In depth study of the electronic properties of NIR emissive κ^3N terpyridine rhenium(I) dicarbonyl complexes

Thomas Auvray,[a] Benedetta Del Secco,[b] Amélie Dubreuil,[a] Nelsi Zaccheroni,[b*] and Garry S. Hanan[a,*]

[a] Département de Chimie, Université de Montréal, Montréal, Canada, H2V-0B3
[b] Dipartimento di Chimica 'G. Ciamician', Università degli Studi di Bologna, Via S. Giacomo 11, 40126 Bologna, Italy

Supporting Information

Experimental Section

Physical measurements

^{1}H and ^{13}C NMR spectra were acquired on a Bruker AV400 (400MHz). Chemical shifts are reported in part per million (ppm) relative to the residual proton (1.94 ppm for CD_3CN, 2.05 ppm for acetone-d^6, 2.50 ppm for DMSO-d^6) or carbon resonances (39.52 ppm for DMSO-d^6) of the solvent. ESI-MS measurements were made on a Bruker Daltonics MicrOTOF II. Infra-red vibration spectroscopy measurements were conducted on a Perkin-Elmer Spectrum2 in ATR mode. Electrochemical measurements involved a three-electrode set-up with a glassy carbon disk (d=3mm) working electrode, a platinum coil as counter electrode and a platinum wire as pseudo-reference. Measurements were made using a SP-50 BioLogic potentiostat interfaced to a computer equipped with the EC-lab software V11.21. The potentials were referenced internally using the ferrocenium/ferrocene couple in DMF (0.45 V *vs*. ECS). The concentration of analyte was approximatively 1 mM while the supporting electrolyte (tetrabutylammonium hexafluorophosphate TBAP) was at 0.1 M.

Photophysical characterization

All photophysical measurements were carried out in deaerated solutions (acetonitrile). Absorption spectra were measured on an Agilent Cary6000i UV-Vis-NIR spectrophotometer or on a UV/Vis Perkin Elmer Lambda-45. All the luminescence spectra were recorded at room temperature on a Perkin-Elmer LS55 fluorescence spectrometer or, for the NIR emitters, on an Edinburgh FLS920 spectrometer (450 W Xe lamp) equipped with an Edinburgh Instruments Ge detector (800-1600 nm spectral

range). All spectra were corrected for the Ge-detector response. Emission quantum yields[1] were obtained using as standard [Re(bpy)$(CO)_3$Cl] in DCM (Φ = 0.005) for visible emitters and IR125 in DMSO (Φ = 0.23) for NIR emitters.[2] Luminescence lifetimes were measured with an Edinburgh FLS920 equipped photomultiplier Hamamatsu R928P and connected to a PCS900 PC card for the TCSPC experiments.

Computational studies

The singlet ground state geometries of the complexes were optimized by DFT method with the PBE0 hybrid functional[3] without symmetry constraints using Gaussian16 Rev. A03.[4] The lowest triplet excited state T_1 geometries were also optimized in the case of the complexes. All elements were assigned the LANL2DZ basis set.[5-8] Frequency calculations were performed to ensure that local minima had been reached and get a model of the IR spectra. The absorption and emission properties were modelled by time dependent DFT (TD-DFT). All calculations were made for acetonitrile solution using a conductor-like polarizable continuum model (CPCM).[9] The results were visualized and tabulated using Gaussview6.0, GaussSum3.0[10] and Chemissian4.53[11].

Materials

$Re_2(CO)_{10}$ was obtained from Pressure Chemical and converted to $Re(CO)_5Br$ via titration with bromine.[12] Solvents were of ACS or spectroscopic grade (for absorption and emission measurements) and used as received, like other reagents, from commercial sources (Millipore Sigma or Fisher Scientific). Acetonitrile for electrochemistry was distilled from CaH_2 and stored under N_2. The ligands **La-e** were prepared following published procedures.[13-15] Complexes **1a**, **1e**, **2a**, **2e**, **3a**, **3e** and **4a** were prepared as previously reported and their spectra matched the literature.[16-18]

Synthetic procedures

All the complexes are hygroscopic and were thus stored in a desiccator with freshly activated $CaSO_4$ (Drierite) and covered with aluminium foil.

Complexes **1a-e** were prepared via the typical Re diimine complex synthesis. $Re(CO)_5Br$ and the desired ligand were combined in a 1:1.05 molar ratio in toluene and refluxed for 4 h (Typical scale: 0.5 mmol in 75 mL). The desired neutral complex, [$Re(CO)_3Br(\kappa^2$N-

tpy)], which precipitated during the reaction, was filtered, washed with cold toluene then diethyl ether and finally air dried. Further drying at 100°C overnight was conducted before storage in a desiccator.

1a *fac*-[Re(CO)$_3$Br(κ^2N-*La*)] Y=94% (550 mg, 1mmol scale) yellow solid. ^{1}H NMR (400 MHz, CD_3CN) δ 9.08 (d, J = 6 Hz, 1H), 8.78 (d, J = 5 Hz, 1H), 8.50 (t, J = 8 Hz, 2H) 8.28 (t, J = 8 Hz, 1H), 8.21 (td, J = 8, 2 Hz, 1H), 7.97 (td, J = 8, 2 Hz, 1H), 7.78 (t, J = 7 Hz, 2H), 7.63 (ddd, J = 8, 6, 2 Hz, 1H), 7.55 (ddd, J = 8, 5, 2 Hz, 1H) ; ESI-MS (MeCN): Calculated 504.0352 for $[M -Br]^+$, Observed 504.0342

1b *fac*-[Re(CO)$_3$Br(κ^2N-*Lb*)] Y=88% (275 mg) yellow solid.; ^{1}H NMR (400 MHz, CD_3CN) δ 8.89 (d, J = 6 Hz, 1H), 8.60 (d, J = 5 Hz, 1H), 8.35(d, J = 6 Hz, 2H), 7.62 (s, 2H), 7.45 (d, J = 5 Hz, 1H), 7.37 (d, J = 6 Hz, 1H), 2.60 (s, 3H), 2.58 (s, 3H), 2.44 (s, 3H) ; ^{13}C NMR (101 MHz, DMSO-d^6) δ 197.5; 194.0, 190.6, 160.7, 157.8, 156.1 156.0, 152.3, 152.1, 151.9, 149.0, 147.6, 128.2, 128.0, 125.8, 125.42, 125.38, 124.2, 20.9, 20.7, 20.5 ; ESI-MS (MeCN): Calculated 546.0822 for $[M-Br]^+$, Observed 546.0869 ; Elemental analysis for $C_{21}H_{17}BrN_3O_3Re,H_2O$ Calculated: C(%) 39.20, N(%) 6.53, H(%) 2.98, Found: C(%) 39.40, N(%) 6.41, H(%) 2.57.

1c *fac*-[Re(CO)$_3$Br(κ^2N-*Lc*)] Y=91% (301 mg) yellow solid. ^{1}H NMR (400 MHz, CD_3CN) δ = 9.10 (d, J = 6 Hz, 1H), 8.81 (d, J = 5 Hz, 1H), 8.75 (d, J = 2 Hz, 1H), 8.68 (d, J = 8 Hz, 1H), 8.24 (t, J = 8 Hz, 1H), 8.05 (d, J = 2 Hz, 1H), 8.03 – 7.98 (m, 3H), 7.85 (d, J = 8 Hz, 1H), 7.68 – 7.54 (m, 5H).; ^{13}C NMR (101 MHz, DMSO-d^6) δ 197.5, 194.0, 190.4, 161,6, 157.9, 157.3, 156.4, 152.8, 150.6, 149.2, 139.9, 137.0, 134.7, 131.0, 129.4, 127.9, 127.5, 125.5, 125.1, 125.0, 124.4, 120.7; ESI-MS (MeCN): Calculated 580.0672 for $[M -Br]^+$, Observed 580.0754; Elemental analysis for $C_{24}H_{15}BrN_3O_3Re,H_2O$, Calculated: C(%) 42.55, N(%) 6.20, H(%) 2.53, Found: C(%) 42.71, N(%) 6.00, H(%) 2.17.

1d *fac*-[Re(CO)$_3$Br(κ^2N-*Ld*)] Y=92% (339 mg) orange-red solid. ^{1}H NMR (400 MHz, CD_3CN) δ = 9.10 (d, J = 6 Hz, 1H), 8.81 (d, J = 5 Hz, 1H), 8.79 (s, 1H), 8.71 (d, J = 8 Hz, 1H), 8.24 (t, J = 8 Hz, 1H), 8.11 (s, 1H), 8.09 (s, 2H), 8.00 (t, J = 8 Hz, 1H), 7.89 (d, J = 8 Hz, 2H), 7.85 (d, J = 8 Hz, 1H), 7.76 (d, J = 7 Hz, 2H), 7.65 (t, J = 7 Hz, 1H), 7.58 (dd, J

= 8, 5 Hz, 1H), 7.52 (t, J = 8 Hz, 2H), 7.44 (t, J = 7 Hz, 1H)·; ^{13}C NMR (101 MHz, DMSO-d^6) δ 197.5, 194.0, 190.4, 161,6, 158.0, 157.3, 156.4, 152.8, 150.0, 149.2, 142.5, 139.9, 138.9, 137.0, 133.6, 129.1, 128.5, 128.2, 127.5, 12.9, 125.5, 125.1, 125.0, 124.2, 120.4 ; ESI-MS (MeCN): Calculated 656.0985 for [M -Br]$^+$, Observed 656.0888 ; Elemental analysis for $C_{30}H_{19}BrN_3O_3Re,H_2O$ Calculated: C(%) 47.81, N(%) 5.58, H(%) 2.81, Found: C(%) 48.09, N(%) 5.42, H(%) 2.60.

1e *fac*-[Re(CO)$_3$Br(κ^2N-*Le*)] Y=95% (313 mg) yellow-orange solid. ^{1}H NMR (400 MHz, CD_3CN) δ = 9.11 (d, J = 5 Hz, 1H), 8.99 (d, J = 7 Hz, 1H), 8.80 (m, 3H), 8.67 (dd, J = 11, 9 Hz, 1H), 8.25 (m, 1H), 8.10 (m, 1H), 7.99 (d, J = 7 Hz, 2H), 7.91 (dd, J = 5, 2 Hz, 1H), 7.85 (m, 1H), 7.66 (m, 1H), 7.58 (m, 1H).; ESI-MS (MeCN): Calculated 581.0624 for [M -Br]$^+$, Observed 581.0675

Complexes **2a-e** were prepared as in our previous report, starting from the corresponding κ^2N-terpyridine complexes. The suitable κ^2N-terpyridine complex (100 mg) was ground into a fine powder then placed in a 20mL Biotage® microwave vial, sealed in a nitrogen purged glovebox with a PTFE-silicon septum. The vial was then heated in a sand bath at 270 °C for 6 h. Once back to RT, the vial was opened, and the black brown solid was dispersed in 10 mL of diethyl ether, filtered, washed with dichloromethane (2*10 mL) and finally air dried. Further drying at 100°C overnight was conducted before storage in a desiccator.

2a [Re(CO)$_2$Br(κ^3N-*La*)] Y=90% (129 mg, starting with 150 mg) dark brown solid.; ^{1}H NMR (400 MHz, DMSO-d^6) δ = 8.89 (dd, J = 6, 1 Hz, 2H), 8.61 (d, J = 8 Hz, 2H), 8.56 (d, J = 8 Hz, 2H), 8.22 (t, J = 8 Hz, 1H), 8.03 (td, J = 8, 1 Hz, 2H), 7.51 – 7.43 (ddd, J = 8, 6, 1 Hz, 2H) ; ESI-MS (MeCN): Calculated 476.0409 for [M -Br]$^+$, Observed 476.0355

2b *mer,cis*[Re(CO)$_2$Br(κ^3N-*Lb*)] Y=74% (72 mg) dark brown solid; ^{1}H NMR (400 MHz, Acetone-d^6) δ = 8.79 (d, J = 6 Hz, 2H), 8.32 (s, 2H), 8.27 (d, J = 1 Hz, 2H), 7.27 (dd, J = 6, 1 Hz, 2H), 2.72 (s, 3H), 2.58 (s, 6H) ; ^{13}C NMR (101 MHz, DMSO-d^6) δ 182.4, 156.4, 156.0, 155.7, 151.2, 149.2, 128.6, 125.0, 122.6, 21.4, 20.5 ; ESI-MS (MeCN): Calculated 518.0879 for [M -Br]$^+$,Observed 518.0859 ; Elemental analysis for

$C_{20}H_{17}BrN_3O_2Re$, Calculated: C(%) 40.21, N(%) 7.03, H(%) 2.87, Found: C(%) 39.92, N(%) 6.78, H(%) 2.79.

2c *mer,cis*[Re(CO)$_2$Br(κ^3N-*Lc*)] Y=73% (69 mg) dark brown solid; ^{1}H NMR (400 MHz, Acetone-d^6) δ = 9.03 (d, J = 5 Hz, 2H), 8.79 (s, 2H), 8.67 (d, J = 8 Hz, 2H), 8.12 (d, J = 7 Hz, 2H), 8.02 (t, J = 8 Hz, 2H), 7.65 (t, J = 7 Hz, 2H), 7.60 (d, J = 7 Hz, 1H), 7.48 (t, J 7 Hz, 2H) ; ^{13}C NMR (101 MHz, DMSO-d^6) δ 181.1, 156.9, 156.7, 156.6, 150.7, 137.5, 135.9, 130.6, 129.2, 128.3, 128.0, 124.8, 119.5; ESI-MS (MeCN): Calculated 552.0722 for [M -Br]$^+$, Observed 552.0734 ; Elemental analysis for $C_{23}H_{15}BrN_3O_2Re$,0.5 H_2O , Calculated: C(%) 43.13, N(%) 6.56, H(%) 2.52, Found: C(%) 43.08, N(%) 6.41, H(%) 2.28.

2d *mer,cis*[Re(CO)$_2$Br(κ^3N-*Ld*)] Y=79% (76 mg) dark brown solid ; ^{1}H NMR (400 MHz, Acetone-d^6) δ = 9.04 (d, J = 6 Hz, 2H), 8.86 (s, 2H), 8.69 (d, J = 8 Hz, 2H), 8.25 (d, J = 9 Hz, 2H), 8.03 (t, J = 8 Hz, 2H), 7.95 (d, J = 8 Hz, 2H), 7.80 (d, J = 7 Hz, 2H), 7.60 – 7.40 (m, 5H) ; ^{13}C NMR (101 MHz, DMSO-d^6) δ 181.1, 156.9, 156.8, 156.7, 150.0, 142.2, 139.0, 137.5, 134.7, 129.1, 128.6, 128.3, 128.2, 127.3, 126.9, 124.8, 119.2; ESI-MS (MeCN): Calculated 628.1036 for [M -Br]$^+$,Observed 628.1021 ; Elemental analysis for $C_{29}H_{19}BrN_3O_2Re$,0.5 H_2O , Calculated: C(%) 48.61, N(%) 5.86, H(%) 2.81, Found: C(%) 48.48, N(%) 5.72, H(%) 2.52.

2e *mer,cis*[Re(CO)$_2$Br(κ^3N-*Le*)] Y=90% (86 mg) dark brown solid ; ^{1}H NMR (400 MHz, DMSO-d^6) δ = 9.03 (s, 2H), 8.92 (d, J = 5 Hz, 2H), 8.89 (d, J = 6 Hz, 2H), 8.81 (d, J = 8 Hz, 2H), 8.21 (d, J = 6 Hz, 2H), 8.10 (t, J = 8 Hz, 2H), 7.52 (ddd, J = 8, 6, 1 Hz, 2H) ; ESI-MS (MeCN): Calculated 533.0675 for [M -Br]$^+$,Observed 533.0736

Complexes **3a-e** were prepared following published procedures for **3a** and **3e**. The suitable precursor complex **2** (50 mg) was dissolved in pyridine (10 mL) under N_2. To this solution, protected from light with aluminum foil, was added 1.25 eq. of silver triflate. The mixture was refluxed for 5 h, still under N_2, turning dark green. Once cooled to RT, it was filtered through Celite and precipitated by addition of an aqueous solution of KPF_6, then filtered and washed with water. The greyish green precipitate was purified on Al_2O_3 (DCM/acetone 2/8). The green fraction was collected, its volume reduced

before being poured in Et_2O to precipitate the final compound. The solid was dried in air and then in a 100°C oven overnight before storage in a desiccator.

3a *mer,cis*[Re(CO)$_2$(py)(*κ*^{3}N-*La*)](PF$_6$) Y=70% (44 mg) ^{1}H NMR (400 MHz, Acetone-d^6) δ = 9.14 (ddd, J = 6, 1, 1 Hz, 2H), 8.67 (d, J = 8 Hz, 2H), 8.60 (ddd, J = 8, 1, 1 Hz, 2H), 8.38 (t, J = 8 Hz, 1H), 8.28 (dd, J = 7, 2 Hz, 2H), 8.18 (td, J = 8, 2 Hz, 2H), 7.91 (tt, J = 8, 2 Hz, 1H), 7.68 (ddd, J = 8, 6, 1 Hz, 2H), 7.36 (ddd, J = 8, 5, 1 Hz, 2H). ; ESI-MS (MeCN): Calculated 555.0826 for $[M - PF_6]^+$, Observed 555.0796

3b *mer,cis*[Re(CO)$_2$(py)(*κ*^{3}N-*Lb*)](PF$_6$) Y=71% (53 mg, starting with 60 mg of **2b**) ^{1}H NMR (400 MHz, Acetone-d^6) δ = 8.93 (d, J = 6 Hz, 2H), 8.54 (s, 2H), 8.45 (d, J = 1 Hz, 2H), 8.24 (dd, J = 7, 1 Hz, 2H), 7.90 (tt, J = 8, 2 Hz, 1H), 7.49 (dd, J = 6, 1 Hz, 2H), 7.35 (ddd, J = 8, 6, 1 Hz, 2H), 2.76 (s, 3H), 2.62 (s, 6H) ; ^{13}C NMR (101 MHz, DMSO-d^6) δ 212.69, 187.76, 156.09, 156.07, 155.80, 152.93, 150.89, 149.97, 139.25, 130.06, 126.57, 126.01, 123.96, 21.62, 20.65 ; ESI-MS (MeCN): Calculated 597.1295 for $[M - PF_6]^+$,Observed 597.1353 ; Elemental analysis for $C_{25}H_{22}N_4O_2RePF_6$, Calculated: C(%) 40.49, N(%) 7.55, H(%) 2.99, Found: C(%) 40.63, N(%) 7.45, H(%) 2.84.

3c *mer,cis*[Re(CO)$_2$(py)(*κ*^{3}N-*Lc*)](PF$_6$) Y=60% (37 mg) ^{1}H NMR (400 MHz, Acetone-d^6) δ = 9.16 (dd, J = 6, 1 Hz, 2H), 8.99 (s, 2H), 8.84 (d, J = 8 Hz, 2H), 8.33 (dd, J = 6, 2 Hz, 2H), 8.21 (td, J = 8, 2 Hz, 2H), 8.13 (dd, J = 8, 2 Hz, 2H), 7.92 (tt, J = 8, 2 Hz, 1H), 7.72 – 7.61 (m, 5H), 7.37 (ddd, J = 8, 6, 1 Hz, 2H) ; ^{13}C NMR (101 MHz, DMSO-d^6) δ 212.90, 186.75, 156.80, 156.76, 156.71, 151.67, 150.10, 139.38, 138.90, 135.33, 131.00, 129.79, 129.25, 128.06, 126.66, 125.71, 120.79 ; ESI-MS (MeCN): Calculated 631.1139 for $[M - PF_6]^+$, Observed 631.1070 ; Elemental analysis for $C_{28}H_{20}N_4O_2Re\ PF_6{,}0.5H_2O$, Calculated: C(%) 42.86, N(%) 7.14, H(%) 2.70, Found: C(%) 42.91, N(%) 6.99, H(%) 2.70.

