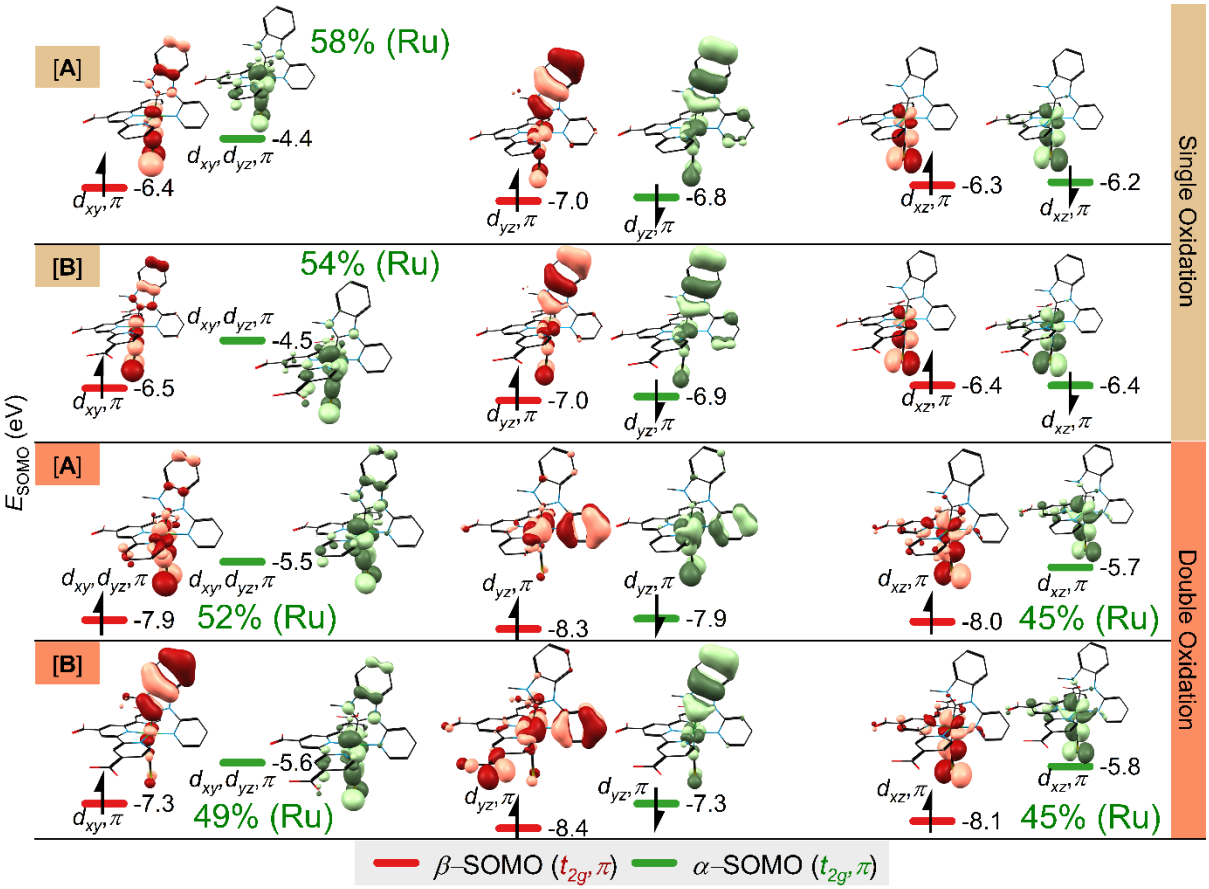


Fig. S71. SOMOs of [**A**] and [**B**] after one- and two-electron oxidation (Contour value: 0.03).

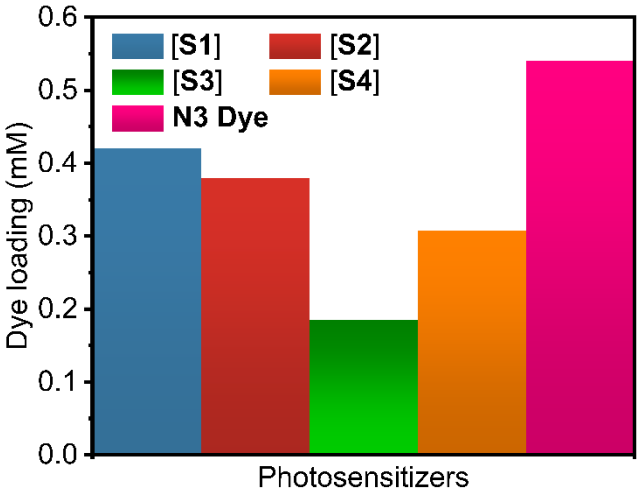
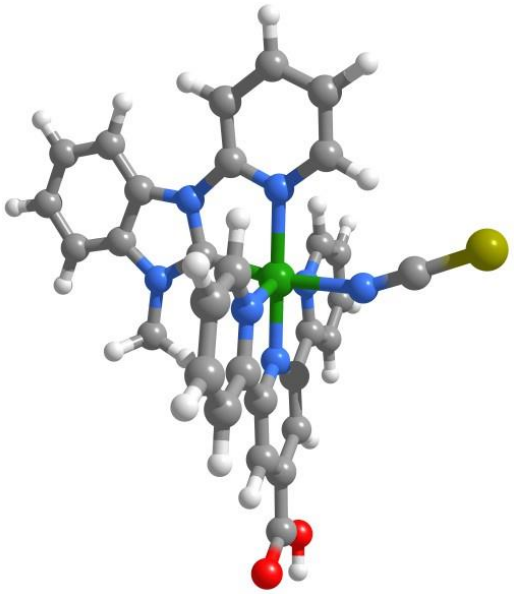


Fig. S72. Dye loading graph of [**S1**] – [**S4**] obtained from calibration curve with N3 dye.

xyz-cartesian coordinates of DFT-D3 optimized geometries. Atoms Ru, C, H, N, S, O, Cl are illustrated in green, grey, white, blue, yellow, red, and green colors, respectively.

Table S9. Final atomic coordinates for the singlet ground state (S_0) of [**A**] in the vacuum phase.

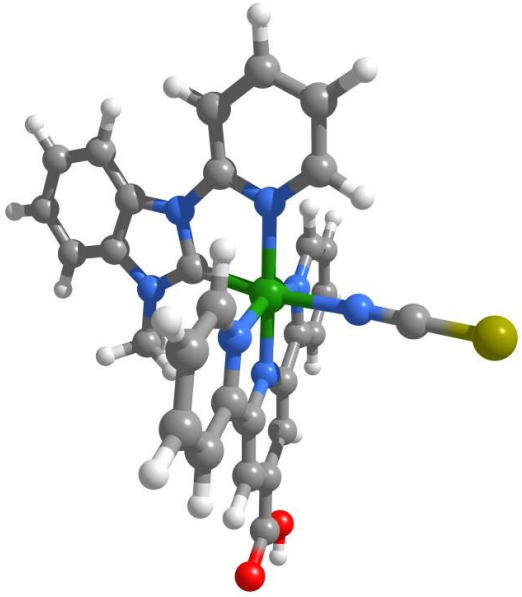
Atom	*x*	*y*	*z*
Ru	0.318268455069	−0.022085898111	0.447714251121
N	0.730680109368	−1.982626140216	−0.109636364252
N	0.686288176710	0.236165026964	−1.453055198289
N	−2.225834478413	−0.509480932577	1.736091879998
N	−0.072529273821	−0.304875708561	2.513468504172
N	0.162010834493	2.049019070041	0.323228576965
N	−2.690333553744	−0.332774362415	−0.397425942332
C	0.734390745720	1.503157643596	−1.941463448984
C	−1.655543171267	−0.298096624976	0.477392830025
C	0.425007251817	2.529042029103	−0.930284288202
C	−1.369404002078	−0.524958997539	2.842484817823
C	−3.622965510654	−0.667671451030	1.635765072460
C	3.315653575174	0.439078121838	1.434295656367
C	−4.658225180614	−0.887302423540	2.547796941580
H	−4.496618759546	−0.978684710779	3.618433659040
C	1.060484961672	−0.841315134605	−2.193506516403
C	1.077768363642	1.718706886993	−3.276603835582
H	1.116825236038	2.722287785460	−3.697497962683
C	1.073593796647	−2.099754029706	−1.428352395576
C	−0.096939375580	4.290273536611	1.129071419620
C	0.855734671504	−0.288915026414	3.493276230368
H	1.884684559435	−0.102891434070	3.185389633551
C	0.418395348376	3.903509521590	−1.187066468107
H	0.630200387313	4.271365233810	−2.191310006997
C	0.758790317905	−3.068766857954	0.676168045086
H	0.494687733852	−2.910165034212	1.723145459931
C	−0.082495064849	2.910755618707	1.320801106505
H	−0.262673288768	2.469037019611	2.302343532889
C	0.154201996059	4.795373066602	−0.149109148658
C	1.113188045162	−4.327749851995	0.197379125135
C	−1.772569623927	−0.744028288716	4.162509030355
H	−2.812992678278	−0.927421779264	4.407350787194
C	0.528913616612	−0.493355689691	4.829078211683
C	−6.229534981360	−0.875830409756	0.671033447405
H	−7.257902302241	−0.961118013965	0.314691929012
C	1.404702990904	−0.672064110567	−3.532044123242
H	1.696216987207	−1.508173843584	−4.167847715821
C	−2.601091109580	−0.165286804174	−1.835535426229
C	1.453022983813	−4.465406071151	−1.150876892627
C	−5.959567642110	−0.989341783380	2.042333675034
H	−6.782095301608	−1.161624346404	2.739232746101
C	1.432496977492	−3.337895536575	−1.969779313694
H	1.704381595531	−3.413272699029	−3.022908186202
C	1.395177529073	0.616915436858	−4.082995793590
C	−3.905522427393	−0.552792051421	0.260183851689
C	−5.198920197824	−0.653368140707	−0.246587748602
H	−5.401861136937	−0.561774651420	−1.314338445978
H	−0.296444473270	4.952147078534	1.973190358593
H	1.126280659943	−5.181209656476	0.877010349234
C	−0.805942772290	−0.726554606877	5.166522574244
H	−1.099764561485	−0.894524434721	6.204748914399
H	1.316665181094	−0.468562328380	5.583068919486
N	2.324052456153	0.239639869358	0.808976844136
S	4.634742500944	0.687073998370	2.324075316763
H	−3.166970698012	0.724217026971	−2.152749613059
H	−1.553144970781	−0.045198104578	−2.116496944306
O	2.034818743020	−0.177237821124	−6.237415163988
C	1.759153688100	0.757476329141	−5.527322048259
O	1.739558092831	2.034623712658	−5.939334109921
H	1.994204161686	2.046666240331	−6.878688825133
H	−3.013900124796	−1.048720124516	−2.345920405029
H	1.737997859681	−5.437193339595	−1.558754038893
H	0.152329971798	5.871345016184	−0.334362331130



[A]

Table S10. Final atomic coordinates for the singlet ground state (S_0) of [**A**] in the acetonitrile phase.