3d *mer,cis*[Re(CO)$_2$(py)(*κ*^{3}N-*Ld*)](PF$_6$) Y=59% (36 mg) ^{1}H NMR (400 MHz, Acetone-d^6) δ = 9.17 (dd, J = 6, 1 Hz, 2H), 9.07 (s, 2H), 8.87 (d, J = 8 Hz, 2H), 8.34 (dd, J = 7, 2 Hz, 2H), 8.27 (d, J = 9 Hz, 2H), 8.22 (td, J = 8, 2 Hz, 2H), 7.97 (d, J = 9 Hz, 2H), 7.92 (tt, J = 8, 2 Hz, 1H), 7.79 (d, J = 7 Hz, 2H), 7.70 (ddd, J = 8, 6, 1 Hz, 2H), 7.54 (t, J = 8 Hz, 2H), 7.45 (tt, J = 7, 2 Hz, 1H), 7.38 (ddd, J = 8, 5, 1 Hz, 2H) ; ^{13}C NMR (101 MHz,

DMSO-d^6) δ 212.94, 186.82, 156.83, 156.75, 151.06, 150.11, 142.54, 139.39, 138.90, 138.80, 134.14, 129.79, 129.10, 128.68, 128.30, 127.64, 127.32, 126.93, 126.67, 125.73, 120.49 ; ESI-MS (MeCN): Calculated 707.1458 for $[M - PF_6]^+$, Observed 707.1436 ; Elemental analysis for $C_{34}H_{24}N_4O_2RePF_6,H_2O$, Calculated: C(%) 46.95, N(%) 6.44, H(%) 3.01, Found: C(%) 47.02, N(%) 6.21, H(%) 3.01.

3e *mer,cis*[Re(CO)$_2$(py)(κ^3N-*Le*)](PF$_6$) Y=50% (30 mg) ^{1}H NMR (400 MHz, Acetone-d^6) δ = 9.18 (dd, J = 6, 1 Hz, 2H), 9.10 (s, 2H), 8.90 – 8.81 (m, 4H), 8.32 (dd, J = 7, 2 Hz, 2H), 8.23 (td, J = 8, 2 Hz, 2H), 8.09 (dd, J = 5, 2, 2H), 7.92 (tt, J = 8, 2 Hz, 1H), 7.72 (ddd, J = 8, 6, 1 Hz, 2H), 7.40 – 7.32 (m, 2H) ; ESI-MS (MeCN): Calculated 632.1097 for $[M - PF_6]^+$, Observed 632.1074.

Complexes **4a** and **4b** were prepared according to literature. The suitable complex **2** (50 mg) were dissolved in THF (50 mL) under N_2. To this solution, protected from light with aluminum foil, was added 1.25 eq. of silver triflate and 10 eq. of triphenylphosphine. The mixture was refluxed for 5 h, still under N_2, turning dark green. The same work-up as for complexes **3** was used to obtain **4** as a green solid.

4a *mer,cis*[Re(CO)$_2$(PPh$_3$)(κ^3N-*La*)](PF$_6$) Y=50% (42 mg) ^{1}H NMR (400 MHz, Acetone-d^6) δ = 9.22 (d, J = 6 Hz, 2H), 8.35 (d, J = 8 Hz, 2H), 8.29 (d, J = 8 Hz, 2H), 8.17 (t, J = 8 Hz, 1H), 7.96 (t, J = 8 Hz, 2H), 7.53 – 7.45 (m, 2H), 7.40 (td, J = 7, 1 Hz, 3H), 7.29 (td, J = 8, 2 Hz, 6H), 7.17 – 7.06 (m, 6H) ; ^{31}P NMR (162 MHz, Acetone-d^6) δ 14.91 ; ESI-MS (MeCN): Calculated 738.1322 for $[M - PF_6]^+$, Observed 738.1291

4b *mer,cis*[Re(CO)$_2$(PPh$_3$)(κ^3N-*Lb*)](PF$_6$) Y=66% (61 mg, starting with 60 mg of **2b**) ^{1}H NMR (400 MHz, Acetone-d^6) δ = 8.99 (d, J = 6 Hz, 2H), 8.19 (s, 2H), 8.15 (m, 2H), 7.40 (m, 3H), 7.30 (m, 8H), 7.14 (m, 6H), 2.72 (s, 3H), 2.53 (s, 6H) ; ^{31}P NMR (162 MHz, Acetone-d^6) δ 14.33 ; ^{13}C NMR (101 MHz, DMSO-d^6) δ 157.05, 155.42, 154.25, 151.54, 149.91, 132.45, 132.35, 130.30, 128.91, 128.82, 125.14, 123.56, 21.19, 20.33 ; ESI-MS (MeCN): Calculated 780.1784 for $[M - PF_6]^+$,Observed 780.1742 ; Elemental analysis for $C_{38}H_{32}N_4O_2ReP_2F_6$, Calculated: C(%) 49.35, N(%) 4.54, H(%) 3.49, Found: C(%) 49.26, N(%) 4.44, H(%) 3.48.

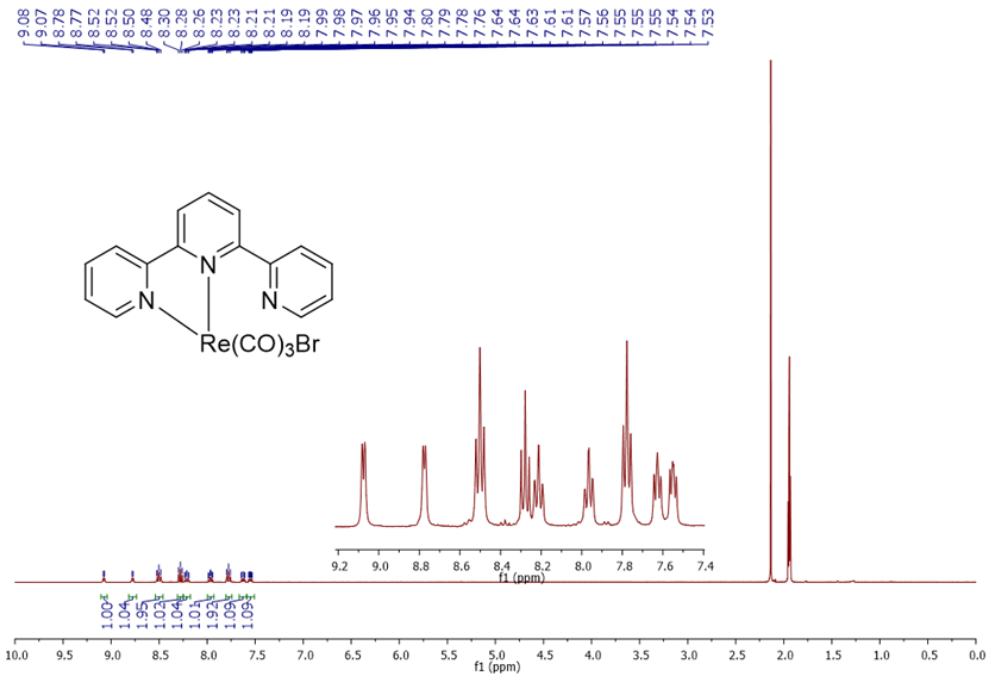


Figure S1 ^{1}H NMR spectra for complex **1a** in CD_3CN

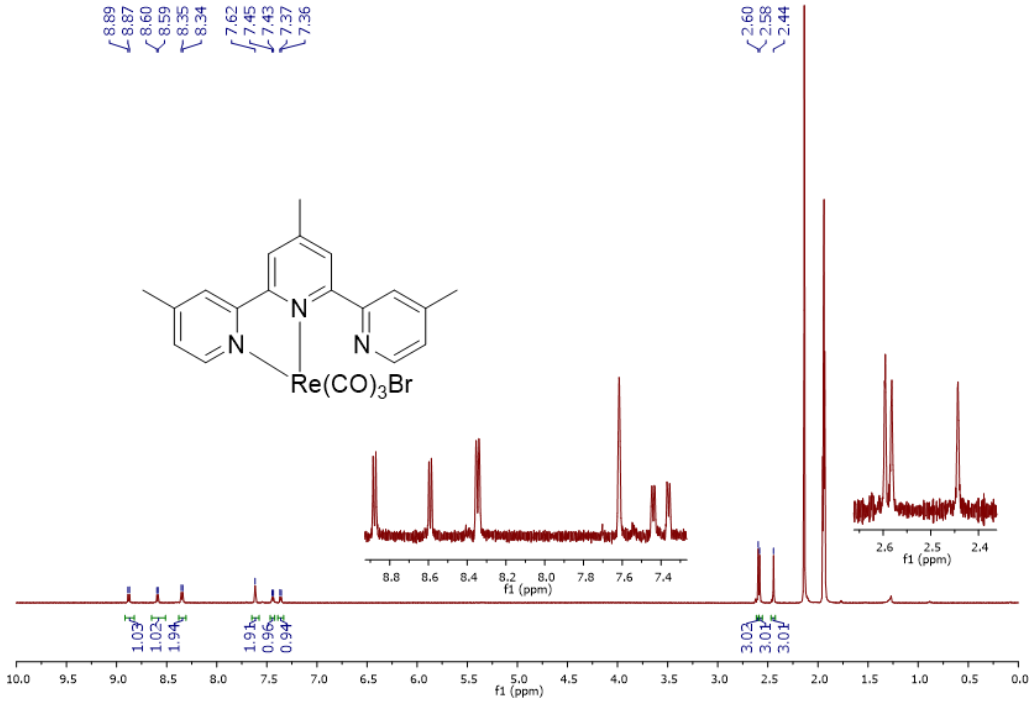


Figure S2. ^{1}H NMR spectra for complex **1b** in CD_3CN

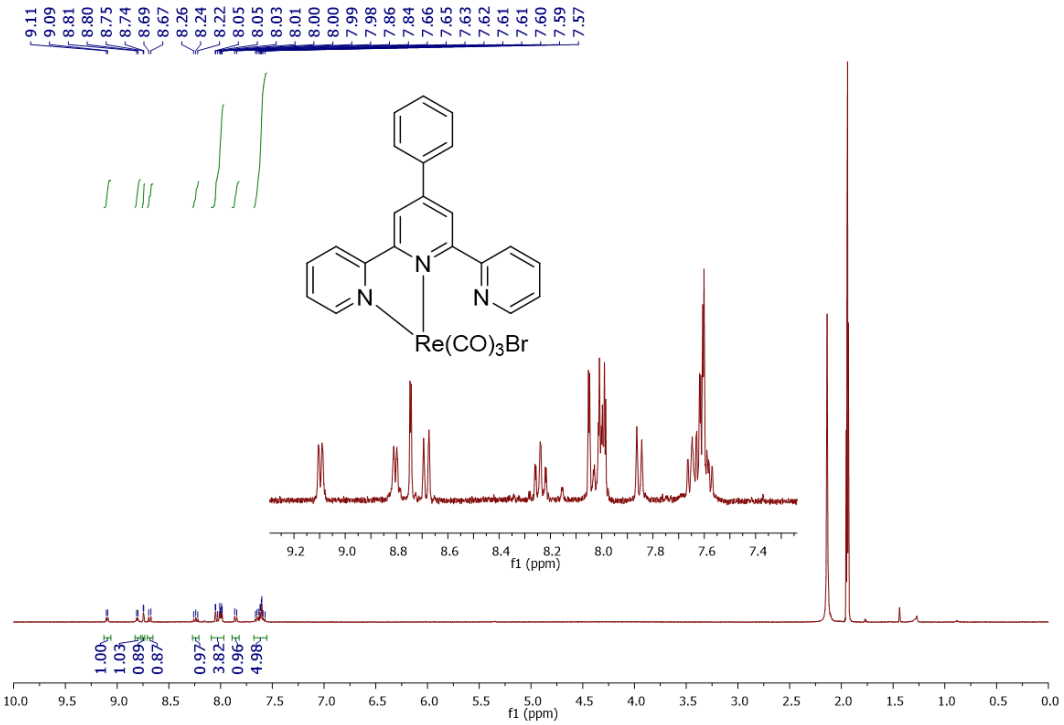


Figure S3. ^{1}H NMR spectra for complex **1c** in CD_3CN

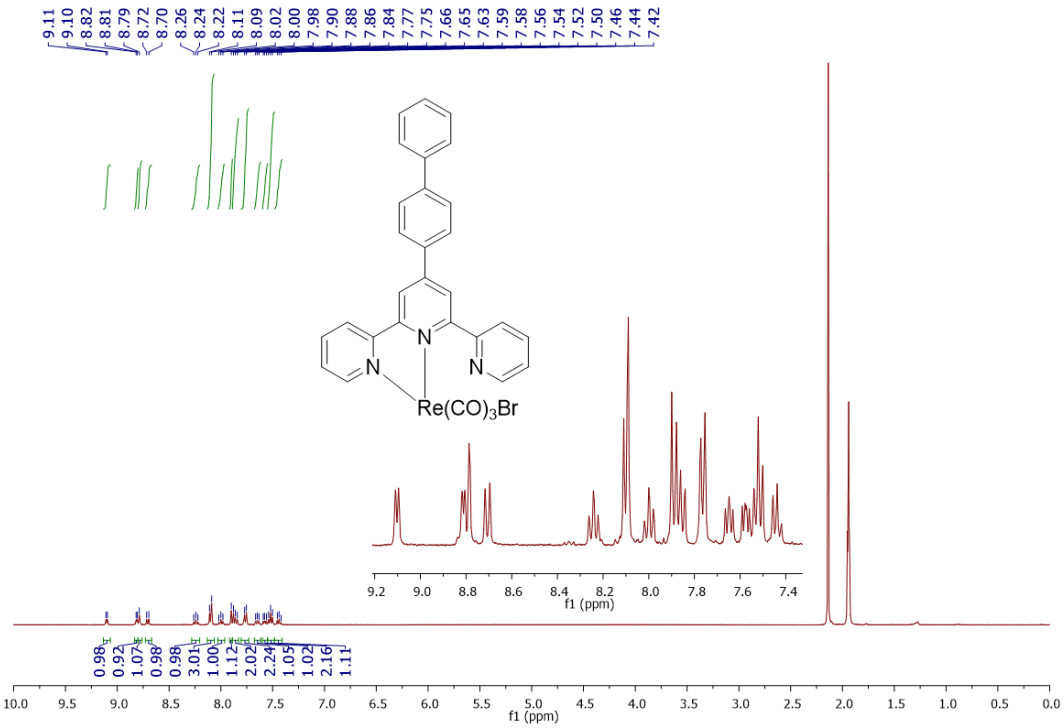


Figure S4. ^{1}H NMR spectra for complex **1d** in CD_3CN

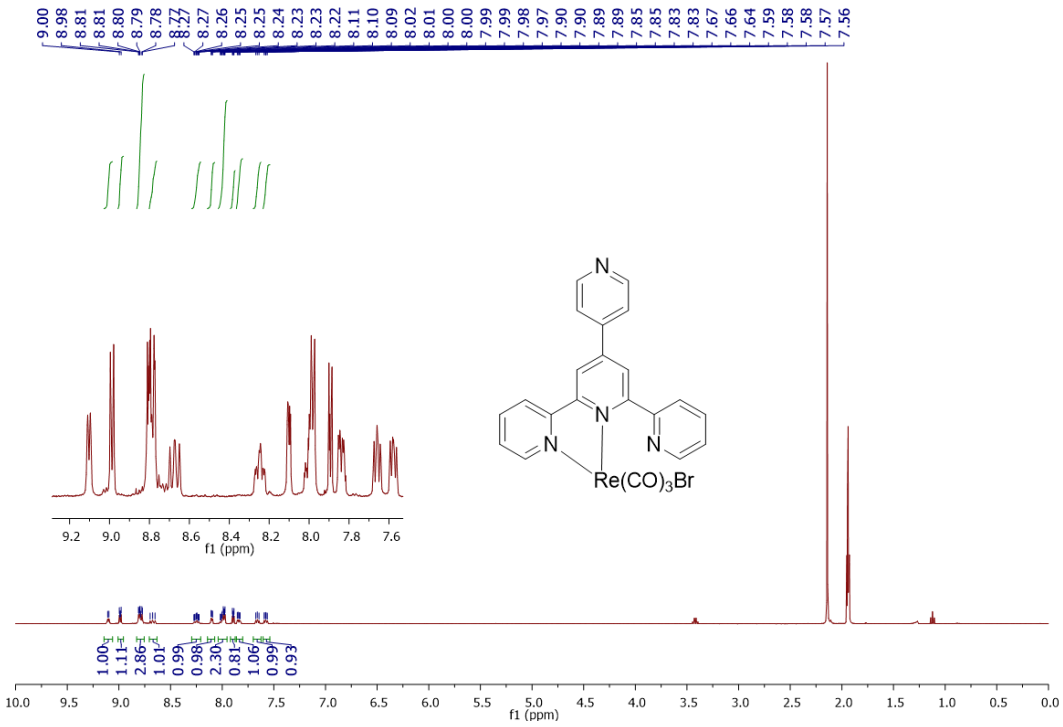


Figure S5. ^{1}H NMR spectra for complex **1e** in CD_3CN

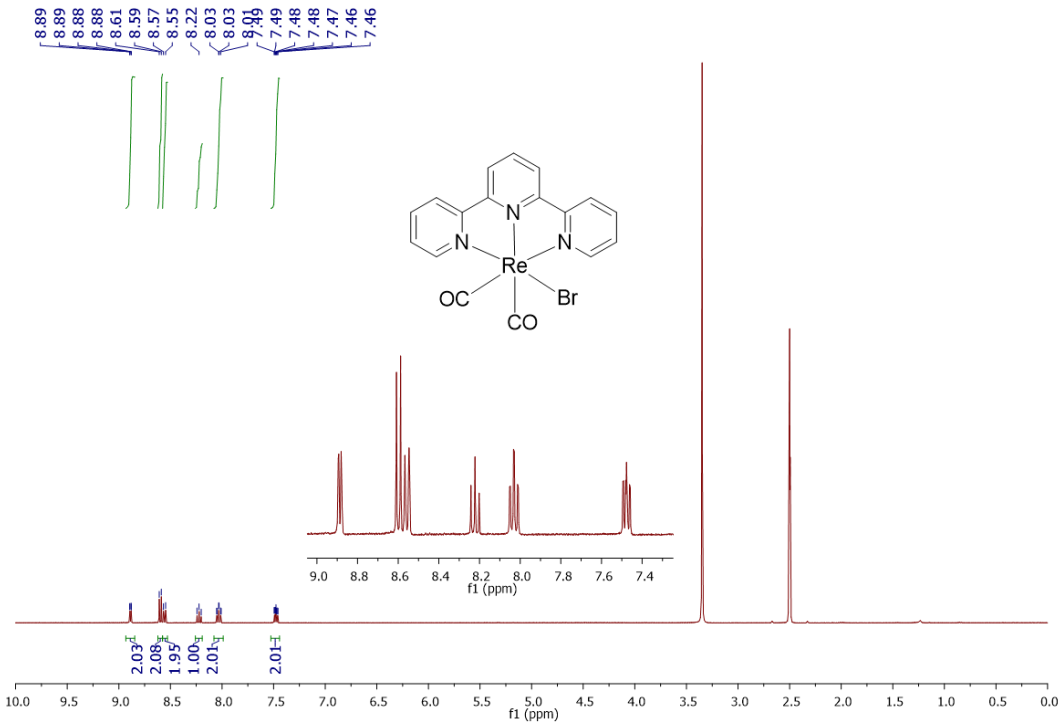


Figure S6. ^{1}H NMR spectra for complex **2a** in (DMSO-d^6)

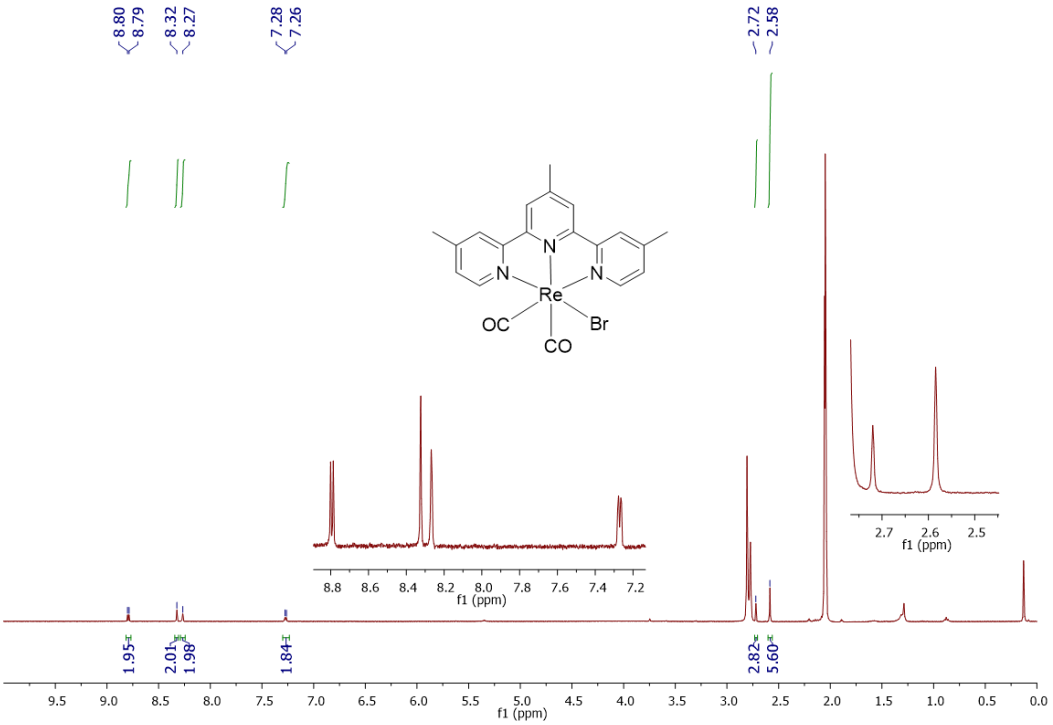


Figure S7. ^{1}H NMR spectra for complex **2b** in (acetone-d^{6})