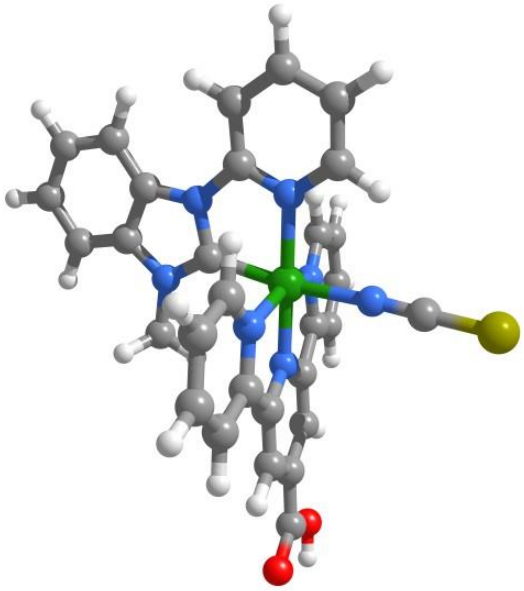
Atom	*x*	*y*	*z*
Ru	0.409371750772	−0.046688409638	0.501120541258
N	0.837996932851	−2.004550775629	−0.065678492795
N	0.789439724602	0.219140383452	−1.405342649765
N	−2.167377171280	−0.509226979601	1.713021204734
N	−0.034004677595	−0.340968283760	2.538087760166
N	0.182372127320	2.021744526080	0.360868202478
N	−2.567125822187	−0.323420809166	−0.434299282720
C	0.766649614616	1.479192524130	−1.903611636714
C	−1.562373170795	−0.316498161611	0.469212088639
C	0.400380402766	2.499126599519	−0.902459222785
C	−1.338804123174	−0.541427460363	2.840434353018
C	−3.563199507697	−0.619610280186	1.575505072655
C	3.603016062998	0.400037110552	1.032770102587
C	−4.627552439460	−0.803011539808	2.462435160941
H	−4.490970769791	−0.903690851438	3.536115615015
C	1.163070822327	−0.853302413988	−2.147997441644
C	1.077420123073	1.699660667534	−3.245313894074
H	1.056011210753	2.703845872461	−3.664764316879
C	1.177541909375	−2.116602807475	−1.386320527435
C	−0.260852915807	4.247458474067	1.125142069180
C	0.877262839430	−0.347244655543	3.530393429396
H	1.910234010400	−0.181858838455	3.223785824556
C	0.285263096248	3.862515689400	−1.185210089173
H	0.458197552238	4.226662324726	−2.198096222736
C	0.840824190790	−3.097722039276	0.710925560175
H	0.570416701977	−2.948348511188	1.757658332199
C	−0.133815958459	2.876820008860	1.343931388253
H	−0.287901451460	2.441344499841	2.332685929245
C	−0.051137868251	4.747718750044	−0.161173740305
C	1.171314638680	−4.358896683013	0.218661512326
C	−1.768446992435	−0.757082469377	4.152840303886
H	−2.815025838445	−0.925746083500	4.384175460629
C	0.528073127078	−0.550279621922	4.859240449688
C	−6.150293730847	−0.720883619203	0.545435050879
H	−7.172732836696	−0.761191987851	0.162912607591
C	1.479602075155	−0.682862875845	−3.494349652707
H	1.769086325043	−1.524946416465	−4.122269683591
C	−2.435537142552	−0.137276650367	−1.869633678053
C	1.513507539989	−4.489366517091	−1.128533898698
C	−5.918958126311	−0.851709985615	1.923715901888
H	−6.764512096498	−0.993518194895	2.600622482437
C	1.517514349531	−3.354129971082	−1.938602415543
H	1.785523836208	−3.425957778181	−2.992693054224
C	1.425064429927	0.603848676908	−4.047688921217
C	−3.805079780460	−0.493133788032	0.192138811876
C	−5.089644767263	−0.536870908984	−0.346725435127
H	−5.257605061392	−0.429251955490	−1.419173051957
H	−0.521556118017	4.903561414497	1.957227283642
H	1.158346427437	−5.219132877829	0.890021452345
C	−0.817966190074	−0.758906492621	5.171241993215
H	−1.133827096792	−0.925071832291	6.203344309861
H	1.300624683562	−0.545521226939	5.629669166079
N	2.443348163201	0.238030521823	0.874255923203
S	5.201647917632	0.630556263850	1.263755498622
H	−2.718845814299	0.887952239866	−2.153052189904
H	−1.403908246238	−0.327479611602	−2.169033672932
O	2.057720419551	−0.156173962779	−6.224647763230
C	1.753812541729	0.762226617022	−5.496653944391
O	1.673929657516	2.033763910687	−5.906835855160
H	1.899284146742	2.063568401310	−6.857271866027
H	−3.090796756737	−0.848967051159	−2.390109871620
H	1.777089972475	−5.463118245970	−1.546621783685
H	−0.145643504665	5.815783636956	−0.367890752479



[A]

Table S11. Final atomic coordinates for the lowest lying singlet excited state (S_1) of [**A**] in the acetonitrile phase.

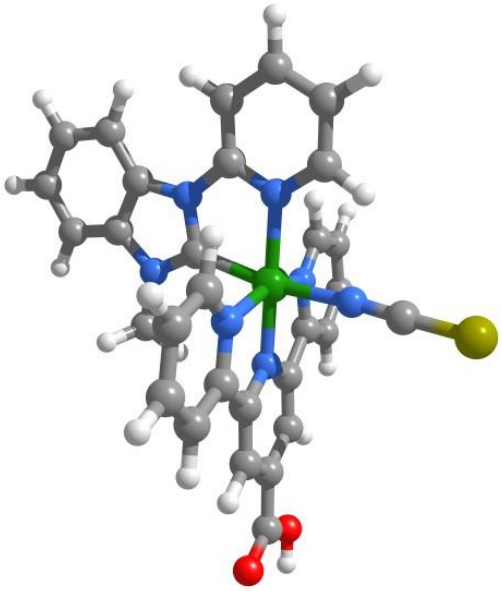
Atom	*x*	*y*	*z*
Ru	0.45617	−0.01898	0.52168
N	0.71569	−1.98971	−0.11593
N	0.83238	0.24494	−1.41854
N	−2.11297	−0.49376	1.75398
N	0.03154	−0.29705	2.5604
N	0.13976	2.03371	0.32151
N	−2.53524	−0.32823	−0.38955
C	0.84886	1.5226	−1.91211
C	−1.53425	−0.29179	0.50559
C	0.43014	2.52174	−0.93244
C	−1.26957	−0.50556	2.87396
C	−3.50453	−0.65388	1.6282
C	3.61262	0.44009	0.90195
C	−4.55647	−0.8683	2.52532
H	−4.41015	−0.94946	3.59916
C	1.19018	−0.84319	−2.16955
C	1.21502	1.74348	−3.23015
H	1.22379	2.75034	−3.64473
C	1.09564	−2.1031	−1.4336
C	−0.43576	4.23037	1.07802
C	0.95143	−0.28111	3.54505
H	1.98059	−0.10818	3.2299
C	0.29959	3.89478	−1.19576
H	0.53407	4.27534	−2.19034
C	0.5624	−3.09195	0.64061
H	0.24806	−2.92864	1.67319
C	−0.28943	2.86578	1.28809
H	−0.51087	2.4091	2.25467
C	−0.13137	4.75175	−0.19067
C	0.798	−4.36744	0.14459
C	−1.68802	−0.70986	4.19095
H	−2.73131	−0.8835	4.43289
C	0.61356	−0.47227	4.87828
C	−6.08924	−0.86971	0.61138
H	−7.11159	−0.95868	0.23728
C	1.56336	−0.66858	−3.49039
H	1.84516	−1.51281	−4.11926
C	−2.40892	−0.16713	−1.83115
C	1.20121	−4.50451	−1.19371
C	−5.84504	−0.97368	1.99279
H	−6.68192	−1.14074	2.67456
C	1.3469	−3.36982	−1.98308
H	1.65072	−3.45179	−3.02708
C	1.58096	0.63945	−4.04239
C	−3.76032	−0.54736	0.24504
C	−5.04437	−0.65283	−0.28919
H	−5.21979	−0.56844	−1.3624
H	−0.78036	4.86969	1.89202
H	0.66802	−5.23369	0.79479
C	−0.72903	−0.69101	5.20147
H	−1.03552	−0.84814	6.23775
H	1.39049	−0.45066	5.64382
N	2.44627	0.24833	0.80893
S	5.20184	0.70453	1.04852
H	−3.02142	0.68466	−2.15961
H	−1.36069	0.01381	−2.07491
O	2.30291	−0.11084	−6.18968
C	1.98139	0.80118	−5.44534
O	1.96338	2.08973	−5.8588
H	2.24182	2.09643	−6.79336
H	−2.75807	−1.07971	−2.33515
H	1.39414	−5.49328	−1.61576
H	−0.2364	5.82043	−0.39042



[A]

Table S12. Final atomic coordinates for the singly oxidized form of [**A**] in the vacuum phase.