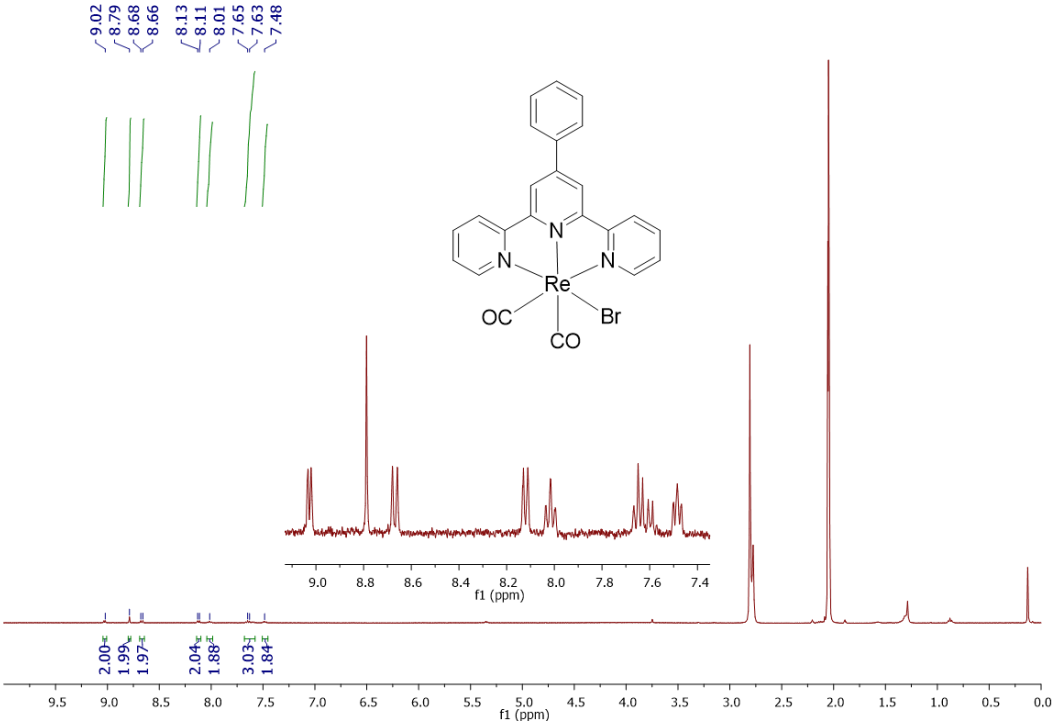


Figure S8.^{1}H NMR spectra for complex **2c** in (acetone-d^{6})

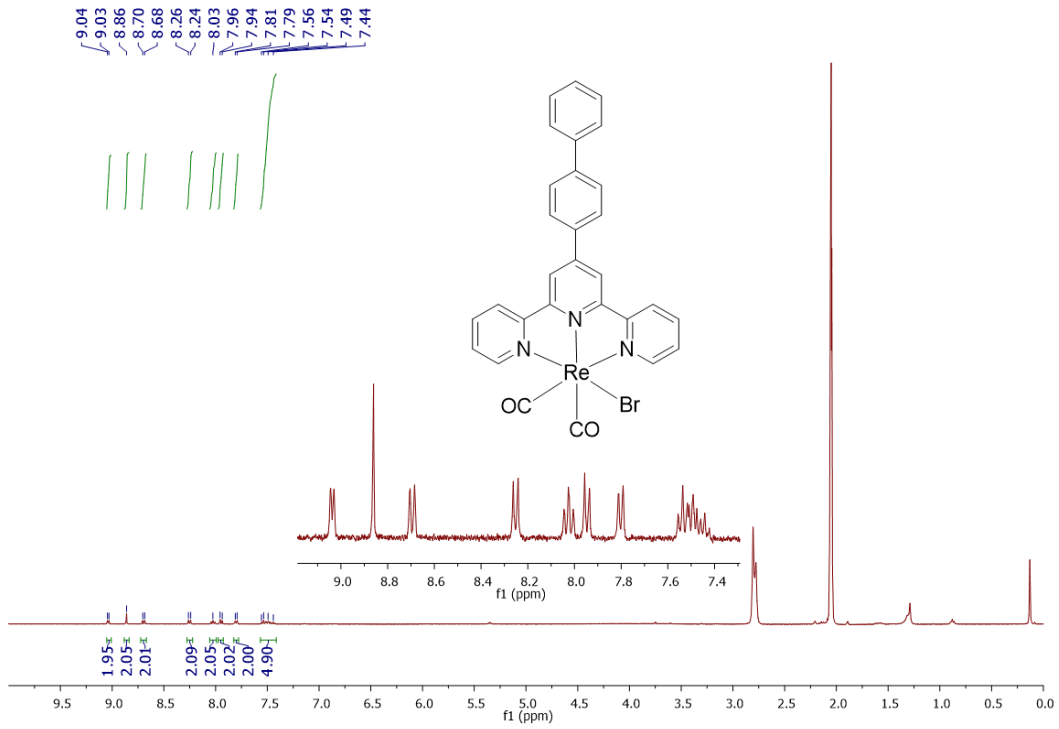


Figure S9. ^{1}H NMR spectra for complex **2d** in (acetone-d^{6})

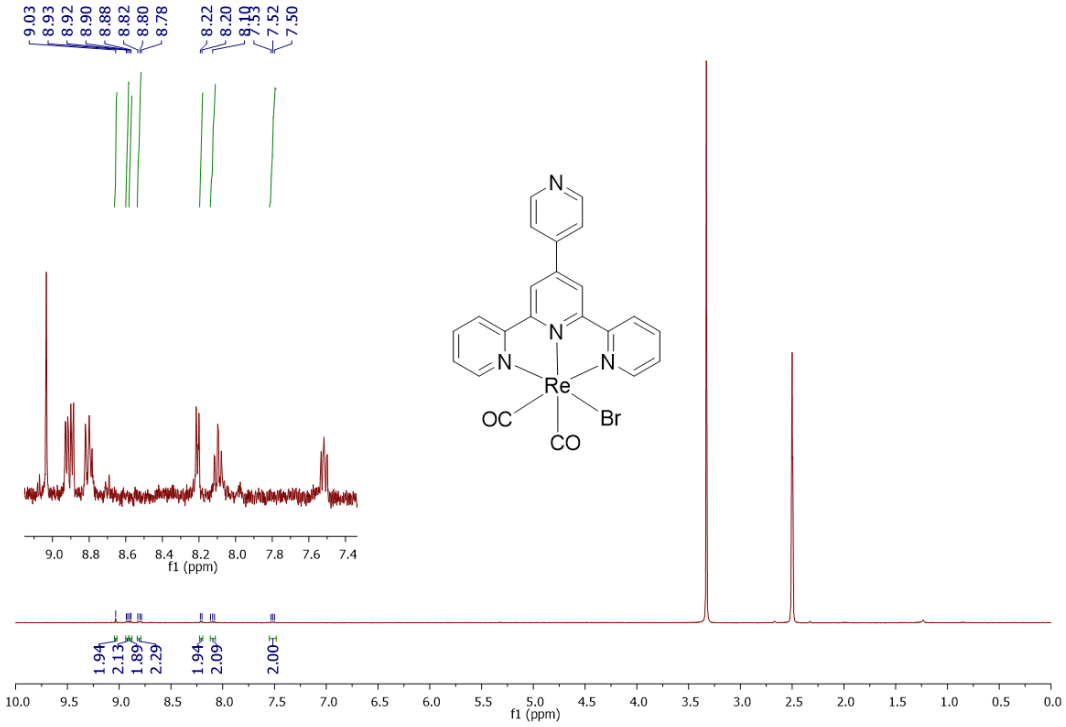


Figure S10. ^{1}H NMR spectra for complex **2e** in (acetone-d^{6})

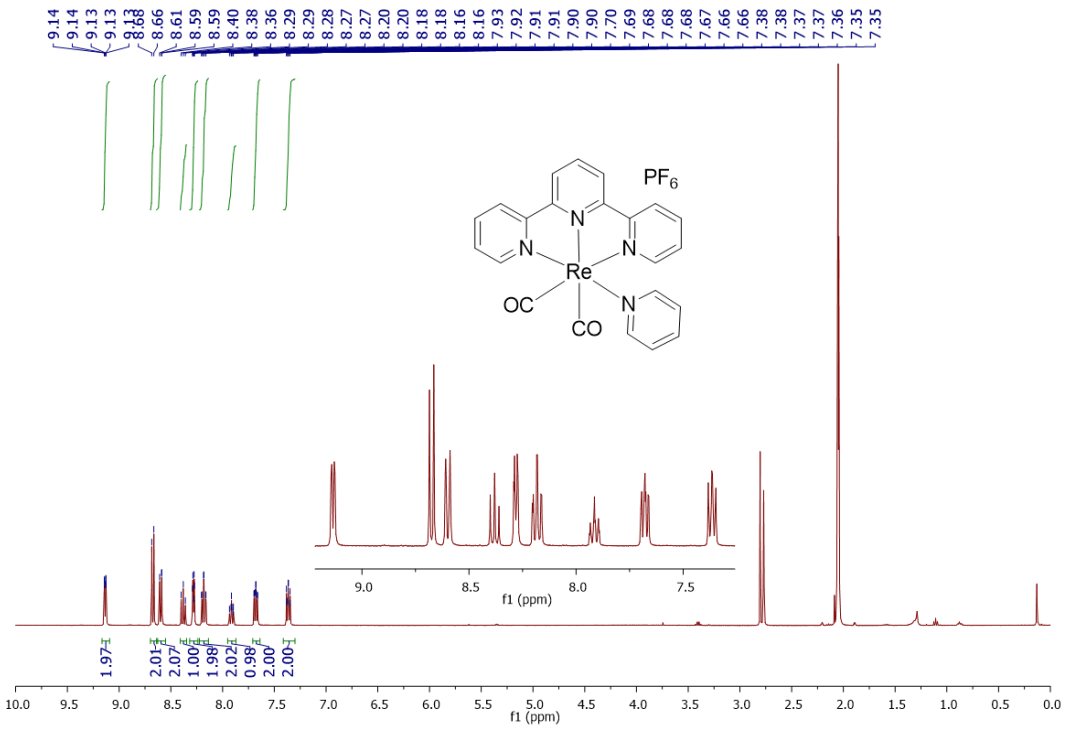


Figure S11. ^{1}H NMR spectra for complex **3a** in (acetone-d^{6})

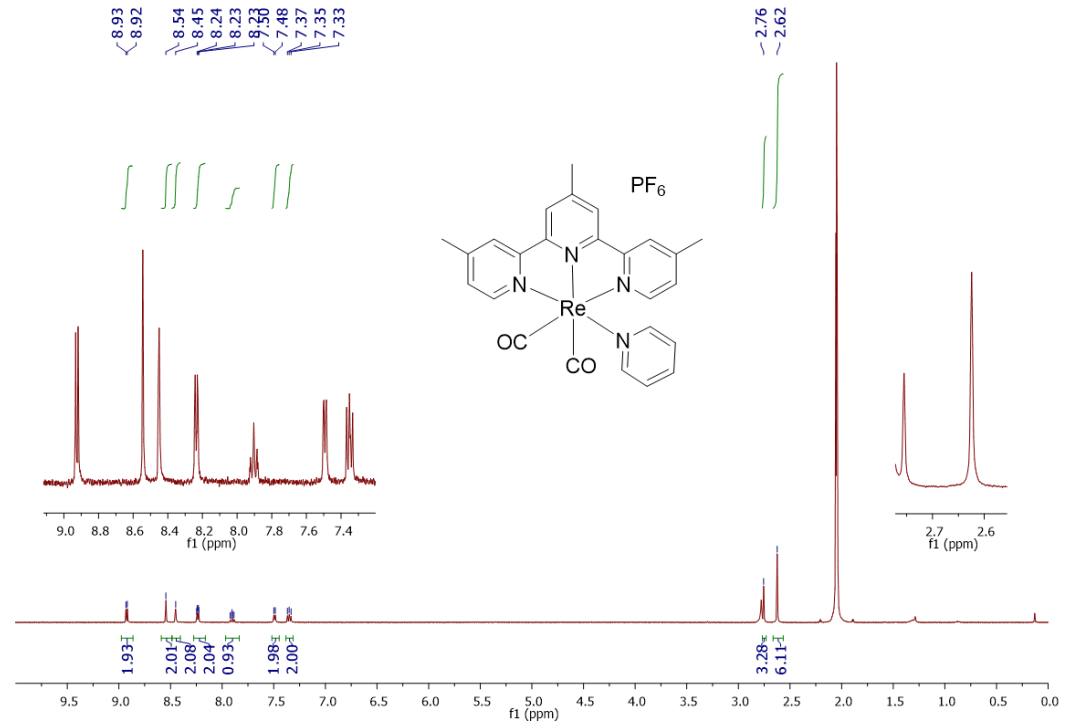


Figure S12. ^{1}H NMR spectra for complex **3b** in (acetone-d^{6})

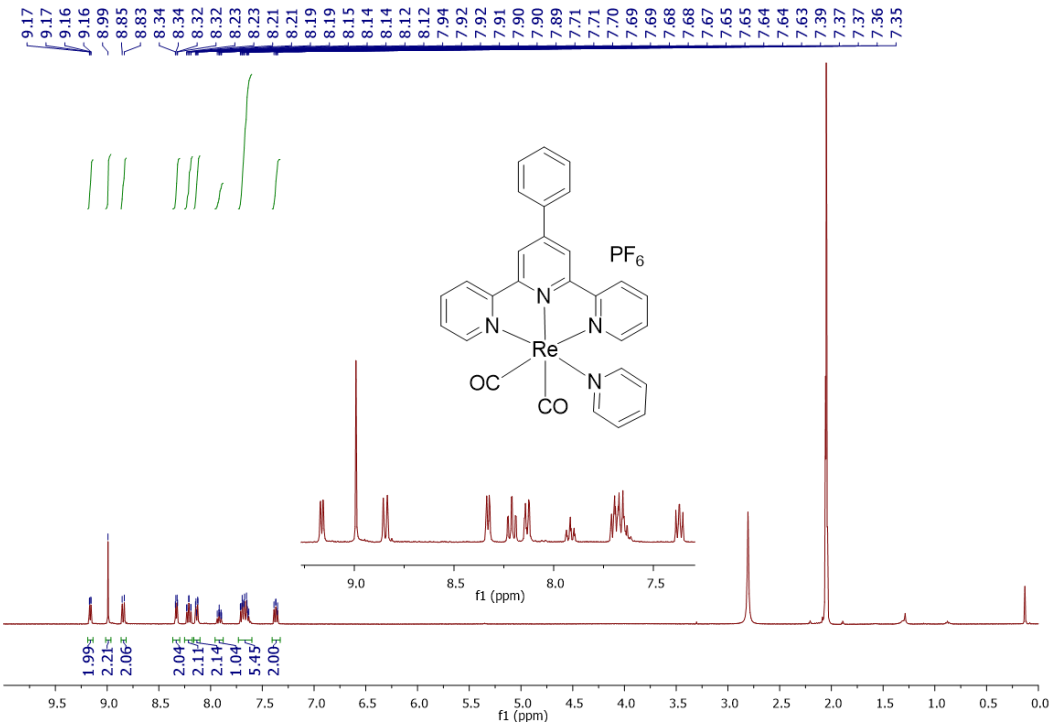


Figure S13. ^{1}H NMR spectra for complex **3c** in (acetone-d^{6})

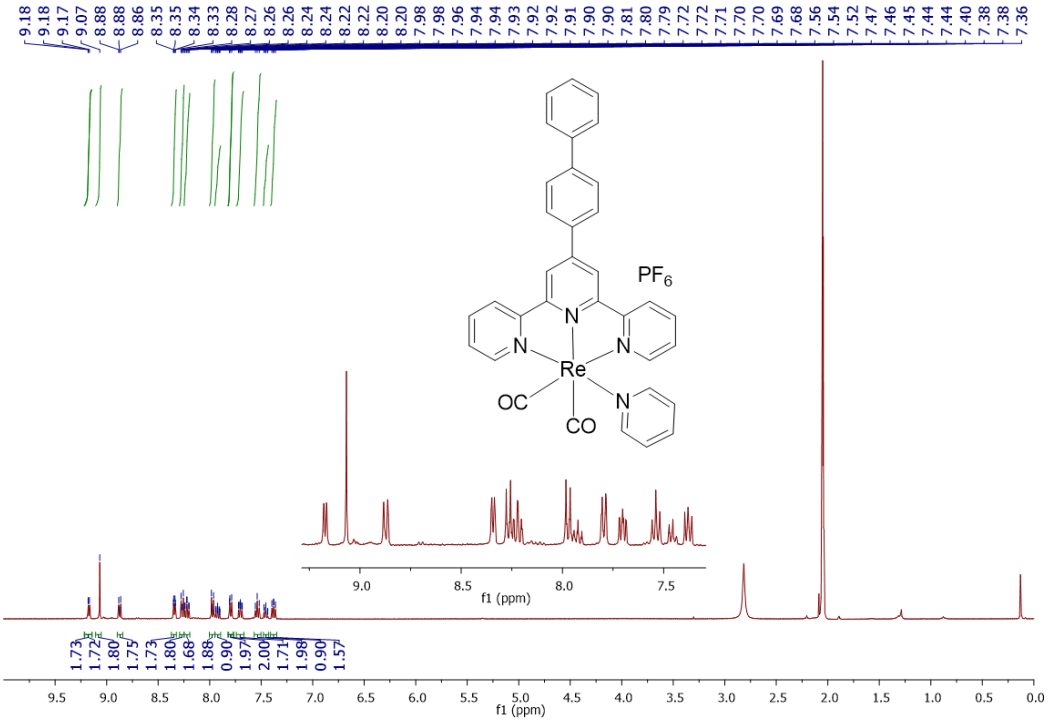


Figure S14. ^{1}H NMR spectra for complex **3d** in (acetone-d^{6})

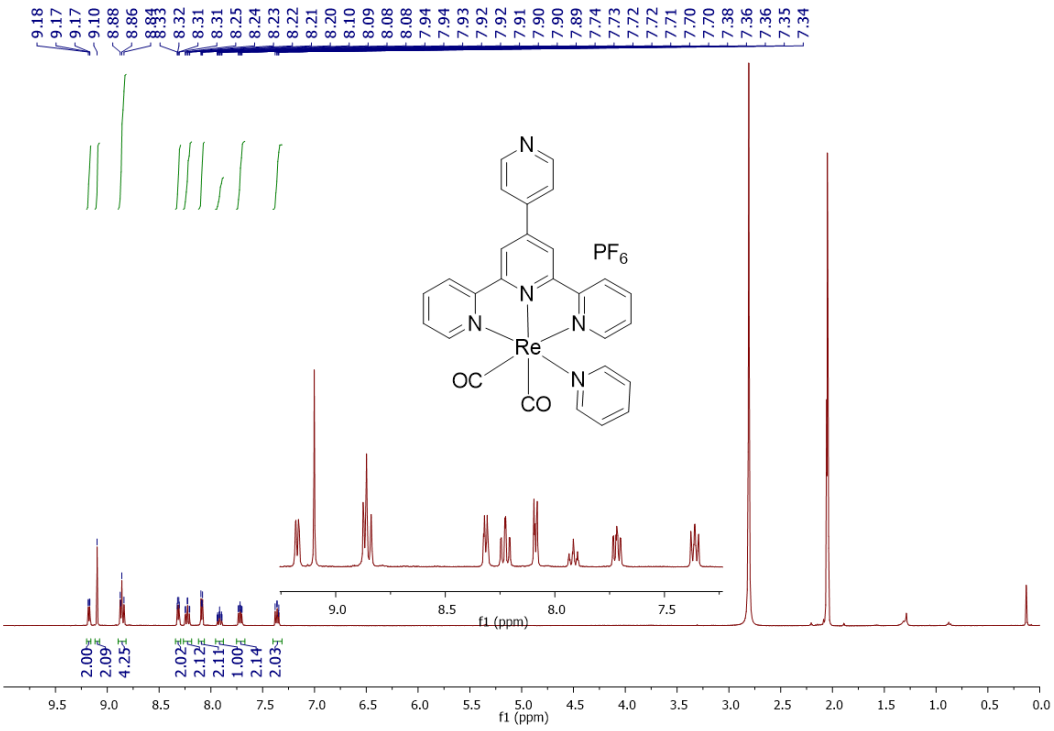


Figure S15. ^{1}H NMR spectra for complex **3e** in (acetone-d^{6})