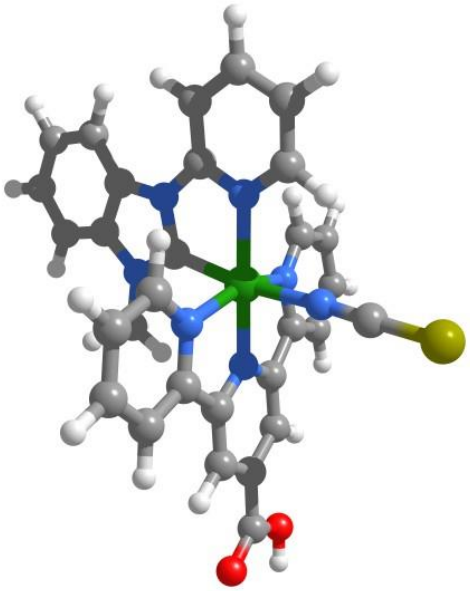
Atom	*x*	*y*	*z*
Ru	0.416035755625	−0.009565332443	0.487715294677
N	0.712014902505	−1.990484878891	−0.119548305197
N	0.817034778656	0.258067794618	−1.437247094638
N	−2.163551323743	−0.497889476360	1.741643621500
N	−0.010034314157	−0.292419518454	2.536371419541
N	0.155015060522	2.060759417293	0.321338638002
N	−2.618162865346	−0.330772257218	−0.390983413105
C	0.850673964324	1.520687752464	−1.917998810934
C	−1.603578190602	−0.287071109223	0.489619741799
C	0.459405115283	2.540820008550	−0.923972395206
C	−1.310046131876	−0.502423198205	2.856368228136
C	−3.559785378399	−0.676017229602	1.636188995009
C	3.537616199388	0.392601783208	0.936314044006
C	−4.596308278193	−0.914792225362	2.545445168710
H	−4.443238338537	−1.009303272112	3.617052600018
C	1.168882801477	−0.821405125806	−2.172705216191
C	1.229236343064	1.743839616663	−3.245346801125
H	1.267330900251	2.746369072397	−3.669806551692
C	1.097298550925	−2.095004602643	−1.428618420477
C	−0.287824496443	4.288242819502	1.081503060610
C	0.913865784252	−0.273314394251	3.519637749813
H	1.941477362631	−0.100551082884	3.200479806073
C	0.396376135113	3.909096982810	−1.195023875860
H	0.643430097400	4.282788403835	−2.189059424566
C	0.622678850939	−3.094199079343	0.637112557767
H	0.318166765704	−2.946829918941	1.674778467092
C	−0.208057265979	2.912527824774	1.291638975464
H	−0.430117272684	2.471071659059	2.264752253734
C	0.019661085601	4.794165955567	−0.182989443806
C	0.914416799170	−4.362482662941	0.137415777941
C	−1.721757173131	−0.699057767976	4.176245653815
H	−2.765347599977	−0.865616307214	4.420283301762
C	0.580903335989	−0.461324720913	4.855183915938
C	−6.153830799852	−0.924422567189	0.652591352561
H	−7.179650163593	−1.026252190578	0.293409605612
C	1.548833183349	−0.649898169990	−3.503746171827
H	1.834731090080	−1.483707798400	−4.146061709363
C	−2.520259824326	−0.165123528907	−1.832937585262
C	1.311290603699	−4.485810427240	−1.195566485798
C	−5.888496991533	−1.035918047649	2.029254959709
H	−6.714114429915	−1.223250931883	2.718591207633
C	1.401786185039	−3.338359971866	−1.985991563868
H	1.712386792077	−3.409655591450	−3.028733100151
C	1.572553800885	0.643491273766	−4.040421104379
C	−3.837006654451	−0.566055601925	0.259096269135
C	−5.126297165372	−0.686285666042	−0.259578137882
H	−5.326799272050	−0.599346700579	−1.328145007205
H	−0.582962650142	4.945574449077	1.901033897318
H	0.833786171958	−5.233594654038	0.789687647767
C	−0.759777479969	−0.677230477321	5.185427474559
H	−1.060943339284	−0.828379926765	6.224250801645
H	1.360697198981	−0.437716528121	5.617780492238
N	2.361087378357	0.226262276170	0.827049287136
S	5.107283717524	0.630538385268	1.128457376718
H	−3.120325022136	0.699429363782	−2.153122298460
H	−1.475478167228	−0.003736284224	−2.105910455203
O	2.266416038941	−0.162857202287	−6.168452559129
C	1.983388930728	0.784283635051	−5.483729697406
O	1.985731733145	2.058342451212	−5.881912426326
H	2.263448113448	2.095505858477	−6.815804067859
H	−2.895764210157	−1.066289604456	−2.339721758509
H	1.550631479050	−5.464076087533	−1.617964778035
H	−0.030594858686	5.866934824041	−0.381325148883



[A]

Table S13. Final atomic coordinates for the singly oxidized form of [**A**] in the acetonitrile phase.

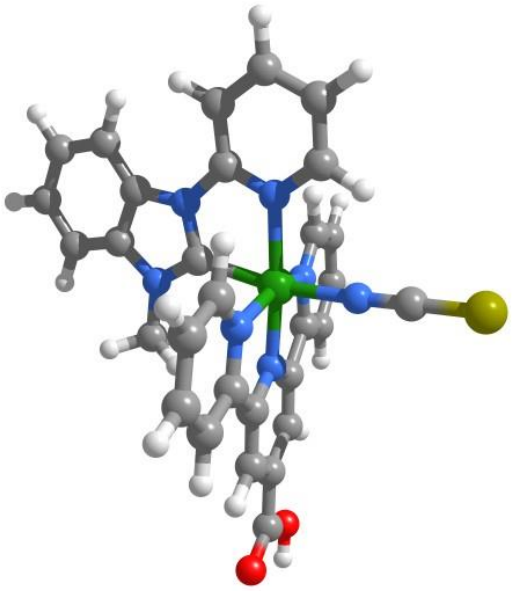
Atom	*x*	*y*	*z*
Ru	0.406429794578	−0.025053507769	0.535137876463
N	0.657647360687	−1.993745434070	−0.098706223300
N	0.820763300295	0.247306285346	−1.398182564037
N	−2.166830164287	−0.495486746936	1.786107418598
N	−0.014888944370	−0.300687120649	2.569979193232
N	0.071092642439	2.020942339533	0.339787785011
N	−2.607164610608	−0.339592664605	−0.353494521754
C	0.825996065213	1.506749316199	−1.878922336455
C	−1.604881051059	−0.303776790653	0.534734165192
C	0.386450748780	2.514036648200	−0.896349647296
C	−1.313223057170	−0.506020515517	2.897647641743
C	−3.561097309263	−0.648728842964	1.674198085536
C	3.551667810196	0.404951168100	0.958939483437
C	−4.605621432132	−0.852920006988	2.582214829392
H	−4.450908057368	−0.930356704754	3.655117795208
C	1.176787421770	−0.827534549622	−2.132046605719
C	1.203253855082	1.737409477835	−3.203195351147
H	1.208283154893	2.744650427849	−3.615694377651
C	1.073915318550	−2.102019132578	−1.397365551231
C	−0.485309506330	4.218015773802	1.092264342894
C	0.918861951090	−0.282248682464	3.542151655719
H	1.944614452475	−0.112732348825	3.216473192248
C	0.275923631961	3.877057736357	−1.167606601296
H	0.530603385297	4.259924961012	−2.155842452917
C	0.502479146570	−3.092999770400	0.653202847783
H	0.163686212094	−2.941338000194	1.678814397541
C	−0.357284902739	2.847276640768	1.305011670733
H	−0.594786134159	2.394312071449	2.268316187919
C	−0.164420305818	4.738809451175	−0.161598867874
C	0.768510089088	−4.365619942418	0.152779062654
C	−1.715174220680	−0.704463904654	4.219402321798
H	−2.755516438123	−0.876289023410	4.474644278889
C	0.594437971307	−0.467577737239	4.878278321784
C	−6.153616332036	−0.853754525541	0.680871811866
H	−7.179822893565	−0.938288648255	0.316665189364
C	1.563232569997	−0.652339564099	−3.460831614506
H	1.850862915719	−1.495465569995	−4.087950775590
C	−2.502078375045	−0.187056541089	−1.796792781338
C	1.202348093006	−4.494216433018	−1.166959191014
C	−5.897672326423	−0.953068037978	2.060597597960
H	−6.729843643075	−1.112495222681	2.749794168898
C	1.355187075728	−3.349869369357	−1.951812817337
H	1.689134196334	−3.425547838246	−2.986479404474
C	1.573837199233	0.642443756602	−3.992822737961
C	−3.828429685343	−0.547602425953	0.293942936845
C	−5.117267711166	−0.647269883104	−0.229822434082
H	−5.302347319334	−0.566474622305	−1.301516392293
H	−0.832767071781	4.857022339659	1.905329021357
H	0.633692634488	−5.234918738625	0.797876413225
C	−0.743776076044	−0.682622376632	5.217272849060
H	−1.038283446800	−0.834797537932	6.257689809692
H	1.380541208700	−0.444019814133	5.634152339549
N	2.382672573195	0.231167943916	0.850581833019
S	5.133077522493	0.652419065431	1.144725958023
H	−3.068355170592	0.699312214329	−2.116487717632
H	−1.453980481959	−0.069601851295	−2.074231292050
O	2.308738184531	−0.110838612374	−6.139691190183
C	1.984288827206	0.809643340350	−5.426658248654
O	1.946920786930	2.084362815395	−5.820624203269
H	2.223297895759	2.129824867278	−6.757651130513
H	−2.911636193529	−1.079513822556	−2.290401212977
H	1.418961844697	−5.478041417709	−1.588208044243
H	−0.256312178035	5.808516359844	−0.360392612015



[A]

Table S14. Final atomic coordinates for the doubly oxidized form of [**A**] in the acetonitrile phase.

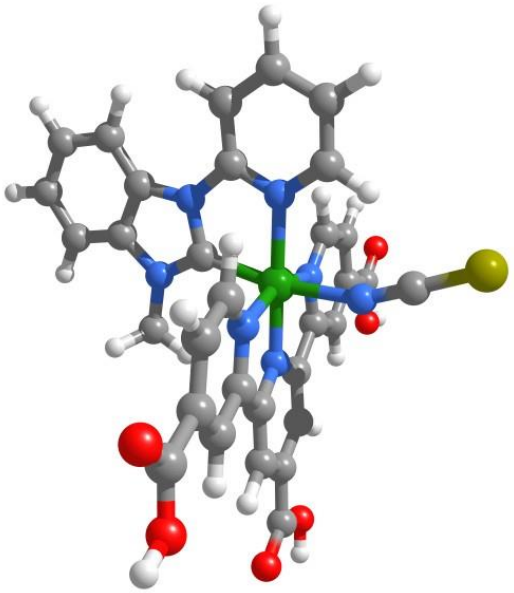
Atom	*x*	*y*	*z*
Ru	0.486133289584	−0.032083076364	0.552739782296
N	0.791554042526	−2.006843415573	−0.033694894080
N	0.795438692110	0.226807696255	−1.390814445491
N	−2.147302786431	−0.492300637179	1.730645790523
N	−0.015713643765	−0.342071863066	2.584353706829
N	0.123094473941	2.014598468029	0.389575602845
N	−2.532453097716	−0.304293838012	−0.419323738628
C	0.722110883820	1.482872680453	−1.879409240899
C	−1.557095764657	−0.310770151824	0.496781908542
C	0.330146481379	2.492651277324	−0.877773023563
C	−1.325193697368	−0.533383843203	2.866810124483
C	−3.540614215236	−0.594445272237	1.585810304961
C	3.504268428053	0.404649988821	1.219656464873
C	−4.612199202937	−0.773761198147	2.469431931744
H	−4.486865061501	−0.877058197940	3.543546587079
C	1.131071775490	−0.859115788239	−2.123127335517
C	0.998261596398	1.697947164687	−3.230030700350
H	0.944626489268	2.696374331766	−3.659992453010
C	1.122827672728	−2.121103207952	−1.358872105626
C	−0.421503746307	4.207227822032	1.151899098213
C	0.888765803109	−0.363750497935	3.584383487246
H	1.929336897033	−0.209587112986	3.307027863477
C	0.165985060212	3.846178920986	−1.158452691347
H	0.332364847709	4.220332301558	−2.168444872795
C	0.740492874026	−3.092955663254	0.748626857066
H	0.472736215101	−2.936318060868	1.794218117626
C	−0.244280295850	2.842568489393	1.375943060332
H	−0.389965262298	2.400025820067	2.362154933813
C	−0.215060068256	4.713244421416	−0.130371697934
C	1.027545169049	−4.362865054988	0.249920231608
C	−1.771001774103	−0.750175278636	4.169428060002
H	−2.820912150495	−0.910356778765	4.388270343926
C	0.518540705337	−0.571268253502	4.904923306751
C	−6.114220592902	−0.679499085201	0.531641948614
H	−7.135476710146	−0.713932472760	0.146544458222
C	1.414510083283	−0.692486404379	−3.476900020696
H	1.680944298495	−1.535852265578	−4.113256165011
C	−2.404000661952	−0.118637266549	−1.860462336342
C	1.369840950405	−4.499042112674	−1.094341702060
C	−5.891754065975	−0.813471141695	1.917430135975
H	−6.745465794642	−0.951164433025	2.584299305824
C	1.417383277713	−3.364720796332	−1.909934858970
H	1.681875048188	−3.447915801189	−2.963790033279
C	1.343733368938	0.596003739314	−4.022833672801
C	−3.773184699139	−0.466313625050	0.199959228463
C	−5.054684267858	−0.501846460882	−0.353653958383
H	−5.215034057048	−0.393049349652	−1.426592645602
H	−0.716658673399	4.851641579891	1.981023209215
H	0.979951811072	−5.223480117979	0.918379118379
C	−0.831896843289	−0.766608278564	5.197939574940
H	−1.162151169515	−0.935038279639	6.224842901696
H	1.283228392333	−0.578994350015	5.682583257142
N	2.352571355636	0.237171813909	0.937682404763
S	5.030155771137	0.623579064149	1.584431662345
H	−2.655886536513	0.917709613837	−2.126617977994
H	−1.388339339081	−0.352575606825	−2.176561881489
O	1.924204148678	−0.181294853207	−6.206941193964
C	1.644219692569	0.748948995722	−5.489841363868
O	1.563910660323	2.016437653116	−5.891888437942
H	1.766778138311	2.059234902327	−6.848203685760
H	−3.092966321251	−0.806060132947	−2.366561514931
H	1.598882613573	−5.480824369260	−1.513618218493
H	−0.348548264302	5.776972692880	−0.337124304355



[**A**]

Table S15. Final atomic coordinates for the singlet ground state (S_0) of [**B**] in the vacuum phase.

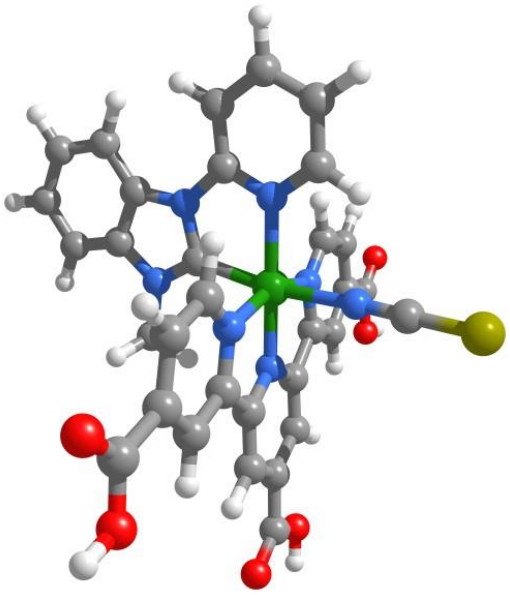
Atom	*x*	*y*	*z*
Ru	0.222708060556	−0.044205262671	0.567050343228
N	0.620313243319	−2.002216655627	0.009541300185
N	0.586566948872	0.214648915780	−1.334609810796
N	−2.317989729706	−0.513567431398	1.874778745035
N	−0.157025138083	−0.325351907310	2.635992844042
N	0.063845847890	2.020504215402	0.446011803283
N	−2.795762613871	−0.342149254348	−0.255618593902
C	0.640009604278	1.481893405004	−1.820149750609
C	−1.756824237747	−0.310869204617	0.612364985553
C	0.330084744414	2.504231460439	−0.806513394173
C	−1.452924553843	−0.533910704048	2.975125681655
C	−3.717073179647	−0.663524497383	1.784778749617
C	3.236407026444	0.381773716478	1.520738818006
C	−4.747381333828	−0.872679727764	2.705031739020
H	−4.579369414825	−0.960791770546	3.775027263515
C	0.962213630198	−0.862125966559	−2.074218373978
C	0.988318516541	1.699532298890	−3.153691208011
H	1.031052199795	2.704215416179	−3.571859245739
C	0.971365288323	−2.119268570319	−1.307974647443
C	−0.211135149314	4.257339562480	1.255571890241
C	0.779406402115	−0.316986365184	3.607862828455
H	1.807259350940	−0.141577809875	3.290503616206
C	0.323474333295	3.877255498501	−1.062199527321
H	0.538631568762	4.259334914251	−2.059164364678
C	0.637983998977	−3.090844943410	0.795317567780
H	0.366658747786	−2.933152996417	1.840298472862
C	−0.191415135170	2.880623240495	1.444981020474
H	−0.375665701383	2.437209762829	2.424676089786
C	0.048743263152	4.767560148837	−0.022171000291
C	0.992265805603	−4.347493193577	0.318925002909
C	−1.847929299919	−0.747127223592	4.298391671075
H	−2.888088839125	−0.920691219151	4.551808797044
C	0.461215227279	−0.516907855428	4.946529355631
C	−6.331134180126	−0.858531207978	0.838434371707
H	−7.362503877736	−0.938726900951	0.489650827718
C	1.311674603258	−0.692479494034	−3.411462053067
H	1.604408378785	−1.528902534008	−4.046491582063
C	−2.713699446582	−0.180804918447	−1.695217243370
C	1.346901644009	−4.484767831032	−1.028632695626
C	−6.052438772442	−0.968227910253	2.208577628732
H	−6.871426960409	−1.132329151096	2.911598244365
C	1.334901574187	−3.354601031114	−1.848565657372
H	1.618748863055	−3.441697562834	−2.896489446734
C	1.305874834647	0.597642322499	−3.960132664300
C	−4.008381998231	−0.552074231829	0.410894153766
C	−5.305743181478	−0.646437644450	−0.087131471325
H	−5.515596112142	−0.557928161473	−1.153817713286
H	−0.417711233573	4.940349193062	2.080623026632
H	1.005554533696	−5.219273586387	0.974482404916
C	−0.873105200316	−0.736941273760	5.294633122856
H	−1.160264313750	−0.900554687496	6.335411085562
H	1.254847659871	−0.499088108023	5.694500699253
N	2.229175628726	0.202769005648	0.913605366948
S	4.579124043653	0.595668695122	2.381445426890
H	−3.277923627317	0.709740905374	−2.012161874012
H	−1.666602652699	−0.066287327808	−1.982444558077
O	1.951506893817	−0.194954600730	−6.113174808925
C	1.674627359987	0.739640851090	−5.403751119897
O	1.659544256282	2.017322436186	−5.812826735380
H	1.917836983055	2.031857414567	−6.751190614863
C	0.028534591926	6.254285592776	−0.217728905945
O	−0.225393779935	7.035302092569	0.662722787798
O	0.322096140639	6.605902085191	−1.478957702994
H	0.298672026538	7.577760482886	−1.529550384587
C	1.736944951898	−5.842178088911	−1.533364614658
O	1.737485849600	−6.830099066515	−0.844906823942
O	2.083187310482	−5.821687580514	−2.829098805021
H	2.332960218447	−6.726746761474	−3.086077152526
H	−3.133085544640	−1.064577838727	−2.199590112813



[**B**]

Table S16. Final atomic coordinates for the singlet ground state (S_0) of [**B**] in the acetonitrile phase.