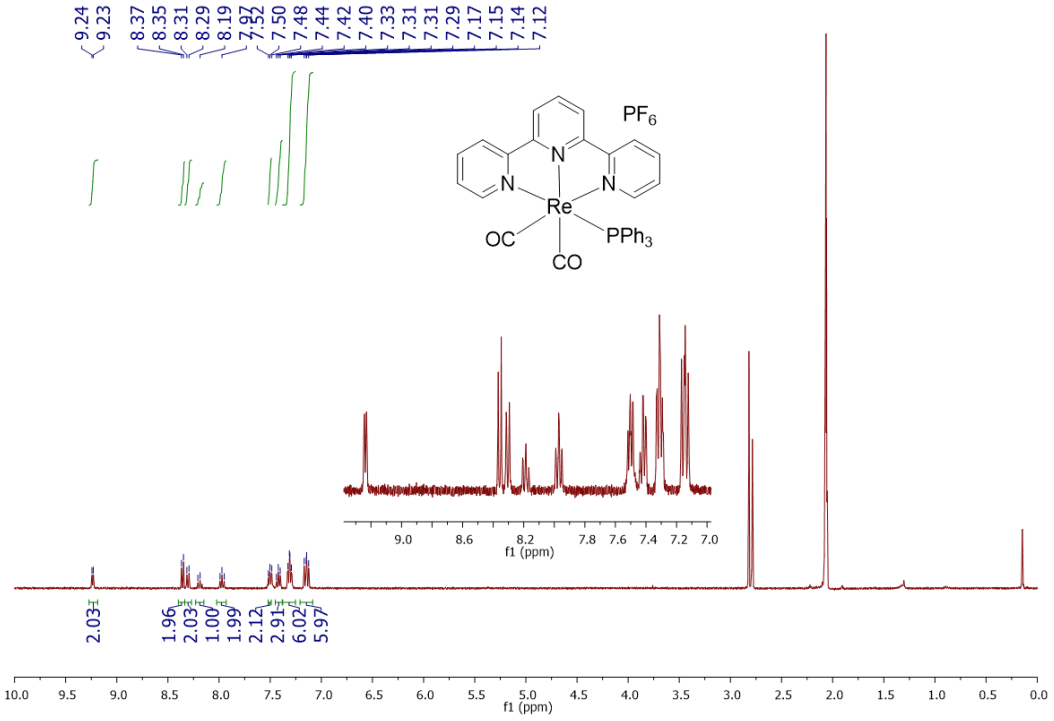


Figure S16. ^{1}H NMR spectra for complex **4a** in (acetone-d^{6})

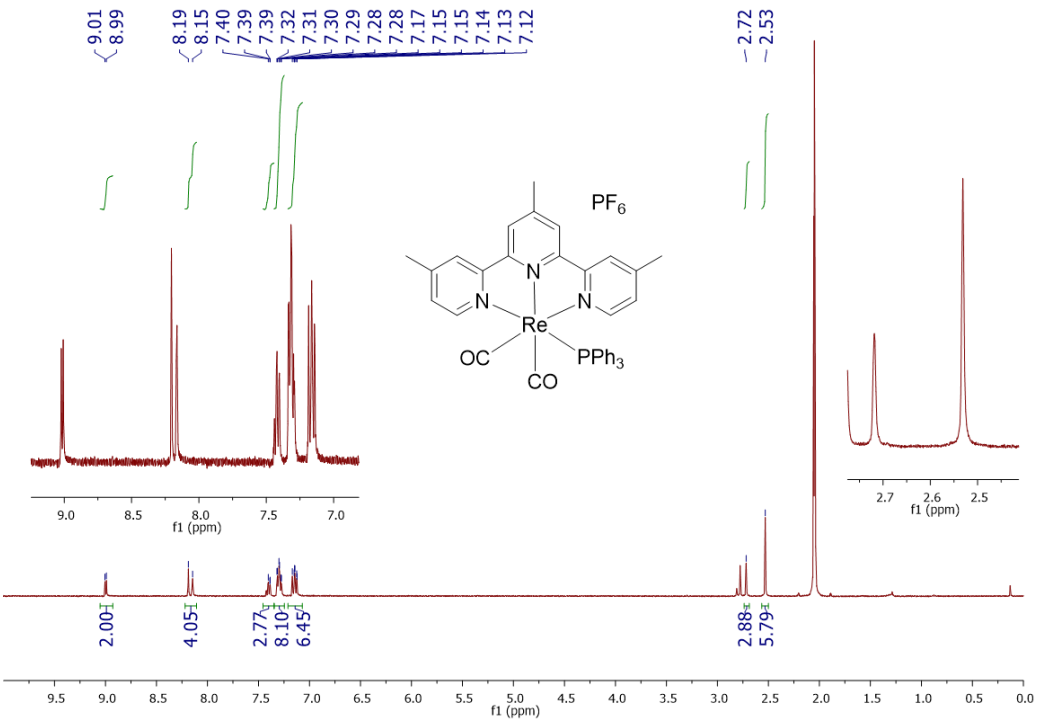


Figure S17. ^{1}H NMR spectra for complex **4b** in (acetone-d^{6})

Theoretical study and correlation with spectroscopic and electrochemical data

A) Vibrational spectroscopy

Table S1. Experimental and theoretical wavenumbers for the carbonyl IR active vibration modes

Compounds	**1a**	**1b**	**1c**	**1d**	**1e**
ν(CO) exp. cm^{-1}	2021, 1913, 1891	2017, 1910, 1881	2013, 1908, 1875	2013, 1905, 1880	2019, 1925, 1880
ν(CO) calc. cm^{-1}	2003, 1881, 1859	2001, 1878, 1854	2003, 1881, 1858	2003, 1881, 1858	2003, 1883, 1860
Compounds	**2a**	**2b**	**2c**	**2d**	**2e**
ν(CO) exp. cm^{-1}	1878, 1796	1880, 1793	1882, 1797	1884, 1801	1884, 1801
ν(CO) calc. cm^{-1}	1872, 1788	1867, 1780	1871, 1788	1871, 1788	1872, 1791
Compounds	**3a**	**3b**	**3c**	**3d**	**3e**
ν(CO) exp. cm^{-1}	1905, 1819	1912, 1837	1897, 1813	1904, 1832	1912, 1859
ν(CO) calc. cm^{-1}	1887, 1805	1881, 1797	1885, 1804	1885, 1804	1887, 1809
Compounds	**4a**	**4b**			
ν(CO) exp. cm^{-1}	1929, 1862	1928, 1859			
ν(CO) calc. cm^{-1}	1895, 1811	1890, 1802			

B) Orbitals data

Table S2. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **1a** (isovalue 0.05 e/Å^3) (bpy: coordinated bipyridine fragment, py: uncoordinated pyridine)

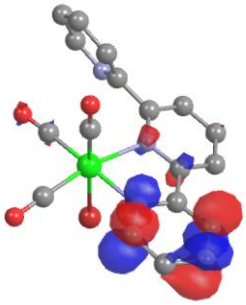
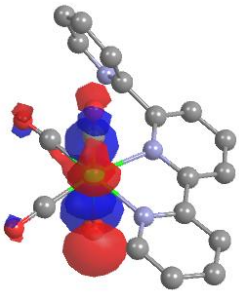
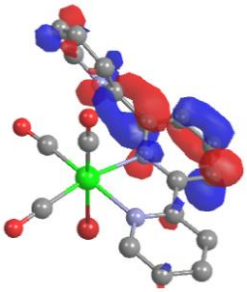
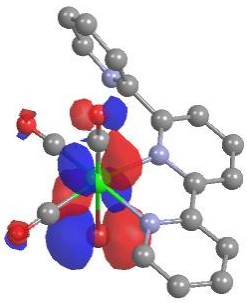
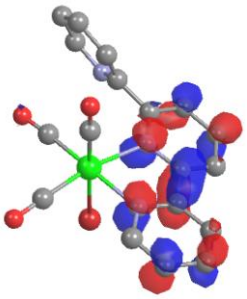
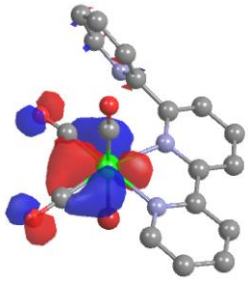
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.593 eV Re: 1% Br: 1% CO: 4% ‘’bpy’’: 93% ‘’py’’: 1%	 HOMO	-6.646 eV Re: 39% Br: 40% CO: 18% ‘’bpy’’: 2% ‘’py’’: 1%
 LUMO+1	-1.912 eV Re: 0% Br: 0% CO: 1% ‘’bpy’’: 71% ‘’py’’: 27%	 HOMO-1	-6.736 eV Re: 35% Br: 46% CO: 15% ‘’bpy’’: 4% ‘’py’’: 0%
 LUMO	-2.694 eV Re: 2% Br: 2% CO: 4% ‘’bpy’’: 89% ‘’py’’: 2%	 HOMO-2	-7.217 eV Re: 61% Br: 2% CO: 26% ‘’bpy’’: 2% ‘’py’’: 8%

Table S3. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **1b** (isovalue 0.05 e/Å^3) (bpy: coordinated bipyridine fragment, py: uncoordinated pyridine)

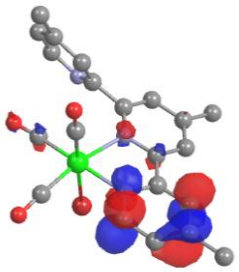
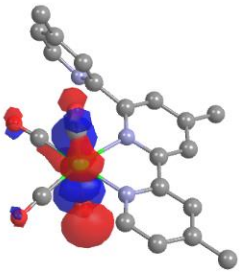
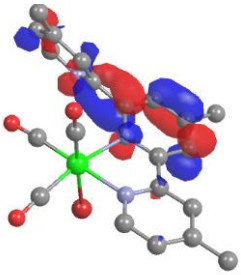
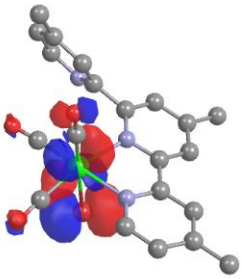
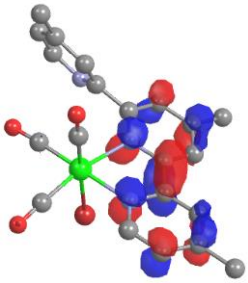
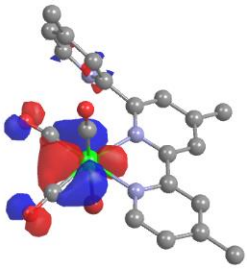
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.437 eV Re: 2% Br: 1% CO: 6% ‘’bpy’’: 89% ‘’py’’: 2%	 HOMO	-6.599 eV Re: 40% Br: 38% CO: 18% ‘’bpy’’: 3% ‘’py’’: 1%
 LUMO+1	-1.785 eV Re: 0% Br: 0% CO: 2% ‘’bpy’’: 71% ‘’py’’: 27%	 HOMO-1	-6.683 eV Re: 36% Br: 43% CO: 16% ‘’bpy’’: 5% ‘’py’’: 0%
 LUMO	-2.543 eV Re: 2% Br: 2% CO: 5% ‘’bpy’’: 89% ‘’py’’: 2%	 HOMO-2	-7.158 eV Re: 60% Br: 3% CO: 26% ‘’bpy’’: 2% ‘’py’’: 10%

Table S4. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **1c** (isovalue 0.05 e/Å^3) (bpy: coordinated bipyridine fragment, py: uncoordinated pyridine)

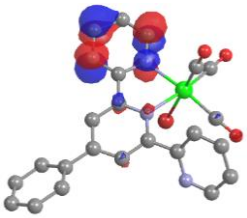
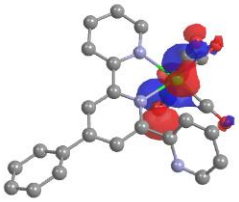
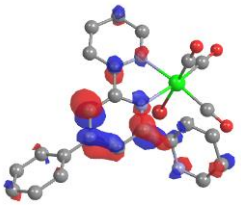
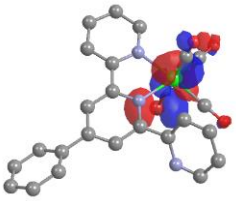
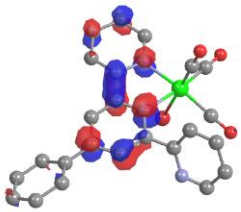
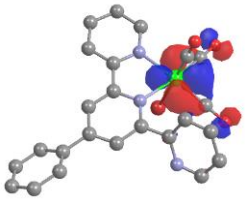
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.618 eV Re: 2% Br: 1% CO: 4% ‘’bpy’’: 90% ‘’py’’: 1% Ph: 2%	 HOMO	-6.636 eV Re: 39% Br: 39% CO: 18% ‘’bpy’’: 2% ‘’py’’: 1% Ph: 1%
 LUMO+1	-2.016 eV Re: 0% Br: 0% CO: 1% ‘’bpy’’: 72% ‘’py’’: 17% Ph: 9%	 HOMO-1	-6.709 eV Re: 35% Br: 42% CO: 16% ‘’bpy’’: 5% ‘’py’’: 0% Ph: 2%
 LUMO	-2.746 eV Re: 2% Br: 2% CO: 4% ‘’bpy’’: 82% ‘’py’’: 3% Ph: 7%	 HOMO-2	-7.207 eV Re: 59% Br: 3% CO: 25% ‘’bpy’’: 3% ‘’py’’: 9% Ph: 2%

Table S5. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **1d** (isovalue 0.05 e/Å^3) (bpy: coordinated bipyridine fragment, py: uncoordinated pyridine)

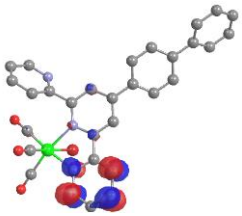
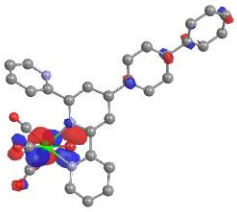
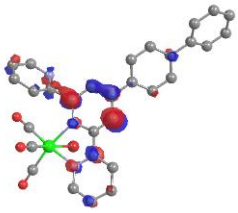
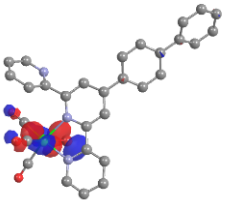
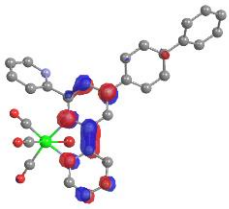
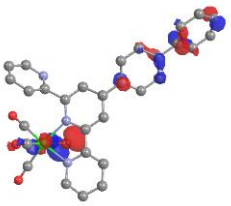
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.630 eV Re: 2% Br: 1% CO: 5% ‘’bpy’’: 85% ‘’py’’: 2% Ph_2: 5%	 HOMO	-6.611 eV Re: 29% Br: 25% CO: 14% ‘’bpy’’: 5% ‘’py’’: 1% Ph_2: 26%
 LUMO+1	-2.052 eV Re: 0% Br: 0% CO: 1% ‘’bpy’’: 70% ‘’py’’: 13% Ph_2: 15%	 HOMO-1	-6.661 eV Re: 32% Br: 33% CO: 14% ‘’bpy’’: 5% ‘’py’’: 1% Ph_2: 16%
 LUMO	-2.763 eV Re: 2% Br: 2% CO: 4% ‘’bpy’’: 80% ‘’py’’: 3% Ph_2: 10%	 HOMO-2	-6.823 eV Re: 12% Br: 29% CO: 5% ‘’bpy’’: 5% ‘’py’’: 1% Ph_2: 48%

Table S6. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **1e** (isovalue 0.05 e/Å^3) (bpy: coordinated bipyridine fragment, py: uncoordinated pyridine)

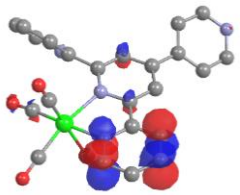
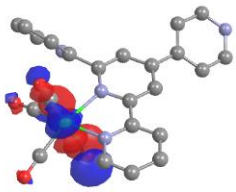
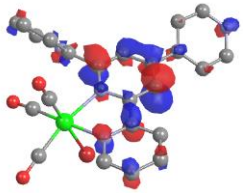
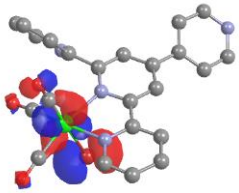
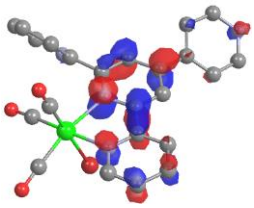
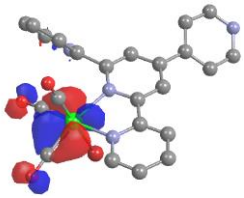
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.669 eV Re: 2% Br: 1% CO: 5% ‘’bpy’’: 84% ‘’py’’: 3% Py: 4%	 HOMO	-6.660 eV Re: 39% Br: 40% CO: 18% ‘’bpy’’: 2% ‘’py’’: 1% Py: 0%
 LUMO+1	-2.167 eV Re: 0% Br: 0% CO: 1% ‘’bpy’’: 73% ‘’py’’: 11% Py: 14%	 HOMO-1	-6.746 eV Re: 35% Br: 45% CO: 15% ‘’bpy’’: 4% ‘’py’’: 0% Py: 1%
 LUMO	-2.877 eV Re: 2% Br: 2% CO: 4% ‘’bpy’’: 78% ‘’py’’: 3% Py: 12%	 HOMO-2	-7.238 eV Re: 61% Br: 2% CO: 26% ‘’bpy’’: 2% ‘’py’’: 8% Py: 0%

Table S7. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **2a** (isovalue 0.05 e/Å^3)

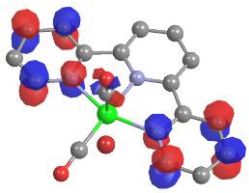
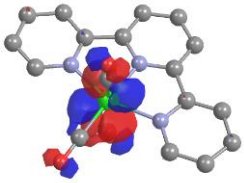
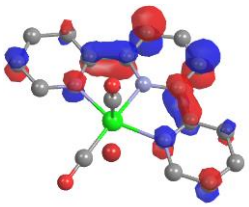
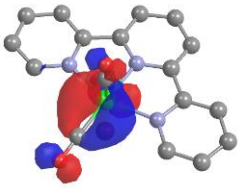
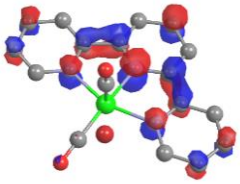
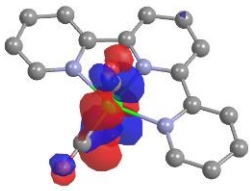
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.390 eV Re: 2% Br: 0% CO: 5% tpy: 93%	 HOMO	-5.733 eV Re: 58% Br: 10% CO: 17% tpy: 15%
 LUMO+1	-2.354 eV Re: 2% Br: 0% CO: 2% tpy: 96%	 HOMO-1	-6.059 eV Re: 66% Br: 0% CO: 27% tpy: 7%
 LUMO	-2.725 eV Re: 3% Br: 3% CO: 5% tpy: 90%	 HOMO-2	-6.306 eV Re: 45% Br: 26% CO: 21% tpy: 8%

Table S8. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **2b** (isovalue 0.05 e/Å^3)

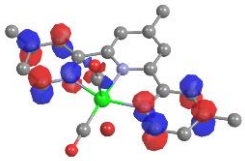
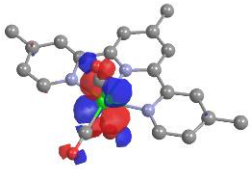
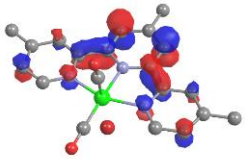
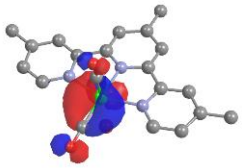
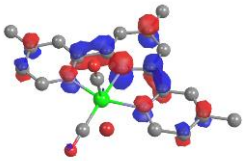
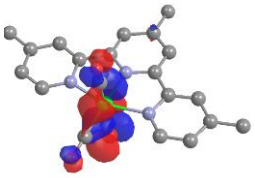
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.229 eV Re: 1% Br: 0% CO: 6% tpy: 93%	 HOMO	-5.637 eV Re: 59% Br: 9% CO: 18% tpy: 15%
 LUMO+1	-2.261 eV Re: 2% Br: 0% CO: 1% tpy: 97%	 HOMO-1	-5.969 eV Re: 65% Br: 0% CO: 27% tpy: 8%
 LUMO	-2.567 eV Re: 3% Br: 3% CO: 4% tpy: 90%	 HOMO-2	-6.225 eV Re: 45% Br: 22% CO: 22% tpy: 8%