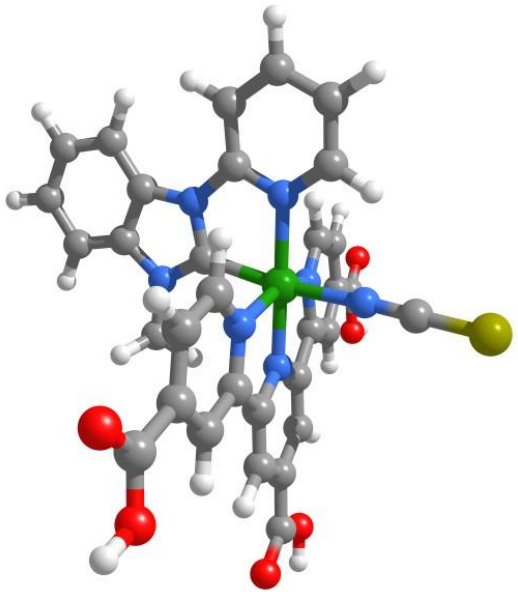
Atom	*x*	*y*	*z*
Ru	0.313034312726	0.007501646702	0.744617963194
N	0.665669833850	−1.958542680949	0.176061322714
N	0.699855811547	0.263423135171	−1.161436449920
N	−2.252470671913	−0.485003732381	1.976064909210
N	−0.117421569355	−0.272010868083	2.788445261710
N	0.133105889835	2.072494033059	0.607506165905
N	−2.672216369892	−0.314382426683	−0.167711635048
C	0.737590781766	1.526070472513	−1.652133712937
C	−1.665553940410	−0.264478355717	0.729821496204
C	0.388019057000	2.549504932709	−0.650054267546
C	−1.416393738152	−0.493518709459	3.098909610959
C	−3.640878457729	−0.671639242210	1.845271348655
C	3.518266923518	0.363698394344	1.251569472624
C	−4.690377491453	−0.912065562530	2.736476875349
H	−4.547117986343	−0.994073067583	3.810747122325
C	1.035327142017	−0.818868150041	−1.905906807357
C	1.077894128361	1.741692589863	−2.987423694353
H	1.106537020161	2.748280080320	−3.400815019445
C	0.989173692357	−2.082760738985	−1.147982665190
C	−0.276689153002	4.302855957051	1.372323005511
C	0.799004571739	−0.251572032577	3.775624832818
H	1.826902626753	−0.068821002650	3.462361506969
C	0.312979140422	3.914028385279	−0.931089420930
H	0.514194075407	4.280032060259	−1.936525770169
C	0.614535699215	−3.054357218763	0.949169325276
H	0.360986833707	−2.897405062889	1.998501358862
C	−0.184734068233	2.932108187942	1.588066999840
H	−0.368649037997	2.499287217009	2.572381248825
C	−0.026299763252	4.805217105093	0.090562402212
C	0.868845427833	−4.327003604632	0.449692424675
C	−1.835330586679	−0.707526932078	4.414710756911
H	−2.877661248395	−0.891615828188	4.653044039786
C	0.460415195313	−0.451747419694	5.107607738766
C	−6.217946869181	−0.943130571096	0.821020397925
H	−7.235996232549	−1.055281158053	0.441128374427
C	1.378467400479	−0.655142048331	−3.246177979611
H	1.641910098946	−1.504679929926	−3.875384426784
C	−2.559019986253	−0.156962501688	−1.607729830515
C	1.193002722553	−4.471624074515	−0.903629672913
C	−5.976616796659	−1.045545113996	2.200291287898
H	−6.810698782237	−1.234764005457	2.879822704245
C	1.255759382576	−3.331648853794	−1.709876307936
H	1.509020431333	−3.415882278385	−2.765392157527
C	1.389192990029	0.636121949355	−3.790987883835
C	−3.894352688286	−0.564445744684	0.462913755251
C	−5.173071531757	−0.698523460955	−0.074708585393
H	−5.347834518166	−0.616659043145	−1.148252083566
H	−0.539580841669	4.974225155576	2.190272068479
H	0.816014836276	−5.197445063653	1.104201126354
C	−0.879507874711	−0.684532446891	5.427838335584
H	−1.186983371968	−0.848979728304	6.462749779678
H	1.236626578661	−0.426133132355	5.873894428359
N	2.352463646008	0.239740943577	1.103118061366
S	5.124724166472	0.536445389836	1.468877944669
H	−3.278481682312	0.598986623083	−1.953240255966
H	−1.549835439754	0.170824057279	−1.858701174621
O	2.023231797510	−0.141300637327	−5.960629541869
C	1.746678622147	0.786916937033	−5.234538563260
O	1.725283368610	2.061829347514	−5.639147560079
H	1.966252011896	2.088107548287	−6.585956660544
C	−0.130400129048	6.279603412993	−0.143280863130
O	−0.436745407060	7.075901357580	0.714125128531
O	0.152677339233	6.620527361786	−1.405222572084
H	0.063628932218	7.590349575588	−1.489037478669
C	1.459619865091	−5.842419392559	−1.441999091387
O	1.396330990471	−6.849820680419	−0.775347633371
O	1.773833583958	−5.831580962323	−2.742011580888
H	1.932833910119	−6.753107837341	−3.027048269977
H	−2.769908145382	−1.112326794349	−2.111309236225



[B]

Table S17. Final atomic coordinates for the lowest lying singlet excited state (S_1) of [**B**] in the acetonitrile phase.

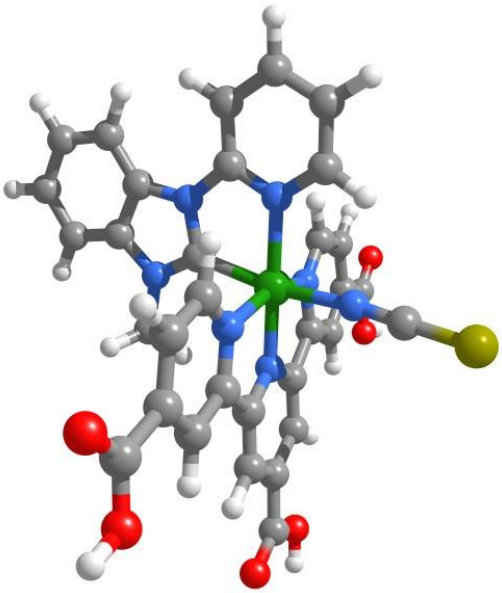
Atom	*x*	*y*	*z*
Ru	0.38927	9.29E−4	0.78608
N	0.64378	−1.97022	0.15847
N	0.77696	0.26341	−1.152
N	−2.18664	−0.47414	2.00358
N	−0.04635	−0.27628	2.82102
N	0.10123	2.05568	0.59642
N	−2.59978	−0.31002	−0.14187
C	0.79025	1.53593	−1.64399
C	−1.60332	−0.26687	0.75838
C	0.38573	2.53769	−0.66381
C	−1.34887	−0.48522	3.12788
C	−3.57563	−0.64723	1.87084
C	3.5496	0.37436	1.20444
C	−4.62984	−0.87263	2.76275
H	−4.48852	−0.95167	3.83735
C	1.10853	−0.82777	−1.90162
C	1.13986	1.75304	−2.97137
H	1.14912	2.75839	−3.38915
C	1.00955	−2.08432	−1.16593
C	−0.45981	4.26006	1.34017
C	0.86809	−0.26038	3.81083
H	1.89915	−0.08715	3.50279
C	0.2626	3.90498	−0.94025
H	0.49285	4.27879	−1.93672
C	0.48689	−3.07861	0.90977
H	0.18606	−2.9205	1.9469
C	−0.3173	2.90093	1.55983
H	−0.5347	2.45483	2.53199
C	−0.1609	4.77614	0.06041
C	0.69964	−4.34961	0.40486
C	−1.77432	−0.69021	4.4423
H	−2.819	−0.86347	4.67815
C	0.523	−0.4527	5.14207
C	−6.1523	−0.89225	0.8406
H	−7.17155	−0.99366	0.46128
C	1.46442	−0.65701	−3.23251
H	1.72834	−1.50347	−3.866
C	−2.46905	−0.15698	−1.58402
C	1.09035	−4.48788	−0.94451
C	−5.91414	−0.99266	2.2235
H	−6.75267	−1.16904	2.90085
C	1.2428	−3.34583	−1.72737
H	1.53623	−3.42724	−2.77293
C	1.48345	0.64581	−3.77798
C	−3.82554	−0.54288	0.48638
C	−5.10554	−0.66371	−0.05459
H	−5.27636	−0.58283	−1.12879
H	−0.79599	4.9203	2.13943
H	0.56908	−5.2277	1.03697
C	−0.82101	−0.67208	5.45818
H	−1.13302	−0.83	6.49266
H	1.2961	−0.43133	5.91147
N	2.37805	0.23649	1.0869
S	5.146	0.56242	1.38038
H	−3.1519	0.63174	−1.92934
H	−1.43993	0.11682	−1.82013
O	2.16511	−0.11609	−5.93614
C	1.86532	0.80295	−5.19864
O	1.84871	2.08629	−5.6072
H	2.11055	2.10159	−6.54742
C	−0.31623	6.23943	−0.18117
O	−0.69168	7.02649	0.6601
O	0.00416	6.5968	−1.43369
H	−0.12262	7.56206	−1.51562
C	1.31822	−5.85702	−1.49023
O	1.17392	−6.87239	−0.84497
O	1.70113	−5.8487	−2.7756
H	1.8281	−6.77496	−3.05966
H	−2.72657	−1.10323	−2.08162



[**B**]

Table S18. Final atomic coordinates for the singly oxidized form of [**B**] in the vacuum phase.

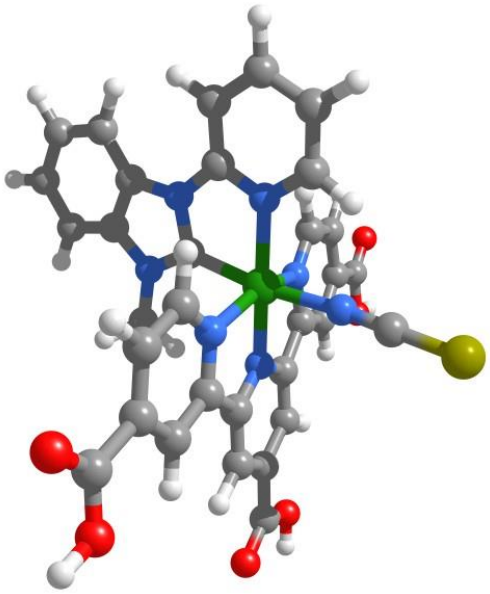
Atom	*x*	*y*	*z*
Ru	0.305978062527	−0.026669351687	0.647310892771
N	0.586181645933	−2.007865225032	0.038918123850
N	0.709310061594	0.239410828664	−1.277103065513
N	−2.271065971986	−0.519456322005	1.905103110281
N	−0.118090210149	−0.302106158857	2.697721546061
N	0.054825645077	2.044127298163	0.481151629393
N	−2.728376818942	−0.360011190546	−0.227520135902
C	0.753681765063	1.501771035020	−1.757056194432
C	−1.714321920391	−0.303695099191	0.652819026982
C	0.366040012577	2.522714958089	−0.763102918295
C	−1.417778740110	−0.509474529734	3.020214967227
C	−3.664423512485	−0.718550115766	1.799949670405
C	3.439796565423	0.319937522705	1.048112821928
C	−4.695854074944	−0.978575746652	2.709143654396
H	−4.539869190438	−1.076589917018	3.780004387373
C	1.056214770508	−0.841154476562	−2.012735118672
C	1.137523857135	1.724053583340	−3.082944177537
H	1.183001360102	2.727406371830	−3.504957161536
C	0.971939688558	−2.113887154979	−1.269843015259
C	−0.390617672550	4.270971440550	1.237445106061
C	0.806172488362	−0.271275035760	3.680363204286
H	1.833519634013	−0.101714001394	3.358542911359
C	0.311974307127	3.889943364504	−1.036803394824
H	0.565074361780	4.275148032283	−2.023999191030
C	0.478966366446	−3.113206055002	0.792902378238
H	0.175003763951	−2.965204122133	1.830463482070
C	−0.313391564182	2.897676375186	1.449594357442
H	−0.541985253610	2.458079661583	2.421845463184
C	−0.070721035476	4.776997536582	−0.026299256309
C	0.751241133966	−4.381912000959	0.289644764709
C	−1.829898717678	−0.686605822575	4.342605234861
H	−2.874226592138	−0.844090533956	4.589551788563
C	0.473395941232	−0.443671096041	5.018040660259
C	−6.253919678180	−1.009518585529	0.816924446059
H	−7.278076734822	−1.127991960567	0.458121694824
C	1.441508652702	−0.671923128211	−3.342528201241
H	1.723311570906	−1.508337691654	−3.983417332123
C	−2.632465940698	−0.192999904918	−1.669414120076
C	1.152364217117	−4.507061413934	−1.044068673913
C	−5.985937850641	−1.120451126480	2.193223817369
H	−6.807728678341	−1.324786437523	2.882280857100
C	1.263311649256	−3.357385331857	−1.831594609054
H	1.577742880479	−3.442999334669	−2.871282131704
C	1.475606497629	0.621824777249	−3.878060416590
C	−3.943753632531	−0.611887092516	0.422967121970
C	−5.231140610426	−0.752607527975	−0.095386966449
H	−5.433650198242	−0.668148273640	−1.163765569923
H	−0.689760124335	4.953611869713	2.034970426660
H	0.662178899752	−5.272519527963	0.914430015882
C	−0.867594191460	−0.652970326282	5.351235540735
H	−1.168949740837	−0.788931056923	6.392103097142
H	1.253237033627	−0.411732520035	5.780282816516
N	2.255866329109	0.186463007950	0.982060659985
S	5.023521622892	0.507309043461	1.167122871601
H	−3.253622177763	0.656095418691	−1.990594529757
H	−1.591675843931	−0.004612981861	−1.940707820236
O	2.169888583953	−0.187600207786	−6.004686112721
C	1.891251389199	0.760931852259	−5.320121656856
O	1.902957673344	2.035234531655	−5.717237949237
H	2.183055227671	2.071171417858	−6.650461397302
C	−0.154277248908	6.266708647934	−0.243247718019
O	−0.512476137662	7.026227992166	0.615874584815
O	0.212367248346	6.611079952934	−1.481285014684
H	0.145352366324	7.579864000961	−1.568487861520
C	1.449279419300	−5.886025773782	−1.576940355748
O	1.326562869191	−6.876881175972	−0.908666424396
O	1.852410326333	−5.850042606198	−2.849882646166
H	2.037688383727	−6.760053061355	−3.146708512465
H	−2.984632089366	−1.103312933524	−2.176706138062



[**B**]

Table S19. Final atomic coordinates for the singly oxidized form of [**B**] in the acetonitrile phase.

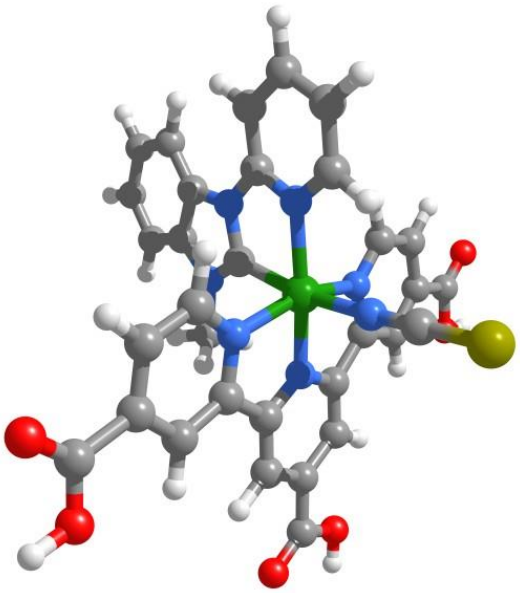
Atom	*x*	*y*	*z*
Ru	0.325991270938	−0.040586123463	0.695197195899
N	0.563178107504	−2.011744790653	0.064049156414
N	0.744500954237	0.227746056892	−1.235780319999
N	−2.250789101129	−0.512825185444	1.940593473582
N	−0.100549137710	−0.315828008242	2.729676279968
N	0.009578938921	2.008677927215	0.501259532995
N	−2.689747532784	−0.347907513711	−0.198758442359
C	0.761065080246	1.486274009174	−1.718086080407
C	−1.688952725092	−0.311503895970	0.690812178398
C	0.328024792596	2.496016173850	−0.735578676887
C	−1.398998709696	−0.524773371009	3.053892048779
C	−3.643571648769	−0.675395215447	1.826152920269
C	3.477274219858	0.324431680037	1.082685957371
C	−4.687650501496	−0.893022366305	2.731783092620
H	−4.533902474808	−0.975008955812	3.804430314220
C	1.091114524821	−0.849258679197	−1.970288025649
C	1.139430972640	1.713970372191	−3.042412622961
H	1.152740810347	2.721233842829	−3.454841402721
C	0.976110397678	−2.121684217876	−1.234697678011
C	−0.538151899840	4.208012852390	1.248247890583
C	0.831207228039	−0.297725397927	3.703642416188
H	1.857286561415	−0.125217451695	3.380455321984
C	0.226574305545	3.857837395710	−1.012482573203
H	0.484586443456	4.238349880003	−1.999338450877
C	0.396154881089	−3.109953505790	0.814735627317
H	0.061349303202	−2.958933529206	1.841406199038
C	−0.414991718961	2.839169826938	1.464584185068
H	−0.654336432772	2.392081545560	2.429919354007
C	−0.212569848291	4.725383745311	−0.008250770058
C	0.644312066711	−4.383201163051	0.312159602933
C	−1.803170942139	−0.728335303534	4.374022954666
H	−2.843565685034	−0.903201590771	4.626730416932
C	0.504460742547	−0.487970706796	5.038546528890
C	−6.232879893057	−0.896931423337	0.828041709227
H	−7.257839082135	−0.988770077118	0.462119409275
C	1.478088115822	−0.678474917761	−3.299454364843
H	1.757487282023	−1.524685275068	−3.926242141312
C	−2.585424180337	−0.187457049560	−1.641460695584
C	1.077578599126	−4.515259940366	−1.009686017485
C	−5.977843417121	−1.001338811540	2.207772595436
H	−6.809531148656	−1.171766806906	2.894903297098
C	1.244313779113	−3.369824214292	−1.793428054908
H	1.576986698036	−3.448694136960	−2.827001501871
C	1.499575784050	0.615647044361	−3.832192985553
C	−3.910074385505	−0.568733899160	0.446102085031
C	−5.197408090265	−0.676605814304	−0.080060429816
H	−5.381440889520	−0.592244710524	−1.151635045311
H	−0.882800351833	4.862377740135	2.049290304409
H	0.503006249399	−5.260442624474	0.943683483487
C	−0.833822419902	−0.707546461510	5.373992705796
H	−1.130193279581	−0.863981641068	6.413243849988
H	1.288988869449	−0.464873706404	5.796060677139
N	2.300008032964	0.185796351221	1.016108518368
S	5.070740853751	0.520382152679	1.200263330607
H	−3.188563265065	0.674590126420	−1.959695113879
H	−1.542886712206	−0.021383045652	−1.914764853342
O	2.222528767753	−0.146748128225	−5.979185993993
C	1.908421475751	0.777933137919	−5.267408742921
O	1.881917864107	2.052635193445	−5.661463155778
H	2.156337866137	2.095541336599	−6.599274099363
C	−0.347965526076	6.203011975769	−0.238949520951
O	−0.736927265198	6.975070098617	0.604623328757
O	0.010013015497	6.558732128287	−1.474443883954
H	−0.100284594298	7.526317131067	−1.565275915170
C	1.345996525765	−5.891930755972	−1.545888017113
O	1.187577320851	−6.899042124778	−0.898041053536
O	1.777312106235	−5.871096397826	−2.808623768138
H	1.933560789468	−6.791950479612	−3.099437306894
H	−2.954192533689	−1.095173603735	−2.139567077055



[B]

Table S20. Final atomic coordinates for the doubly oxidized form of [**B**] in the acetonitrile phase.