Table S9. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **2c** (isovalue 0.05 e/Å^3)

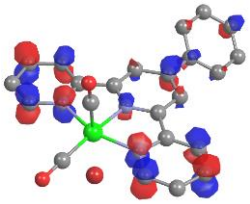
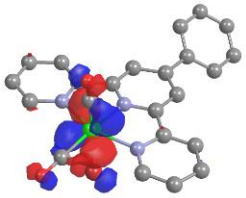
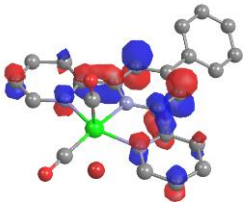
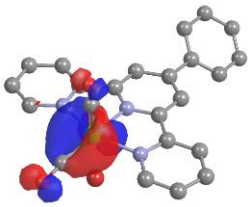
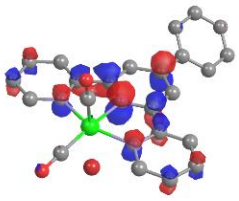
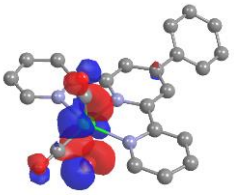
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.499 eV Re: 0% Br: 0% CO: 0% tpy: 85% ph: 15%	 HOMO	-5.729 eV Re: 59% Br: 10% CO: 17% tpy: 14% ph: 0%
 LUMO+1	-2.359 eV Re: 2% Br: 0% CO: 1% tpy: 96% ph: 1%	 HOMO-1	-6.052 eV Re: 65% Br: 0% CO: 27% tpy: 8% ph: 0%
 LUMO	-2.774 eV Re: 3% Br: 3% CO: 5% tpy: 84% ph: 6%	 HOMO-2	-6.266 eV Re: 44% Br: 23% CO: 21% tpy: 8% ph: 3%

Table S10. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **2d** (isovalue 0.05 e/Å^3)

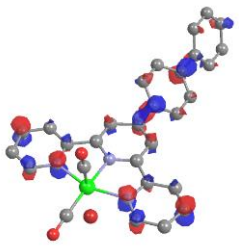
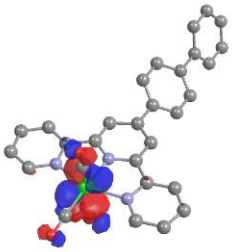
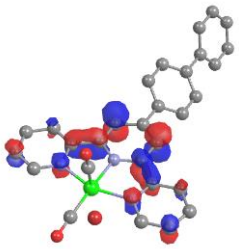
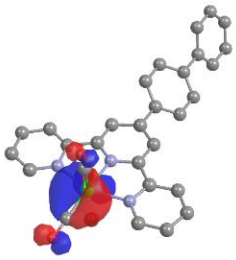
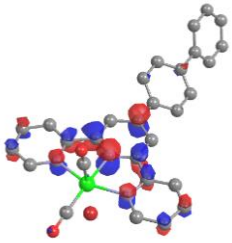
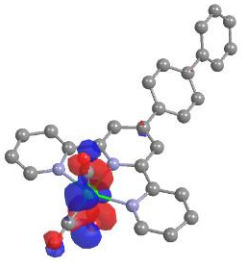
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.614 eV Re: 0% Br: 0% CO: 0% tpy: 60% ph2: 39%	 HOMO	-5.729 eV Re: 59% Br: 10% CO: 17% tpy: 14% ph2: 0%
 LUMO+1	-2.359 eV Re: 2% Br: 0% CO: 2% tpy: 96% ph2: 0%	 HOMO-1	-6.051 eV Re: 65% Br: 0% CO: 27% tpy: 8% ph2: 0%
 LUMO	-2.790 eV Re: 3% Br: 3% CO: 4% tpy: 82% ph2: 8%	 HOMO-2	-6.241 eV Re: 42% Br: 20% CO: 20% tpy: 8% ph2: 10%

Table S11. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **2e** (isovalue 0.05 e/Å^3)

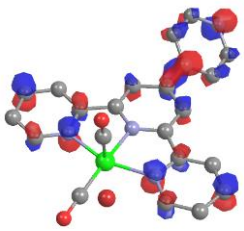
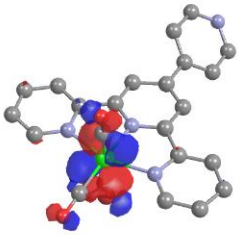
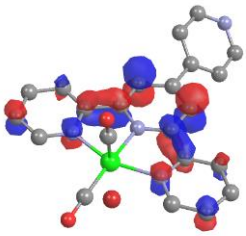
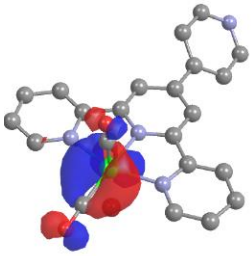
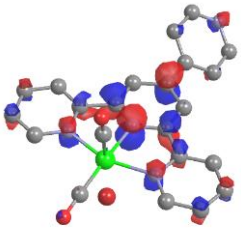
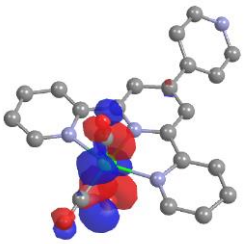
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.703 eV Re: 0% Br: 0% CO: 0% tpy: 63% py: 37%	 HOMO	-5.758 eV Re: 58% Br: 10% CO: 17% tpy: 14% py: 0%
 LUMO+1	-2.425 eV Re: 2% Br: 0% CO: 2% tpy: 96% py: 0%	 HOMO-1	-6.085 eV Re: 65% Br: 0% CO: 27% tpy: 8% py: 0%
 LUMO	-2.891 eV Re: 3% Br: 3% CO: 5% tpy: 80% py: 10%	 HOMO-2	-6.317 eV Re: 44% Br: 25% CO: 21% tpy: 8% py: 1%

Table S12. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **3a** (isovalue 0.05 e/Å^3)

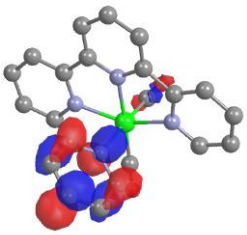
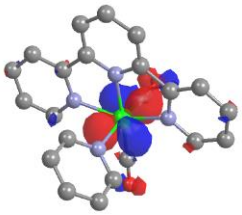
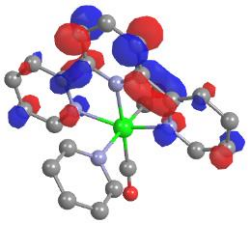
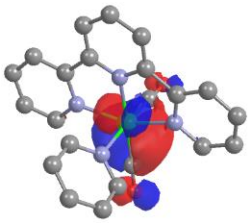
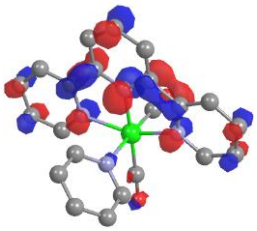
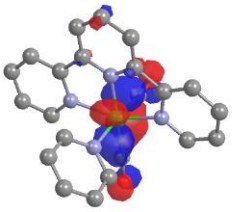
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.778 eV Re: 2% CO: 6% tpy: 4% py: 88%	 HOMO	-6.044 eV Re: 64% CO: 17% tpy: 17% py: 2%
 LUMO+1	-2.558 eV Re: 2% CO: 1% tpy: 96% py: 1%	 HOMO-1	-6.294 eV Re: 66% CO: 26% tpy: 8% py: 0%
 LUMO	-2.949 eV Re: 3% CO: 5% tpy: 91% py: 1%	 HOMO-2	-6.726 eV Re: 58% CO: 27% tpy: 12% py: 3%

Table S13. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **3b** (isovalue 0.05 e/Å^3)

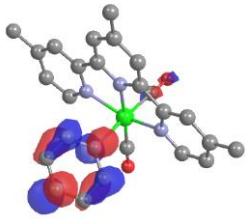
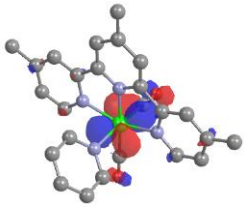
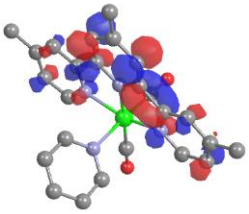
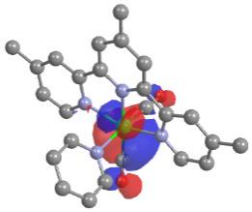
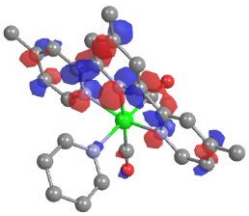
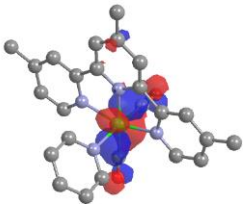
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.741 eV Re: 2% CO: 5% tpy: 3% py: 90%	 HOMO	-5.929 eV Re: 63% CO: 17% tpy: 18% py: 2%
 LUMO+1	-2.440 eV Re: 1% CO: 1% tpy: 97% py: 1%	 HOMO-1	-6.194 eV Re: 66% CO: 27% tpy: 8% py: 0%
 LUMO	-2.762 eV Re: 3% CO: 5% tpy: 92% py: 1%	 HOMO-2	-6.613 eV Re: 57% CO: 27% tpy: 13% py: 3%

Table S14. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **3c** (isovalue 0.05 e/Å^3)

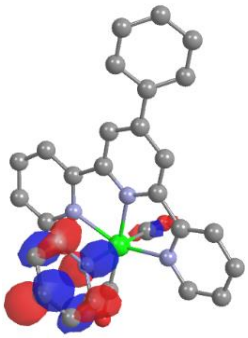
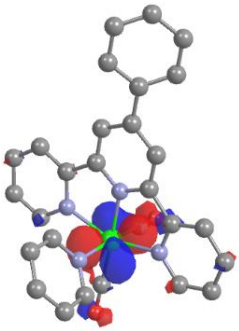
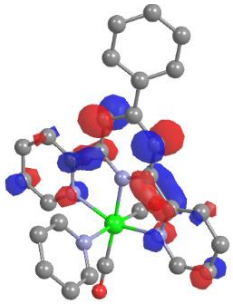
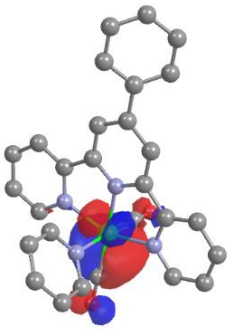
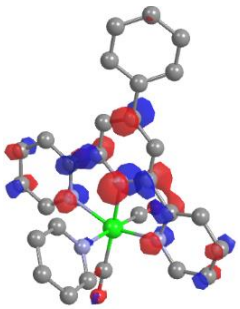
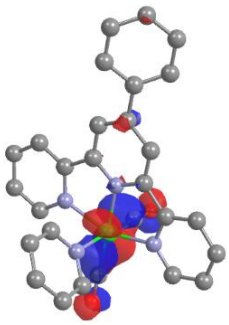
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.741 eV Re: 2% CO: 5% tpy: 5% ph: 0% py: 87%	 HOMO	-6.038 eV Re: 64% CO: 17% tpy: 17% ph: 0% py: 2%
 LUMO+1	-2.558 eV Re: 2% CO: 1% tpy: 96% ph: 0% py: 1%	 HOMO-1	-6.281 eV Re: 66% CO: 26% tpy: 8% ph: % py: 0%
 LUMO	-2.986 eV Re: 3% CO: 5% tpy: 86% ph: 6% py: 1%	 HOMO-2	-6.644 eV Re: 53% CO: 25% tpy: 12% ph: 7% py: 3%

Table S15. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **3d** (isovalue 0.05 e/Å^3)

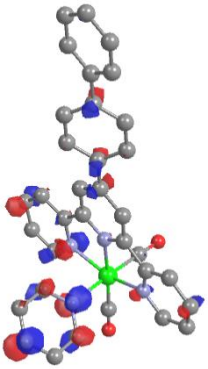
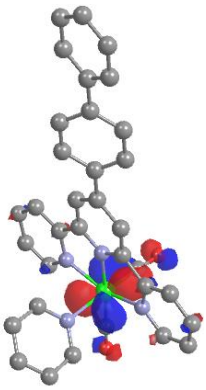
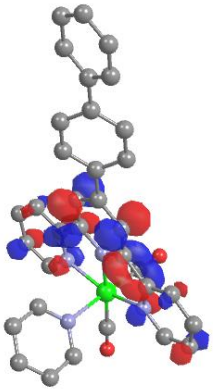
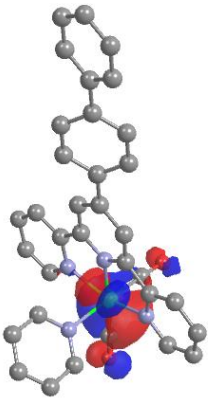
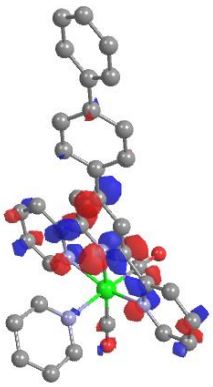
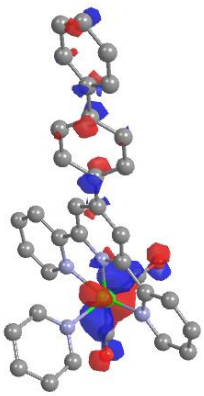
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.764 eV Re: 1% CO: 3% tpy: 38% ph2: 20% py: 38%	 HOMO	-6.036 eV Re: 64% CO: 17% tpy: 17% ph2: 0% py: 2%
 LUMO+1	-2.555 eV Re: 2% CO: 1% tpy: 96% ph2: 0% py: 1%	 HOMO-1	-6.279 eV Re: 66% CO: 26% tpy: 8% ph2: 0% py: 0%
 LUMO	-2.999 eV Re: 3% CO: 5% tpy: 84% ph2: 8% py: 1%	 HOMO-2	-6.560 eV Re: 37% CO: 18% tpy: 11% ph2: 32% py: 2%

Table S16. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **3e** (isovalue 0.05 e/Å^3)

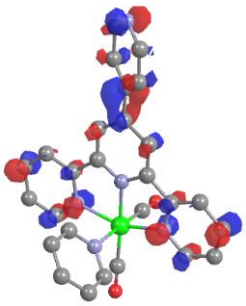
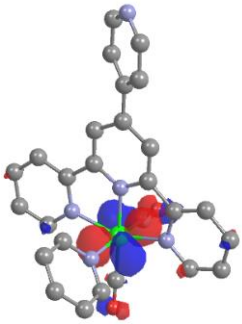
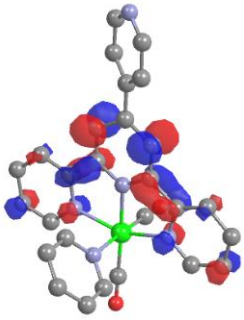
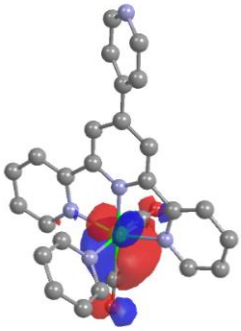
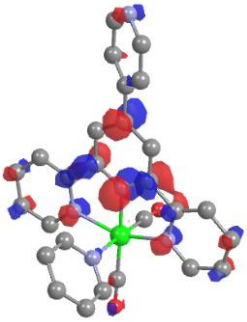
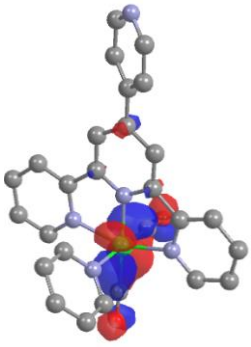
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.863 eV Re: 0% CO: 0% tpy: 66% 4py: 31% py: 2%	 HOMO	-6.071 eV Re: 64% CO: 17% tpy: 17% 4py: 0% py: 2%
 LUMO+1	-2.628 eV Re: 2% CO: 1% tpy: 96% 4py: 0% py: 1%	 HOMO-1	-6.315 eV Re: 66% CO: 26% tpy: 8% 4py: 0% py: 0%
 LUMO	-3.101 eV Re: 3% CO: 5% tpy: 82% 4py: 9% py: 1%	 HOMO-2	-6.726 eV Re: 57% CO: 26% tpy: 12% 4py: 3% py: 3%

Table S17. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **4a** (isovalue 0.05 e/Å^3)

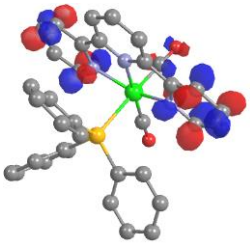
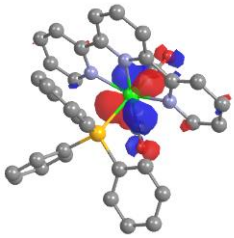
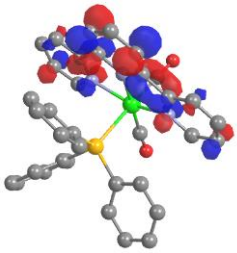
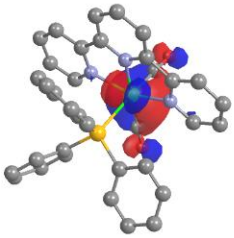
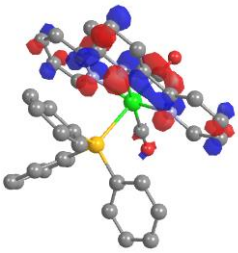
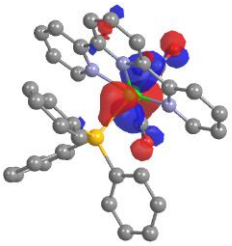
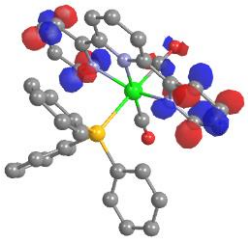
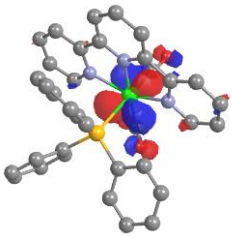
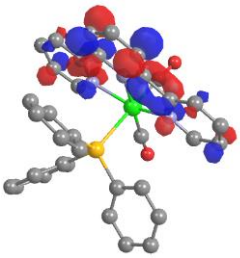
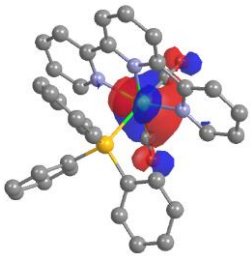
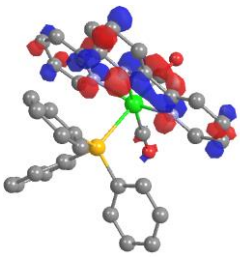
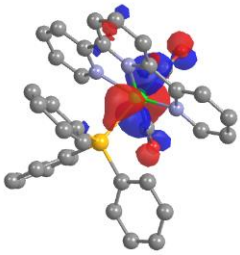
Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.778 eV Re: 2% CO: 7% tpy: 86% PPh3: 4%	 HOMO	-6.186 eV Re: 64% CO: 17% tpy: 17% PPh3: 2%
 LUMO+1	-2.553 eV Re: 2% CO: 1% tpy: 96% PPh3: 1%	 HOMO-1	-6.403 eV Re: 65% CO: 25% tpy: 10% PPh3: 0%
 LUMO	-2.907 eV Re: 2% CO: 5% tpy: 90% PPh3: 3%	 HOMO-2	-6.863 eV Re: 53% CO: 24% tpy: 15% PPh3: 8%

Table S18. Selected molecular orbitals with relative Mulliken contributions of each fragments and energies for complex **4b** (isovalue 0.05 e/Å^3)

Orbital	Energy and contributions	Orbital	Energy and contributions
 LUMO+2	-1.444 eV Re: 2% CO: 6% tpy: 83% PPh3: 10%	 HOMO	-6.092 eV Re: 63% CO: 16% tpy: 18% PPh3: 2%
 LUMO+1	-2.435 eV Re: 1% CO: 1% tpy: 97% PPh3: 1%	 HOMO-1	-6.318 eV Re: 65% CO: 26% tpy: 9% PPh3: 0%
 LUMO	-2.723 eV Re: 2% CO: 4% tpy: 91% PPh3: 2%	 HOMO-2	-6.777 eV Re: 57% CO: 25% tpy: 16% PPh3: 6%

C) Absorption and emission data (experimental and theoretical)

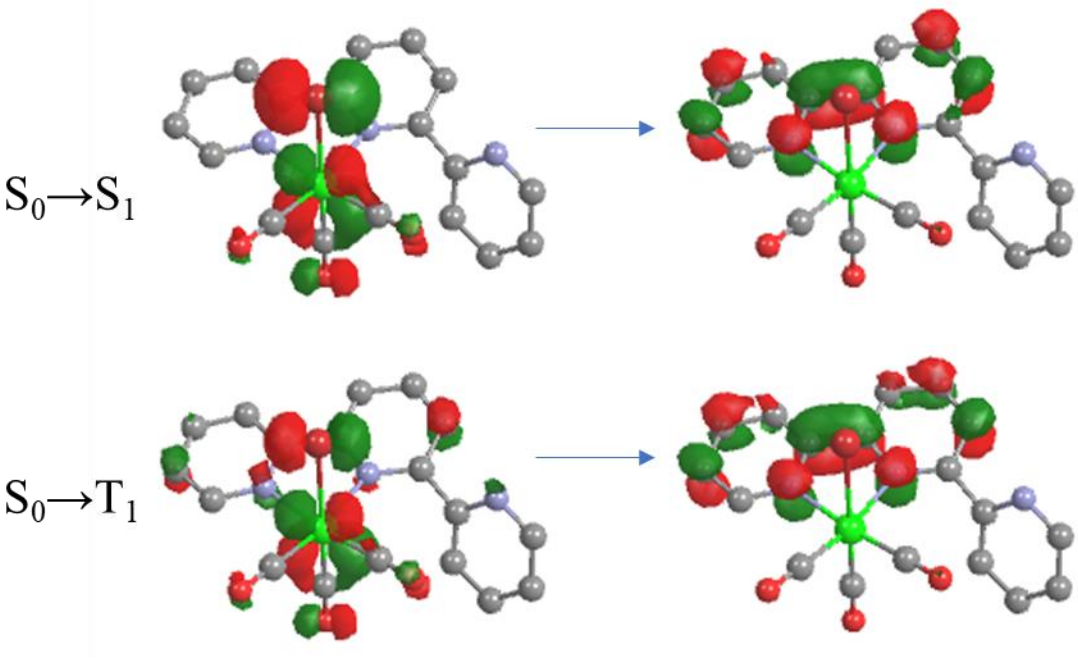


Figure S18. Natural transition orbitals for **1a** lowest energy transitions.

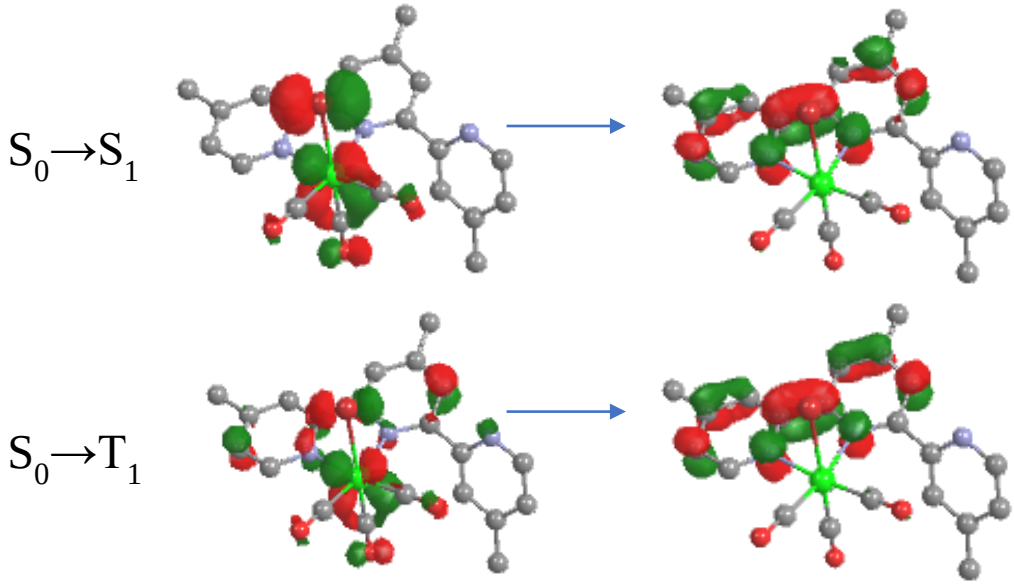


Figure S19. Natural transition orbitals for **1b** lowest energy transitions.

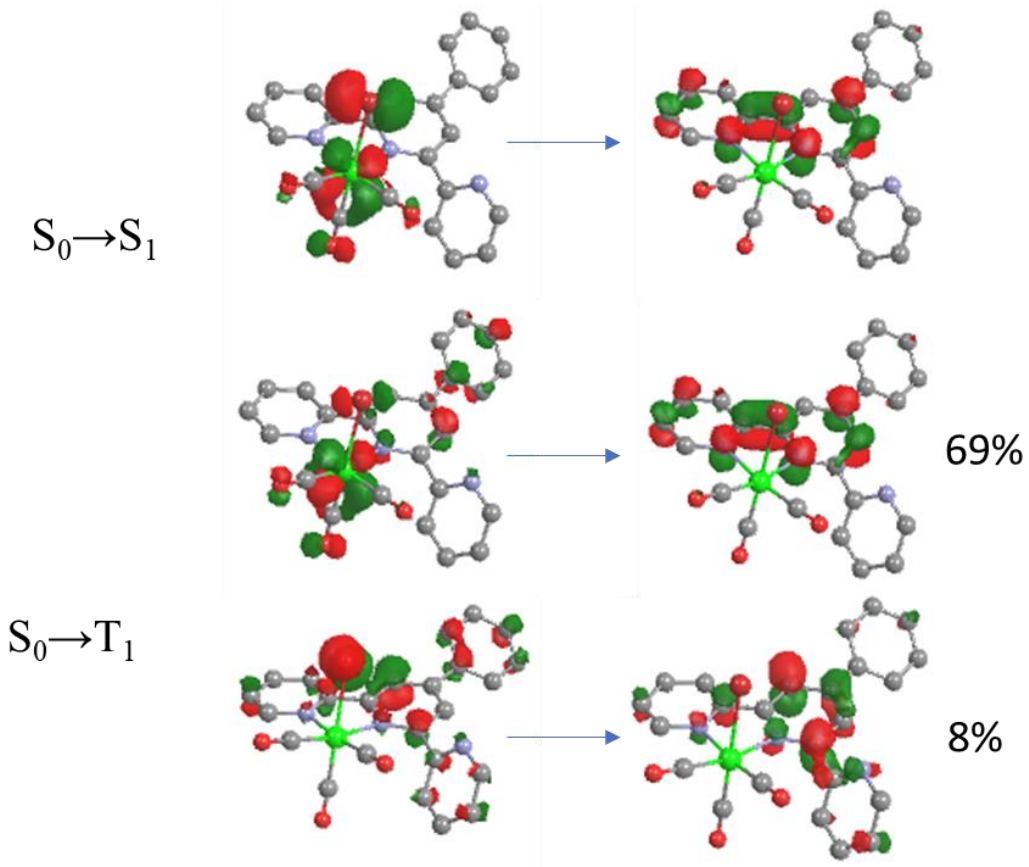


Figure S20. Natural transition orbitals for **1c** lowest energy transitions.

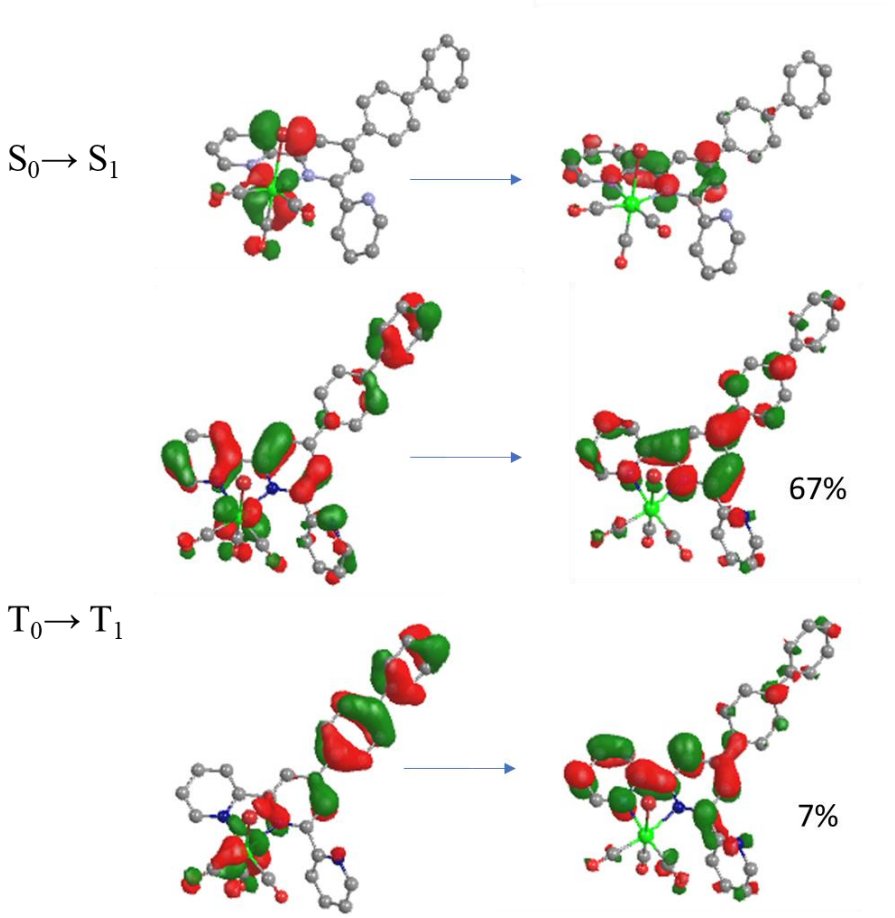


Figure S21. Natural transition orbitals for **1d** lowest energy transitions.

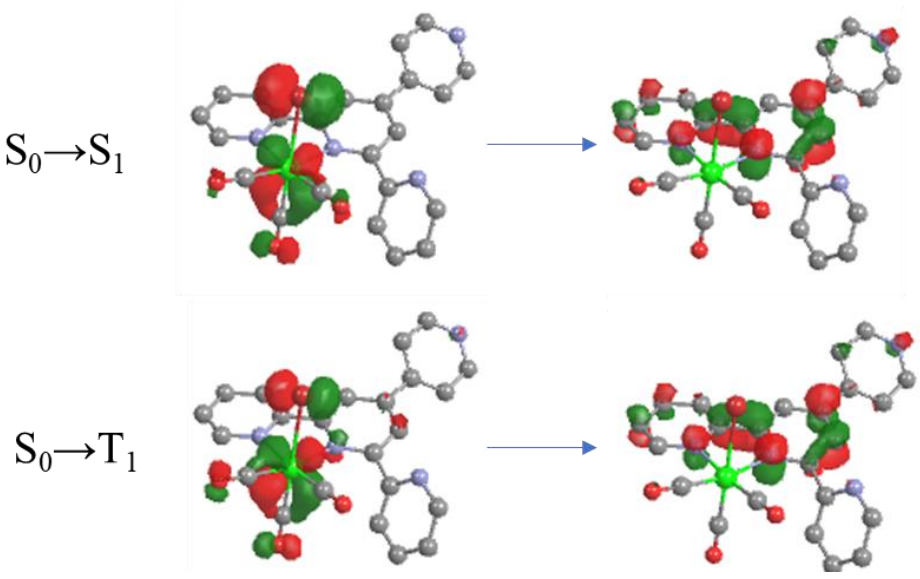


Figure S22. Natural transition orbitals for **1e** lowest energy transitions.

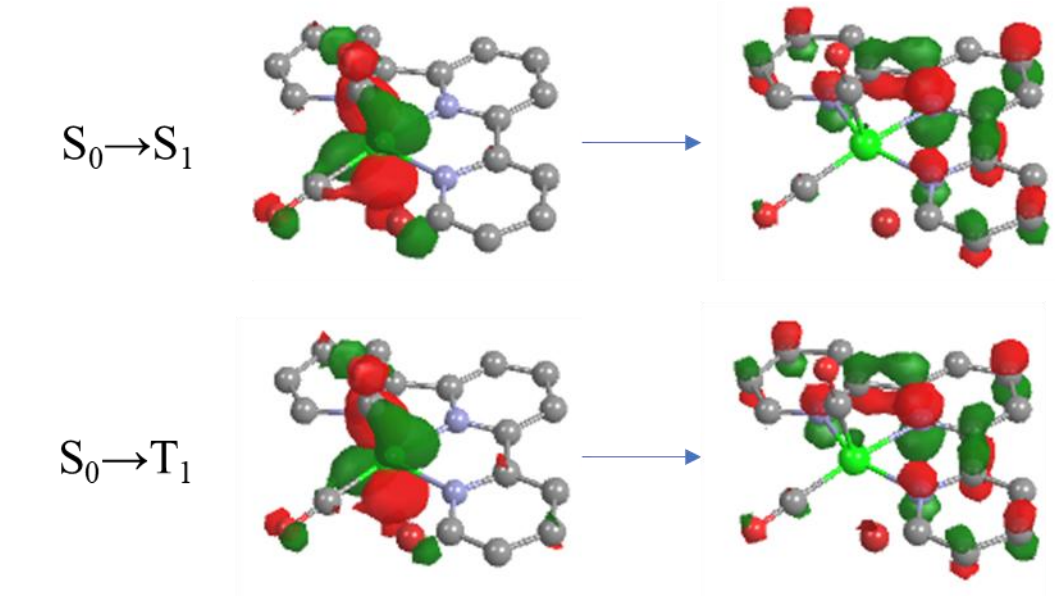


Figure S23. Natural transition orbitals for **2a** lowest energy transitions.

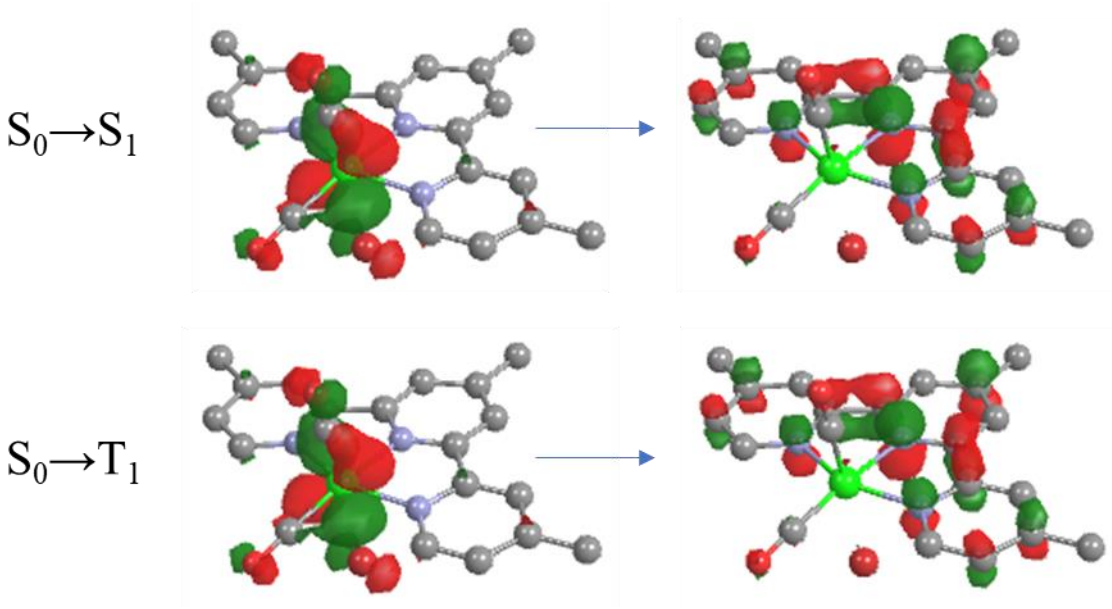


Figure S24. Natural transition orbitals for **2b** lowest energy transitions.

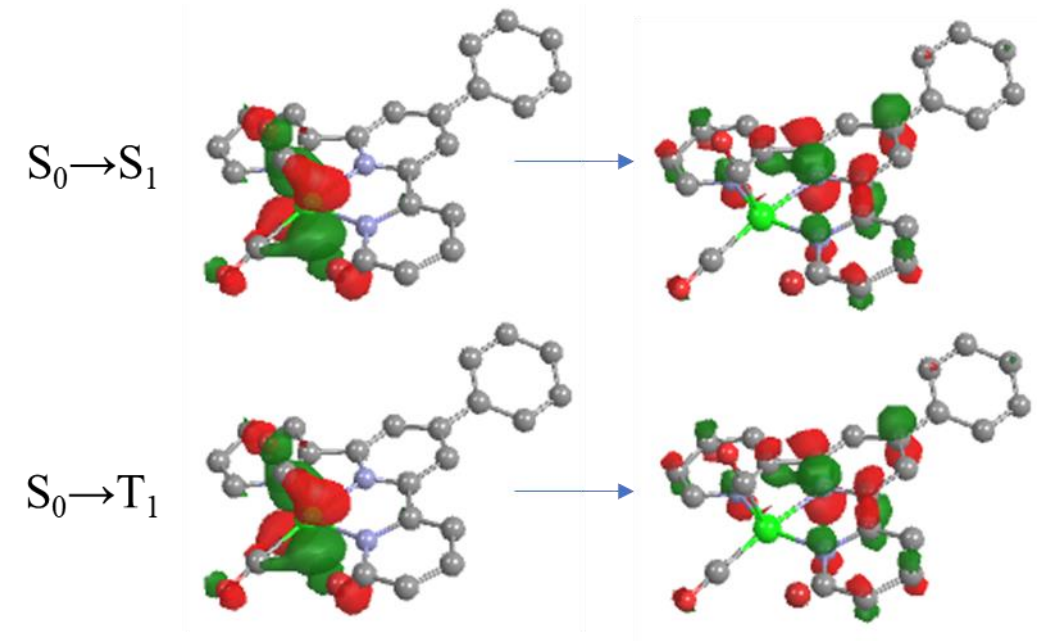


Figure S25. Natural transition orbitals for **2c** lowest energy transitions.

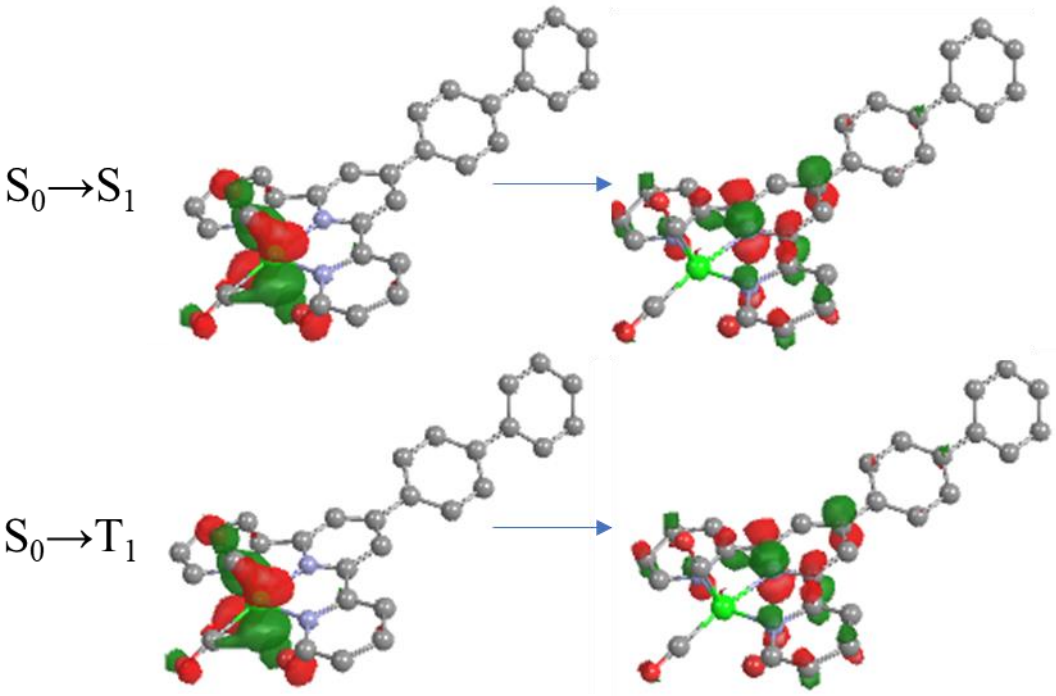


Figure S26. Natural transition orbitals for **2d** lowest energy transitions.