Atom	*x*	*y*	*z*
Ru	0.418389472430	−0.057592800292	0.690898648932
N	0.709136175416	−2.033898002529	0.094626498281
N	0.712188751940	0.207983440211	−1.253705074771
N	−2.225040988160	−0.470984324731	1.855480461609
N	−0.095627974485	−0.368644674849	2.720586753489
N	0.081698438577	1.999934550944	0.541442170559
N	−2.582043210714	−0.314468679983	−0.304118352608
C	0.648651449381	1.465463199004	−1.737164610315
C	−1.619436392934	−0.316084293079	0.627132497509
C	0.274831170852	2.475028648907	−0.727839510420
C	−1.411414597803	−0.519427618581	2.998790865318
C	−3.615632456592	−0.558145957569	1.695099116722
C	3.438883547682	0.379093114995	1.346719075495
C	−4.695339790895	−0.710599578935	2.574234326360
H	−4.577398400041	−0.797796250859	3.650592154048
C	1.027674527467	−0.876640602804	−1.994778690225
C	0.915096338841	1.684824518290	−3.089042722588
H	0.870331357488	2.686114102949	−3.513391098101
C	1.013866846148	−2.142640819789	−1.235967100891
C	−0.438172443315	4.194732657945	1.310082191588
C	0.804177933214	−0.412518682199	3.723468401904
H	1.850472657921	−0.294632436155	3.449125088957
C	0.112692741587	3.827762178006	−1.010948713107
H	0.265181606271	4.200654964264	−2.022298465839
C	0.656398173071	−3.123151353505	0.871361005754
H	0.411725595988	−2.971166677440	1.923154799020
C	−0.263912060872	2.830548008166	1.532615764935
H	−0.397801687560	2.392501531041	2.522283151929
C	−0.251091279592	4.698810470271	0.022245904551
C	0.909342627919	−4.393434169132	0.358887096275
C	−1.869772354024	−0.708371363844	4.300885760123
H	−2.925285661230	−0.831087801536	4.516796675351
C	0.421850957446	−0.598472593819	5.044276981136
C	−6.180331265640	−0.629639474103	0.624634564158
H	−7.198964840238	−0.657220606324	0.232158890876
C	1.300592362066	−0.708565276258	−3.350261805342
H	1.552387436018	−1.551482500038	−3.993103175934
C	−2.391799831620	−0.170167023664	−1.746263320604
C	1.222069296867	−4.526383608180	−0.994618029009
C	−5.970617666801	−0.744138340782	2.014938804369
H	−6.831073469735	−0.860384594261	2.677145264248
C	1.276259198389	−3.385478295092	−1.803693354618
H	1.519145666789	−3.467529218890	−2.861648087457
C	1.240245151985	0.582971441188	−3.890052739166
C	−3.832746328336	−0.449912950963	0.302196193621
C	−5.113844498185	−0.479371884090	−0.255892962691
H	−5.272682444449	−0.385593497946	−1.330254476410
H	−0.717407958691	4.853319411333	2.132823862390
H	0.861416064696	−5.266699822838	1.009845336475
C	−0.935272831716	−0.745301045882	5.333591837959
H	−1.274836559259	−0.892508668869	6.360707973808
H	1.182850212520	−0.626158848744	5.825101992532
N	2.285810028136	0.199829285374	1.076222719814
S	4.961603705579	0.621014897389	1.707660632797
H	−2.194926308956	0.880498937865	−1.999073951898
H	−1.568615009527	−0.809684128160	−2.077174332085
O	1.795800766791	−0.192538497993	−6.080446703720
C	1.531356310059	0.738625202629	−5.358936479582
O	1.460632579025	2.008117894871	−5.754964583595
H	1.655654595448	2.053805811421	−6.712767314617
C	−0.449647593118	6.170174602752	−0.213975266660
O	−0.743789237205	6.946949108610	0.662147855061
O	−0.264946357934	6.506369324836	−1.490986750048
H	−0.405235448278	7.469974209748	−1.586271666871
C	1.486140764523	−5.901093910810	−1.543615331033
O	1.422767054445	−6.903988061591	−0.874411035918
O	1.792452412936	−5.876752839417	−2.841162373316
H	1.951443968691	−6.793557066869	−3.143871102778
H	−3.303057210181	−0.498753141662	−2.256034769497



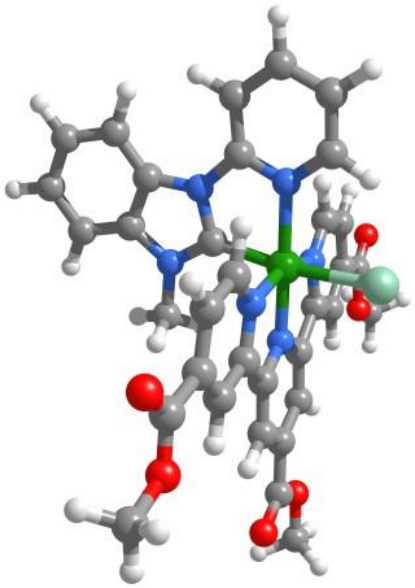
[B]

Table S21. Final atomic coordinates for the ground state of

KSCN				KCl			
Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
N	0.000000013014	−0.000000000429	−3.386792286082	Cl	0.000000000000	0.000000000000	−1.456602995093
C	−0.000000009279	0.000000001053	−2.210740968563	K	0.000000000000	0.000000000000	1.320728563205
S	−0.000000020483	−0.000000000820	−0.552212272659				
K	0.000000016748	0.000000000195	2.344879097000				

Table S22. Final atomic coordinates for the ground state of [**3**]/[**4**].

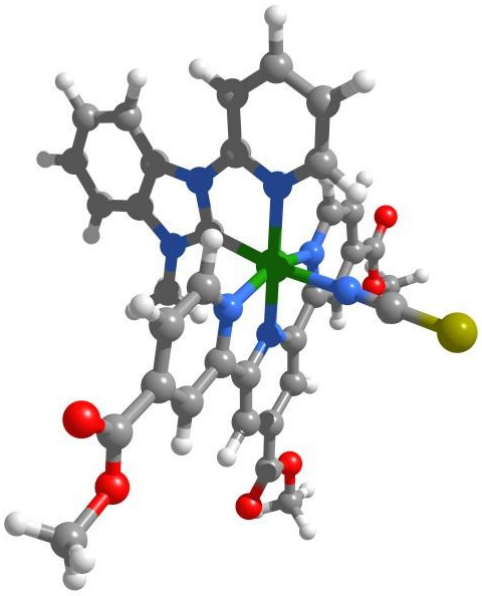
Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
Ru	0.412442700454	−0.030249800278	0.986935245060	C	0.249380092719	7.952897719114	−1.542983355348
N	0.731442175584	−2.002661439518	0.431738537637	H	0.941304148619	8.536440530772	−0.918270441809
N	0.792114495940	0.207163948641	−0.916376973761	H	0.539093041237	8.014804116650	−2.598038274182
N	−2.144853338920	−0.580209309661	2.190094834292	H	−0.773616539131	8.331173180202	−1.401624798583
N	−0.035444090973	−0.290960021093	3.039470281419	C	2.095107870373	2.197109821600	−6.798175517602
N	0.247640602231	2.029916072542	0.840122542266	H	2.029644239564	3.282258729893	−6.936326323164
N	−2.520979766703	−0.403144099621	0.036705973090	H	3.109433249907	1.839688894168	−7.028241669258
C	0.846671741140	1.466370006078	−1.415795978867	H	1.373158712824	1.681804388118	−7.448411447275
C	−1.541472582904	−0.318738942251	0.962648530608	C	1.895487426554	−7.193407798549	−3.097498696389
C	0.513976398130	2.499263638763	−0.418656831458	H	2.095982468620	−6.984901203263	−4.154466950026
C	−1.335153136842	−0.536305455069	3.330557880829	H	2.757811782147	−7.693861287238	−2.633141638149
C	−3.513639201055	−0.855484059198	2.020015091176	H	1.005988557782	−7.831450665334	−2.992037850288
C	−4.557223529656	−1.194119059112	2.885193502079				
H	−4.423718929458	−1.298358333576	3.958858006021				
C	1.096708850069	−0.884300099836	−1.660350820116				
C	1.175379725578	1.668659722999	−2.756142202436				
H	1.216763664792	2.671231620121	−3.178564686605				
C	1.033926122693	−2.143111107987	−0.895879208991				
C	−0.167981061927	4.267398170424	1.583553184070				
C	0.857324452440	−0.218843388112	4.045797392305				
H	1.885136560823	−0.020533407162	3.737025571163				
C	0.449767153416	3.862185508669	−0.708664505712				
H	0.662257784353	4.222298128444	−1.714032759867				
C	0.652659277399	−3.093550866035	1.209896958744				
H	0.411427967019	−2.923246912326	2.260381262346				
C	−0.082189092771	2.897730385725	1.810185819297				
H	−0.282734025141	2.470695180893	2.794041371750				
C	0.102229659290	4.762382187619	0.302294483591				
C	0.862981623386	−4.375729981657	0.712935645075				
C	−1.782930387200	−0.709911474351	4.642058317573				
H	−2.829769043911	−0.893401694269	4.861205295145				
C	0.491768021241	−0.386746121361	5.376140540496				
C	−6.039766182940	−1.298152546858	0.939885637283				
H	−7.038152327509	−1.478538878711	0.535351471456				
C	1.426273924185	−0.733833016594	−3.005509128432				
H	1.664975027853	−1.591130698447	−3.634114507996				
C	−2.340100956453	−0.212248637799	−1.395577137204				
C	1.167963778719	−4.536653698527	−0.643361186227				
C	−5.820010138253	−1.411459708657	2.321785609856				
H	−6.649952481082	−1.679064583928	2.979375326550				
C	1.255946858025	−3.401644322817	−1.454782629431				
H	1.491545651660	−3.501634450277	−2.513091706811				
C	1.455068037487	0.553759903259	−3.558988024647				
C	−3.741791032329	−0.742883948984	0.632249933384				
C	−4.998185895370	−0.962500282071	0.069778718757				
H	−5.162400595853	−0.882040837020	−1.005382004369				
H	−0.441894659068	4.945817586569	2.391971080553				
H	0.789555216745	−5.242980872732	1.369573264900				
C	−0.850712716988	−0.634254750334	5.675485967111				
H	−1.178607730859	−0.766049443368	6.708775611519				
H	1.249080932248	−0.320293076348	6.158605472027				
H	−3.308992709405	0.026264736629	−1.849273273588				
H	−1.660911254569	0.627216289863	−1.572439476484				
O	2.054748621415	−0.257386679374	−5.725512216170				
C	1.797421961296	0.686742278366	−5.009342056108				
O	1.782982629084	1.955023198368	−5.418419787215				
C	0.003242263172	6.236843274391	0.057995272283				
O	−0.326762440341	7.035311336586	0.907717538362				
O	0.317260277507	6.562008509302	−1.195393407712				
C	1.386276591575	−5.919426846782	−1.177405115568				
O	1.310465634040	−6.918714168493	−0.496084676763				
O	1.669111430959	−5.917966647352	−2.479288863795				
H	−1.935778485142	−1.122014091224	−1.863242567984				
Cl	2.850712799638	0.222497409652	1.395928878728				



[**3**]/[**4**]

Table S23. Final atomic coordinates for the ground state of [**7**]/[**8**].