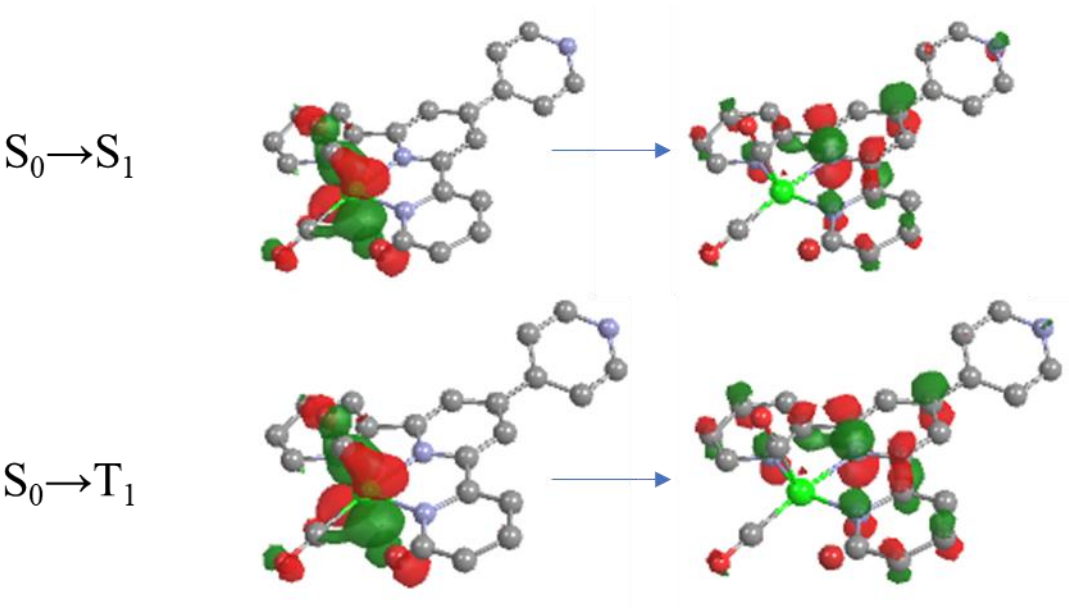


Figure S27. Natural transition orbitals for **2e** lowest energy transitions.

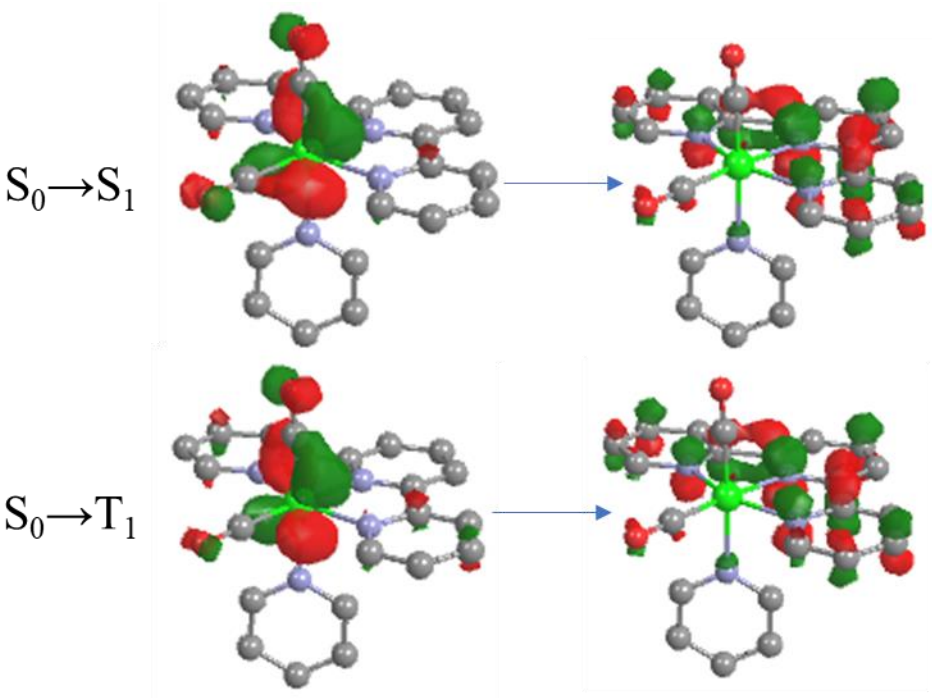


Figure S28. Natural transition orbitals for **3a** lowest energy transitions.

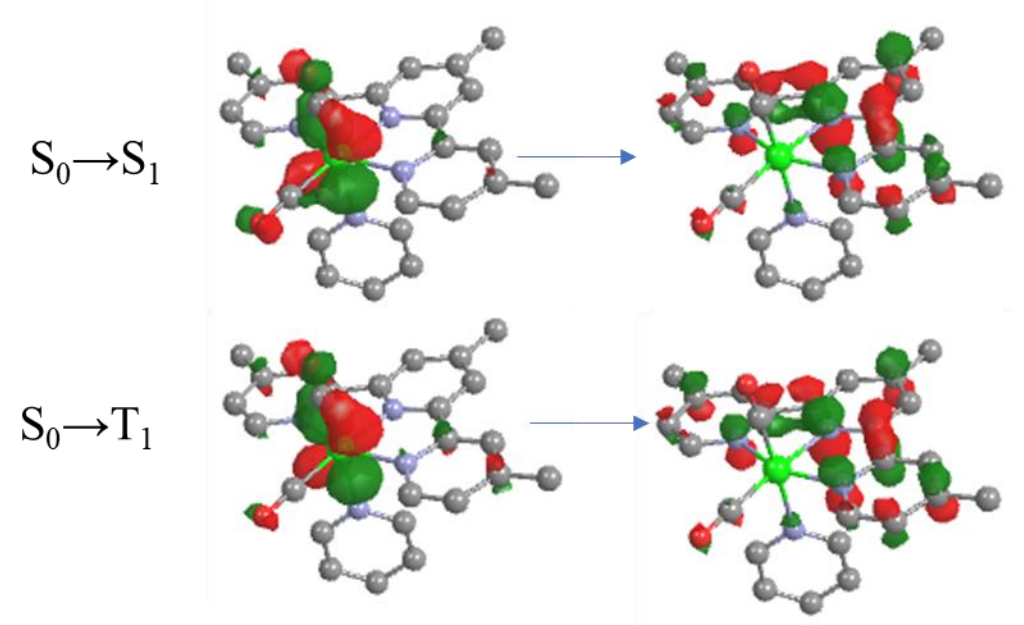


Figure S29. Natural transition orbitals for **3b** lowest energy transitions.

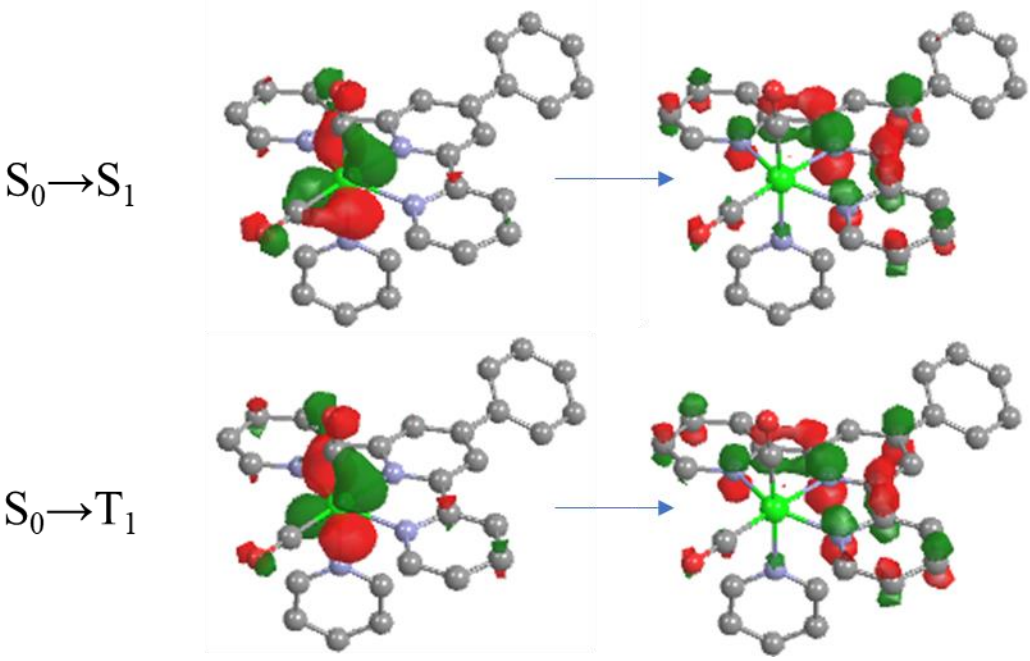


Figure S30. Natural transition orbitals for **3c** lowest energy transitions.

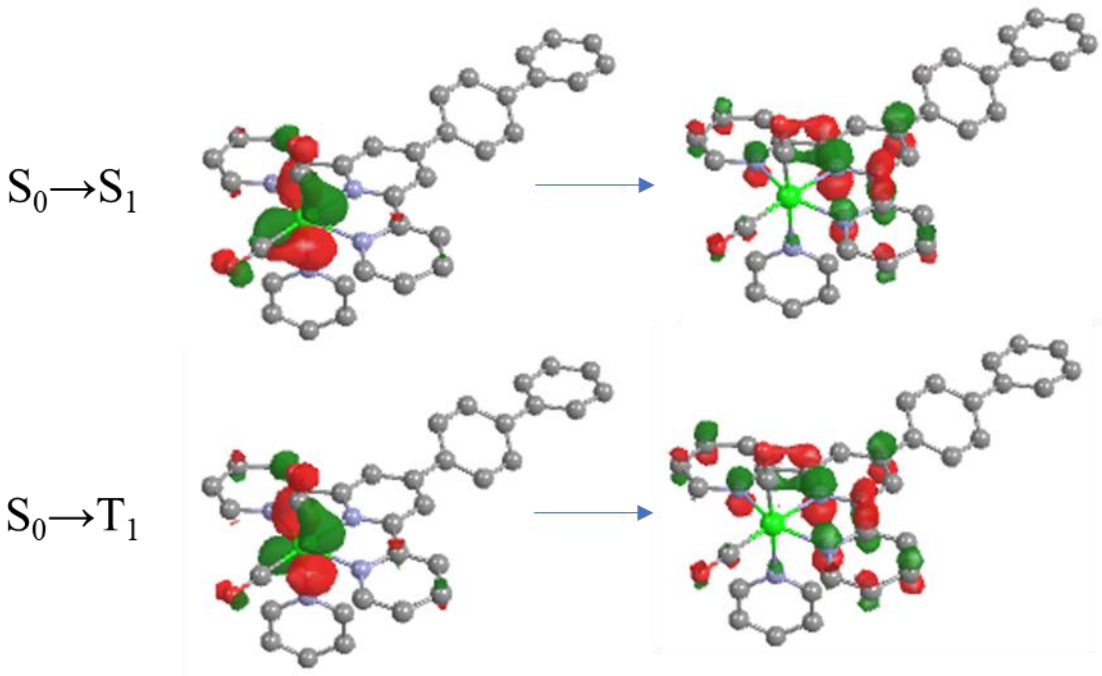


Figure S31. Natural transition orbitals for **3d** lowest energy transitions.

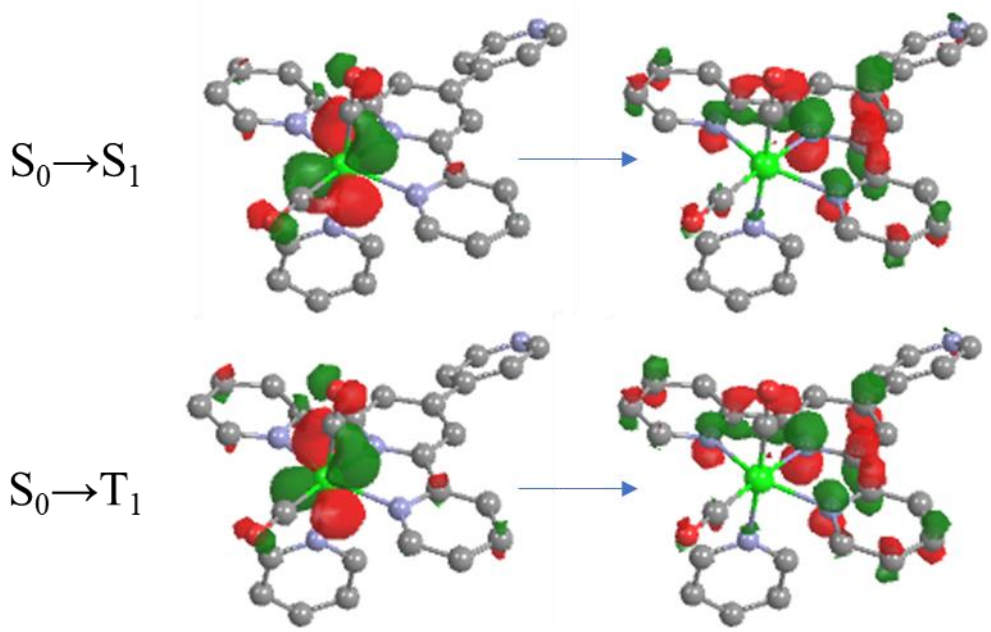


Figure S32. Natural transition orbitals for **3e** lowest energy transitions.

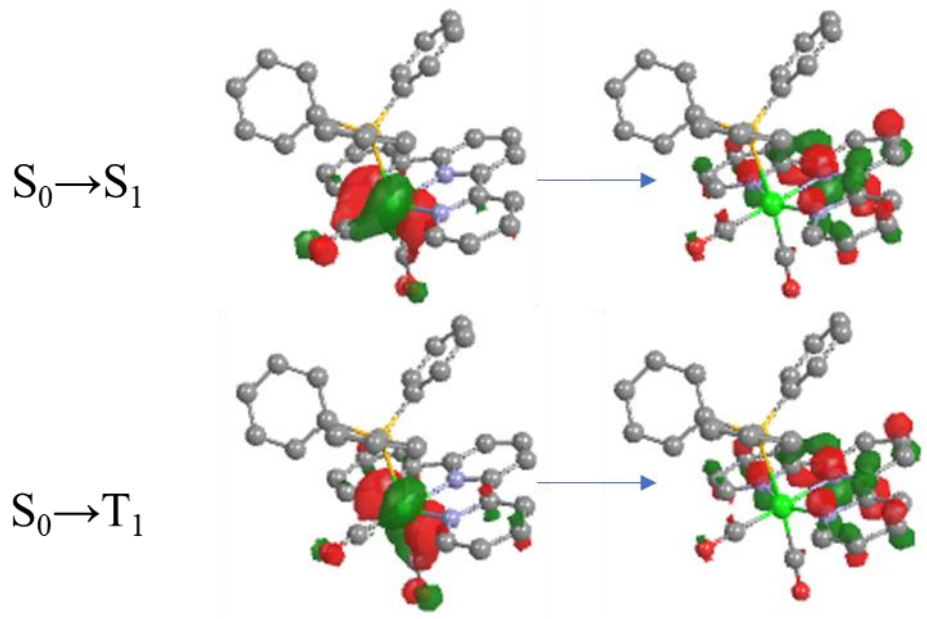


Figure S33. Natural transition orbitals for **4a** lowest energy transitions.

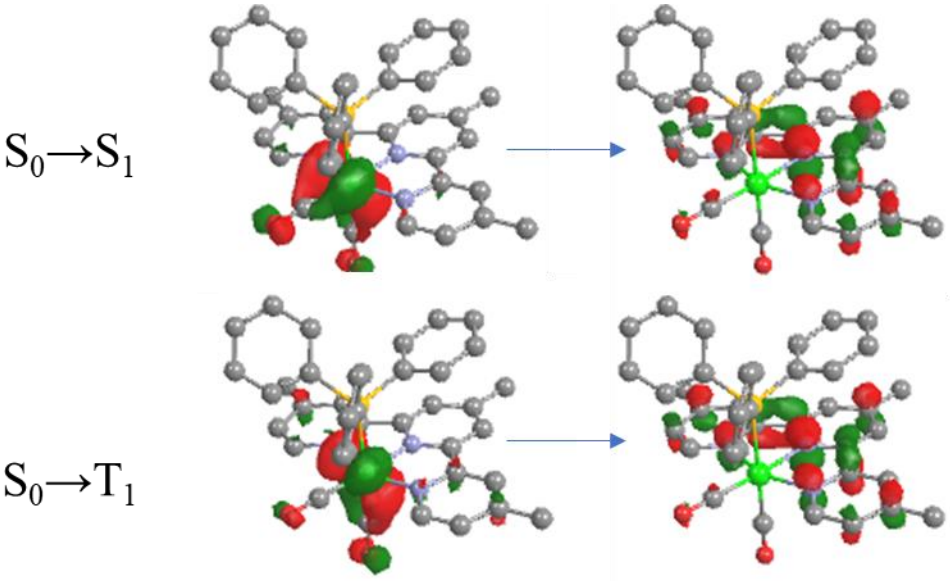


Figure S34. Natural transition orbitals for **4b** lowest energy transitions.

Table S19. Complete list of absorption maxima and molar absorption coefficients for all complexes measured in acetonitrile.

Complex	λ_{max} (nm) (ε (10^{-3} / L $mol^{-1}cm^{-1}$))
1a	367 (2.2), 322 (11.1, sh), 310 (12.6), 247 (17.0), 210 (31.1, sh)
1b	360 (2.8), 319 (13.2, sh), 308 (14.5), 248 (20.9)
1c	386 (3.7), 328 (12.8, sh), 266 (25.5), 218 (32.8, sh)
1d	364 (12.6, sh), 320 (33.3), 276 (28.3), 248 (28.0)
1e	388 (5.1), 322 (14.6), 265 (28.7), 251 (29.9)
2a	690 (1.1), 547 (1.2), 446 (3.3), 395 (3.3), 330 (21.0, sh), 323 (22.0), 278 (16.5), 241 (20.2, sh) 229 (22.9, sh)
2b	660 (1.6), 534 (1.8, sh), 454 (4.2, sh), 390 (4.3, sh), 326 (27.2, sh), 318 (27.8, sh), 241 (27.4), 214 (42.7, sh)
2c	700 (1.2), 473 (6.0), 398 (4.6), 334 (22.5, sh), 323 (24.8), 286 (41.4), 239 (23.8, sh)
2d	705 (1.4), 475 (8.8), 401 (5.8), 328 (46.6), 287 (37.6), 234 (32.4)
2e	721 (0.6), 481 (3.5), 402 (2.8), 328 (13.5), 283 (23.9), 227 (24.6, sh)
3a	647 (1.5), 516 (1.7), 440 (4.8), 380 (6.0), 322 (37.3), 281 (22.7), 274 (19.6, sh), 227 (29.5, sh)
3b	621 (2.0), 514 (2.2), 428 (6.1), 379 (7.7), 318 (46.4), 283 (24.7), 274 (22.8), 234 (40.0, sh)
3c	661 (1.2), 448 (7.0), 382 (6.1), 323 (31,8), 285 (38.4), 240 (21.9)
3d	661 (1.3), 449 (10.0), 325 (46.4), 285 (43.2), 235 (30.7)
3e	678 (1.4), 454 (8.2), 385 (7.2), 326 (33.8), 284 (44.5), 277 (38.0, sh), 263 (28.9), 242 (29.0)
4a	590 (1.1), 488 (1.4), 421 (3.8), 374 (3.2), 320 (27.7), 273 (21.0)
4b	579 (1.5, sh), 487 (1.8), 415 (4,5), 371 (4.3), 317 (32.8), 286 (19.1, sh), 274 (22.7)