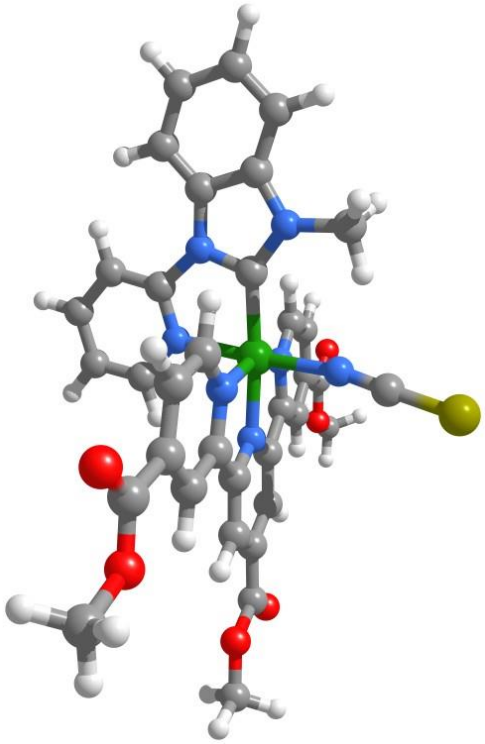
Atom	*x*	*y*	*z*
Ru	0.196155303753	−0.080907077174	0.913029430301
N	0.542248521181	−2.050332282313	0.352625820146
N	0.590186603327	0.165848519410	−0.994621493869
N	−2.362883130451	−0.590761012441	2.146848060931
N	−0.230346036043	−0.347604029452	2.958252869494
N	0.005323132215	1.982197396134	0.762120932186
N	−2.788860534521	−0.424882667742	0.004627626298
C	0.637986774631	1.426557863961	−1.488358418638
C	−1.780822816074	−0.362047172621	0.899825582124
C	0.279889490222	2.454053807682	−0.493488126088
C	−1.529171566622	−0.568136932463	3.270640268729
C	−3.746931224113	−0.809517728661	2.017858268290
C	3.400058351364	0.292596860334	1.412037024447
C	−4.785643363572	−1.091826563122	2.909184813407
H	−4.636469291890	−1.193537335859	3.980867925040
C	0.928473151627	−0.919923611676	−1.731816064732
C	0.992078213912	1.636910683824	−2.821217482484
H	1.029142993842	2.640579687604	−3.241311523038
C	0.868484302715	−2.181330550697	−0.970497576310
C	−0.431314040388	4.215973651998	1.504052890154
C	0.683519263754	−0.304751014869	3.947672940439
H	1.711281876417	−0.125370294490	3.632571512223
C	0.210947272958	3.816896118924	−0.782311354448
H	0.433054172222	4.180296608622	−1.784350819532
C	0.470671302266	−3.144874707835	1.125980055613
H	0.213496563460	−2.982887747463	2.173929024835
C	−0.339064630110	2.846232199133	1.729906135726
H	−0.544177864745	2.417712046677	2.712168158017
C	−0.150487324577	4.713802226792	0.226721227766
C	0.708182889984	−4.422040430721	0.627848705787
C	−1.953738922595	−0.743721784950	4.589822985050
H	−2.998909932206	−0.908714862799	4.829449913892
C	0.340962919874	−0.476293650295	5.283022407586
C	−6.317396719261	−1.142478349549	0.997267830700
H	−7.333015645307	−1.277640901006	0.618889200274
C	1.285362639965	−0.761474752586	−3.069593093897
H	1.551785422921	−1.613171368318	−3.694621241024
C	−2.683174035698	−0.260619301504	−1.436044550739
C	1.035281152212	−4.573432933507	−0.724080208152
C	−6.069510152968	−1.254430205037	2.374775296230
H	−6.895581447105	−1.476734044712	3.053811020845
C	1.118412486974	−3.434304528657	−1.530081151600
H	1.372584066983	−3.526924569064	−2.584749795858
C	1.306165414310	0.527831546901	−3.619026472315
C	−4.005485774464	−0.700628256336	0.636889680553
C	−5.281412403220	−0.863282450392	0.100924948236
H	−5.461942454199	−0.778986777756	−0.971432263693
H	−0.715725818993	4.891766579907	2.311009497838
H	0.639044188441	−5.292369913255	1.280852081237
C	−1.000925257967	−0.696809822436	5.605582828973
H	−1.311849931289	−0.831058239862	6.643722333954
H	1.114701130265	−0.433719278328	6.050790130524
N	2.235987655902	0.159401876144	1.266438210561
S	5.008376282167	0.477539631837	1.627896664385
H	−3.405752583196	0.495860914632	−1.773751695380
H	−1.675388506832	0.069691747301	−1.689985876094
O	1.963419659643	−0.267811448318	−5.774779346643
C	1.679608631949	0.670849227088	−5.061742778636
O	1.656531652830	1.939867623123	−5.466047430469
C	−0.249951518770	6.189120893150	−0.015678517802
O	−0.598788951320	6.983186523270	0.830516441923
O	0.087074938134	6.518487194597	−1.261370940240
C	1.281547020735	−5.951110732272	−1.260120584519
O	1.213259642820	−6.953124422719	−0.582089246615
O	1.580632034092	−5.940443144519	−2.557861068494
H	−2.895284395251	−1.214398803811	−1.941758734202
C	0.023017453932	7.910521396499	−1.606312236667
H	0.701021966708	8.493284023024	−0.965870300426
H	0.333473702002	7.976372177302	−2.655159449504
H	−1.003353054763	8.286081419767	−1.483688781916
C	1.996532395142	2.192299743754	−6.837702457113
H	1.297835460385	1.668179831639	−7.505937273900
H	1.917750591944	3.276797858962	−6.973492896617
H	3.021137838955	1.850765646505	−7.045137660550
C	1.835046162294	−7.209937991420	−3.177915294972
H	2.049205955288	−6.994095860963	−4.230676643801
H	2.696668121399	−7.700253731137	−2.701681453731
H	0.953138072045	−7.860939827155	−3.089024394131



[**7**]/[**8**]

Table S24. Final atomic coordinates for the ground state of Isomer-[**7**]/[**8**].

Atom	*x*	*y*	*z*
Ru	0.175796404237	0.174501066896	0.643688704447
N	0.586621130757	1.998921498405	−0.260997551217
N	0.126113163951	−0.341867261030	−1.301856771117
N	−1.223534223659	1.136728615501	2.982104287320
N	−1.835884658669	0.666981629178	0.817516174814
N	−0.296867705540	−1.844065804558	0.782058840073
N	0.843550404261	0.870848241582	3.652583790678
C	−0.109814936048	−1.630966424188	−1.614294637742
C	0.051047822963	0.736226409819	2.568209797956
C	−0.377319039563	−2.477080574962	−0.431380071093
C	−2.250286180028	1.092655028972	2.036993073464
C	−1.212974232652	1.524510408382	4.335145024811
C	3.260863454154	−0.611179081552	0.302486107244
C	−2.173147484714	2.000401073919	5.231665745286
H	−3.213880315174	2.156338827950	4.959388146380
C	0.411009743861	0.602359950834	−2.220367509448
C	−0.089909050023	−2.033040478797	−2.951538811370
H	−0.278878222333	−3.066182698379	−3.237398523738
C	0.652835412858	1.935489747987	−1.628966814446
C	−0.883237807496	−3.891217210242	1.881058482770
C	−2.732225794452	0.576818902784	−0.184479734643
H	−2.349766737467	0.230767929697	−1.144801873783
C	−0.707838426528	−3.828900272526	−0.518654308458
H	−0.769395044253	−4.319656823695	−1.488569845383
C	0.780544487361	3.179222370477	0.350426553044
H	0.717645256580	3.177636383864	1.439216416441
C	−0.545885391468	−2.541667498994	1.902782832371
H	−0.469278581002	−1.993793589840	2.842522678365
C	−0.965816484726	−4.550390133389	0.650855224004
C	1.051715741724	4.347652198196	−0.354617565693
C	−3.582348779344	1.436951213381	2.281072479200
H	−3.906021955289	1.773027237250	3.260626795976
C	−4.071989976168	0.902024509276	−0.018738614269
C	−0.423277877098	2.104510768520	6.943397858509
H	−0.135432947280	2.338061412337	7.970863409948
C	0.445773715870	0.258327511263	−3.572116263684
H	0.670827807512	0.989224392983	−4.348210490858
C	2.265192049632	0.571689762942	3.713186195640
C	1.125567309264	4.296954184427	−1.750009938157
C	−1.754737428870	2.285554934696	6.537630262385
H	−2.490069793239	2.658527298472	7.253995682052
C	0.921822564763	3.071494683379	−2.391294742433
H	0.971791915140	3.008673517812	−3.477063885636
C	0.188033446046	−1.071371653422	−3.933645714576
C	0.122221010298	1.347286755696	4.751583096024
C	0.541966471267	1.629308271336	6.049696602875
H	1.579659637587	1.485392960339	6.353813970081
H	−1.079442669669	−4.426928425172	2.810132587814
H	1.205637118686	5.288781358145	0.173926296239
C	−4.500350905155	1.338558664420	1.237826052267
H	−5.545639546481	1.602121017390	1.411748131666
H	−4.759511593128	0.812099561477	−0.860665366555
N	2.156162538514	−0.292332733197	0.568593654968
S	4.800958184676	−1.044623106254	−0.028154212352
H	2.449812268907	−0.206890684323	4.468452166295
H	2.588812032991	0.220528287207	2.730457347809
O	0.463298356838	−0.612345250722	−6.263811974745
C	0.226082898837	−1.419712548363	−5.391349739982
O	−0.029856029380	−2.707824202895	−5.609392908522
C	−1.329741936023	−6.003672809305	0.631678131971
O	−1.555299834074	−6.647561676243	1.633165920867
O	−1.376584908091	−6.495356291558	−0.604844561091
C	1.420489119701	5.556198768063	−2.506541594550
O	1.619444218925	6.624453199389	−1.970233764769
O	1.437983065163	5.361103293801	−3.823835352429
H	2.824664962127	1.477968320251	3.989345301695
C	1.717118711348	6.503980212690	−4.646914507129
H	2.709563523107	6.912403878374	−4.406607003178
H	1.689498946425	6.144610926459	−5.681710676379
H	0.956819955564	7.282597559599	−4.487919403571
C	−0.021198428410	−3.152312526838	−6.974448551860
H	−0.248910315731	−4.223709492429	−6.944045682939
H	−0.782818369206	−2.611936287977	−7.555406075508
H	0.967372699669	−2.980616355018	−7.424546811041
C	−1.716243917461	−7.883619611716	−0.740888025103
H	−2.719533292737	−8.071661656944	−0.331419051170
H	−1.693219215731	−8.096046328908	−1.815572088902
H	−0.984904917609	−8.508459472353	−0.207843135866



Isomer-[**7**]/[**8**]

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