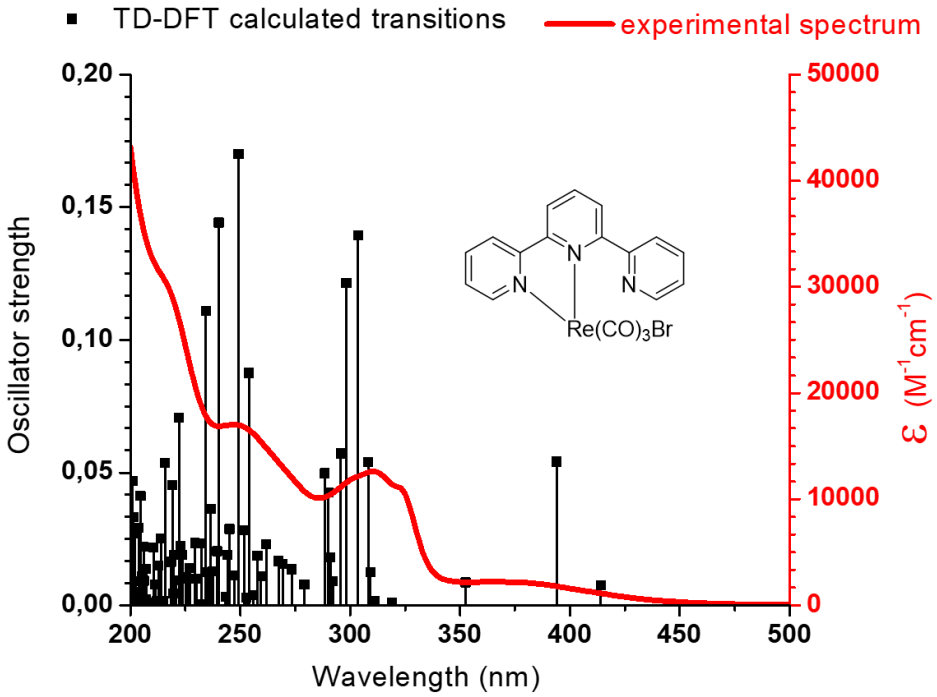


Figure S35. Theoretical and experimental absorption spectra for complex **1a**

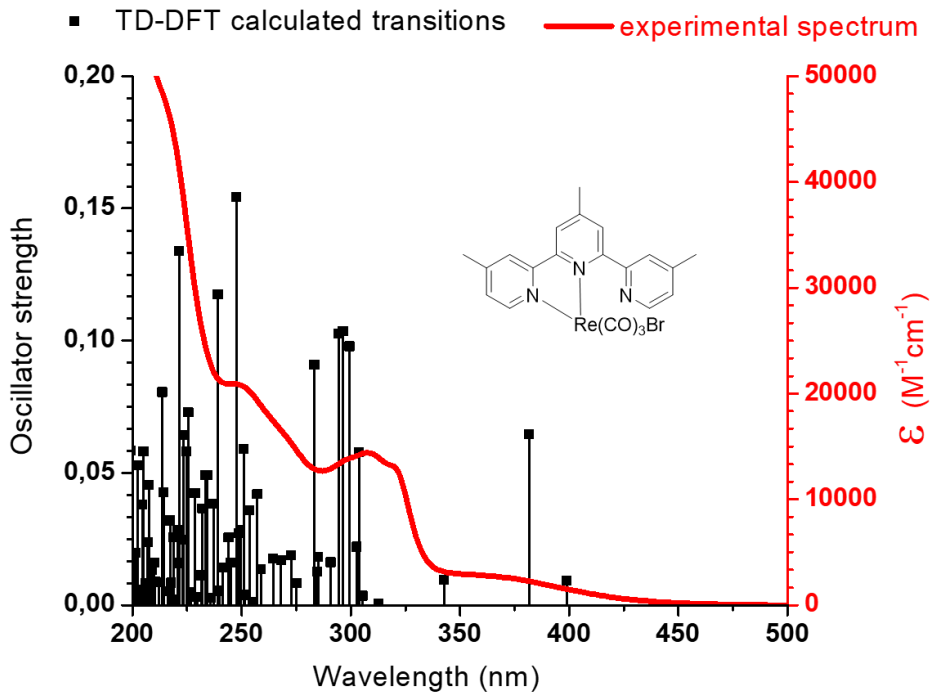


Figure S36. Theoretical and experimental absorption spectra for complex **1b**

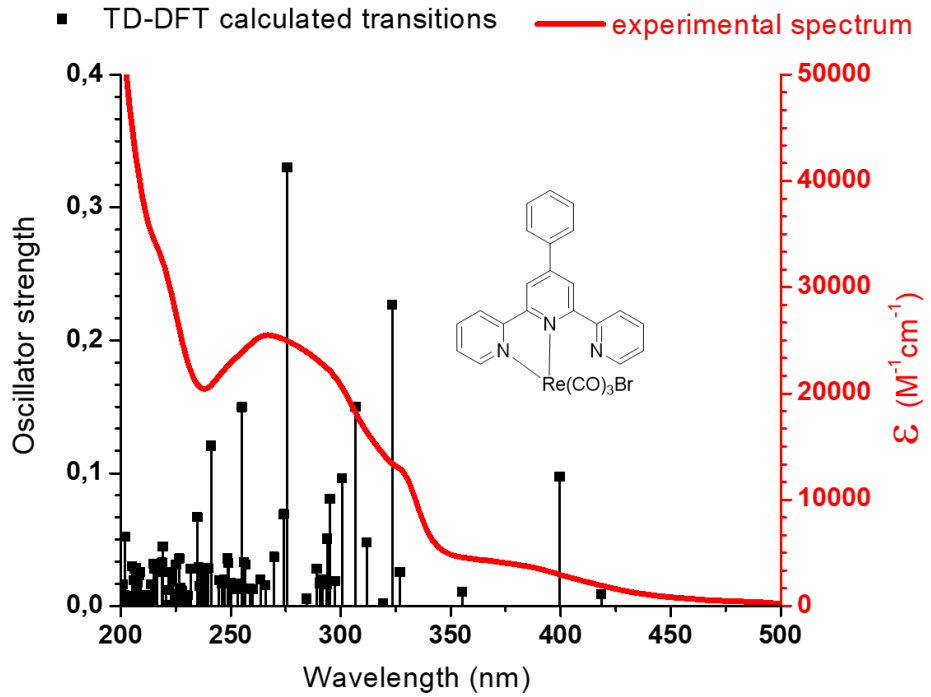


Figure S37. Theoretical and experimental absorption spectra for complex **1c**

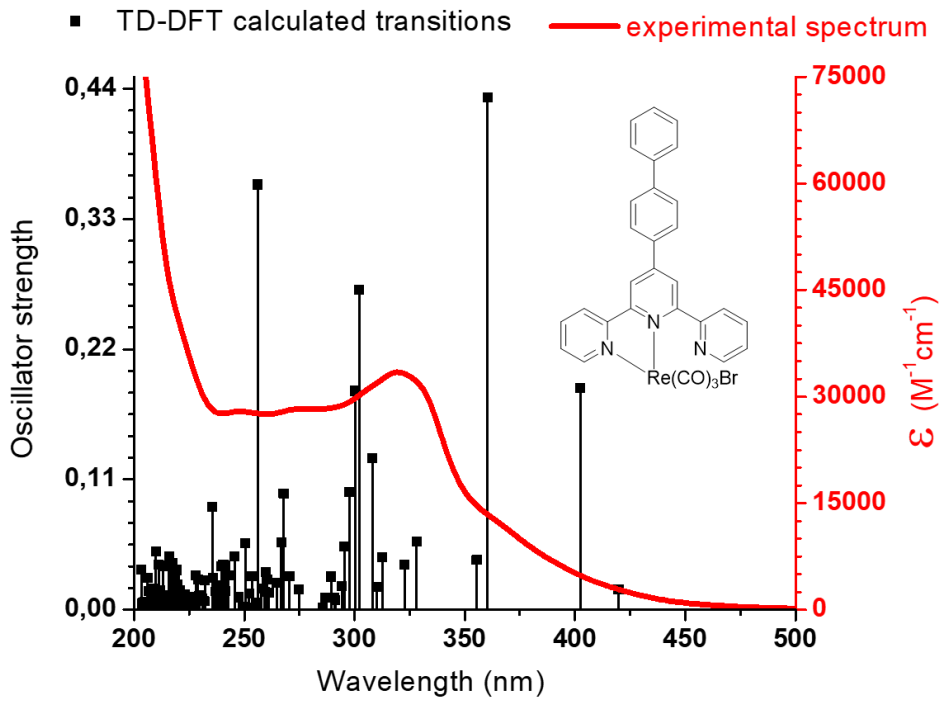


Figure S38. Theoretical and experimental absorption spectra for complex **1d**

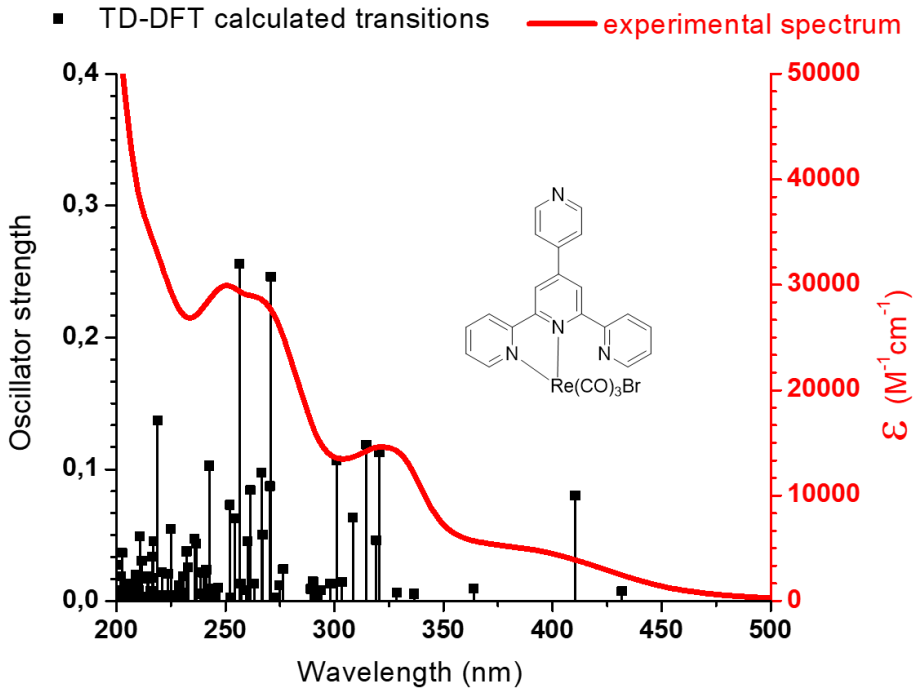


Figure S39. Theoretical and experimental absorption spectra for complex **1e**

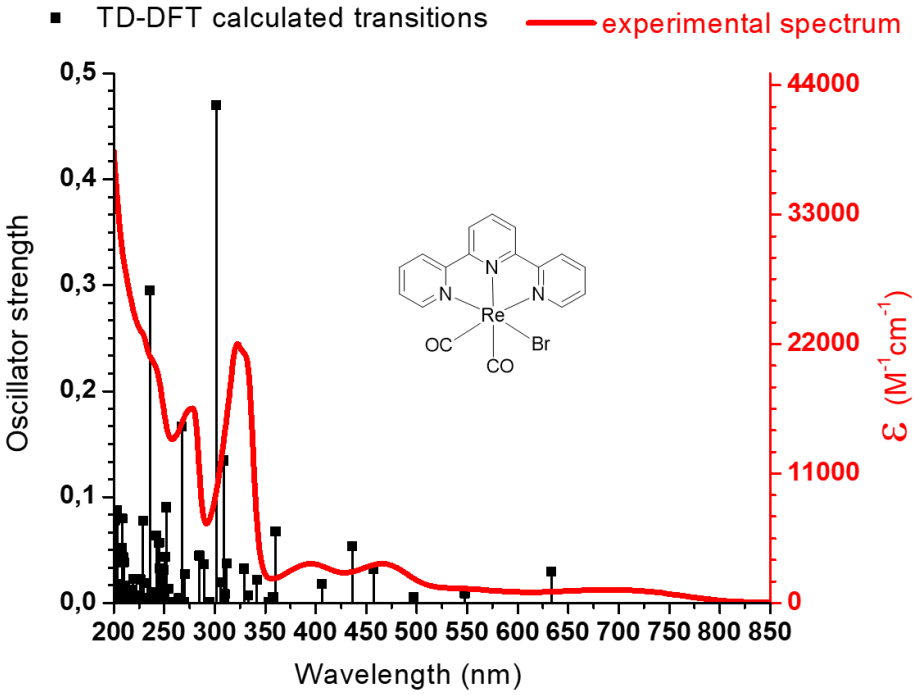


Figure S40. Theoretical and experimental absorption spectra for complex **2a**

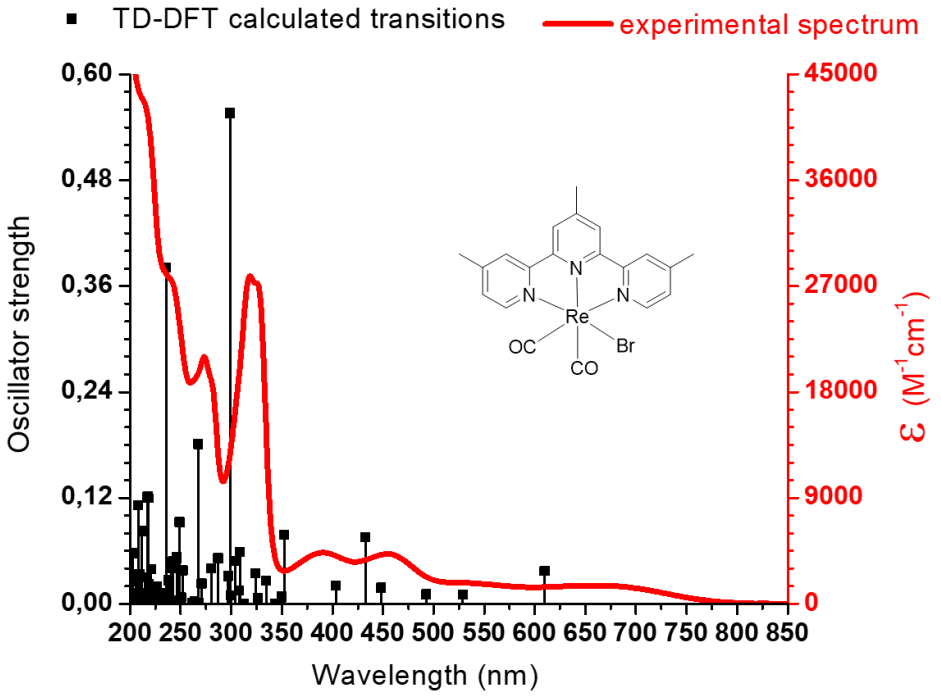


Figure S41. Theoretical and experimental absorption spectra for complex **2b**

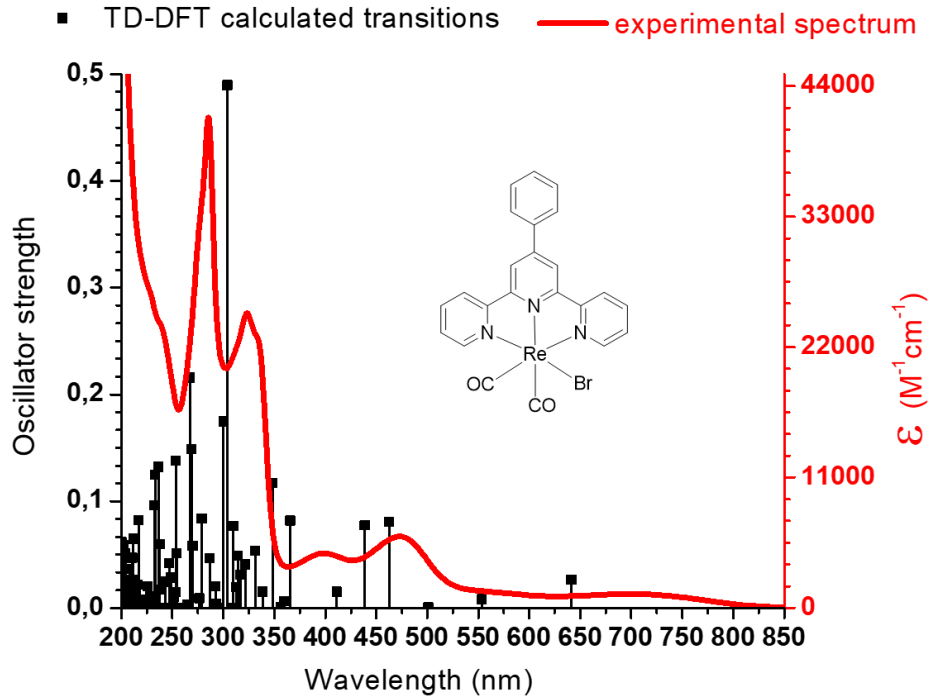


Figure S42. Theoretical and experimental absorption spectra for complex **2c**

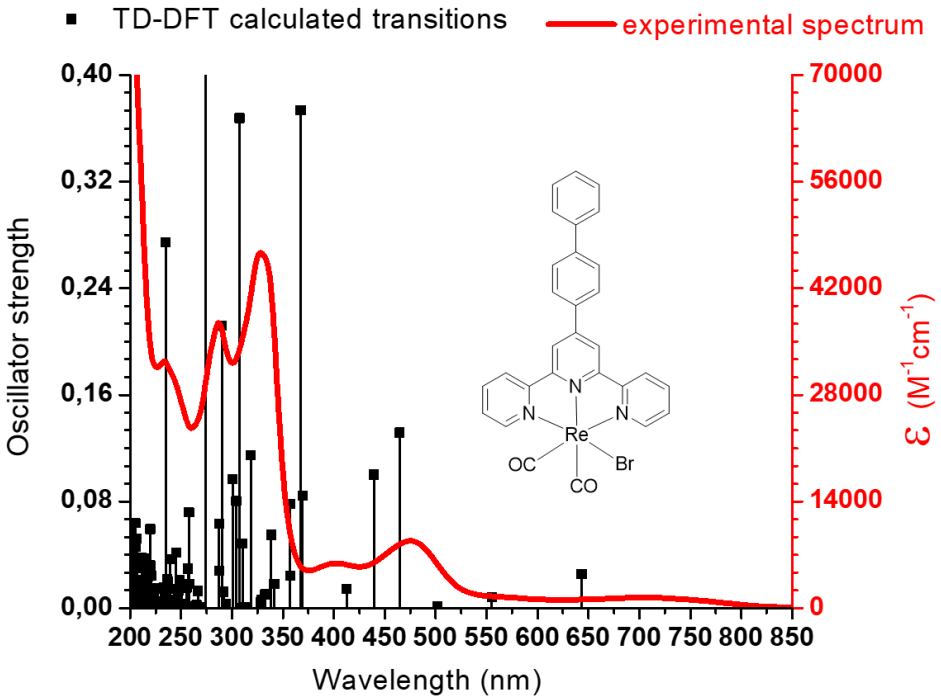


Figure S43. Theoretical and experimental absorption spectra for complex **2d**

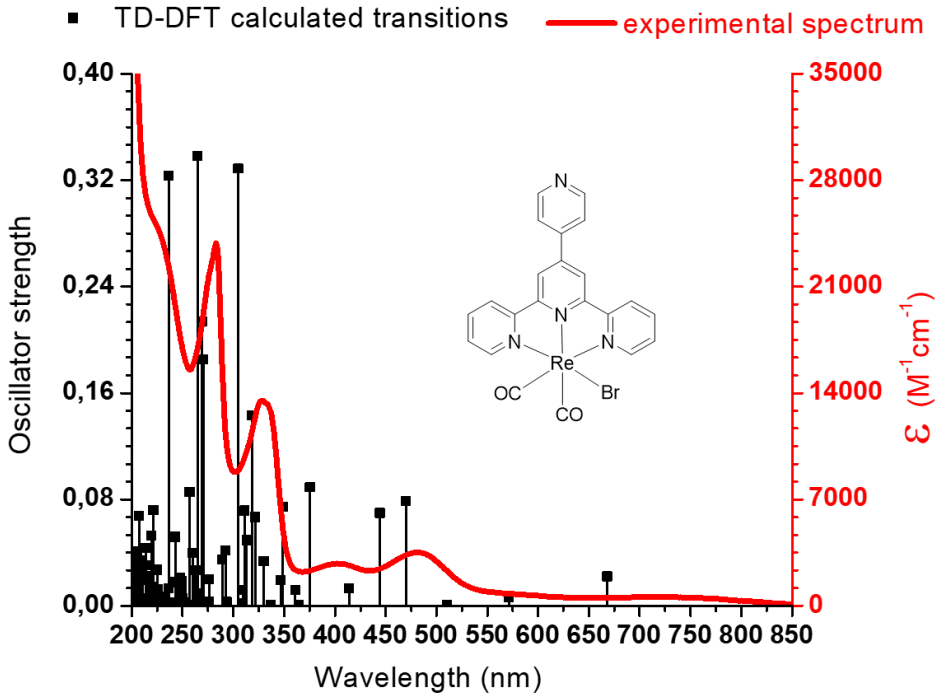


Figure S44. Theoretical and experimental absorption spectra for complex **2e**

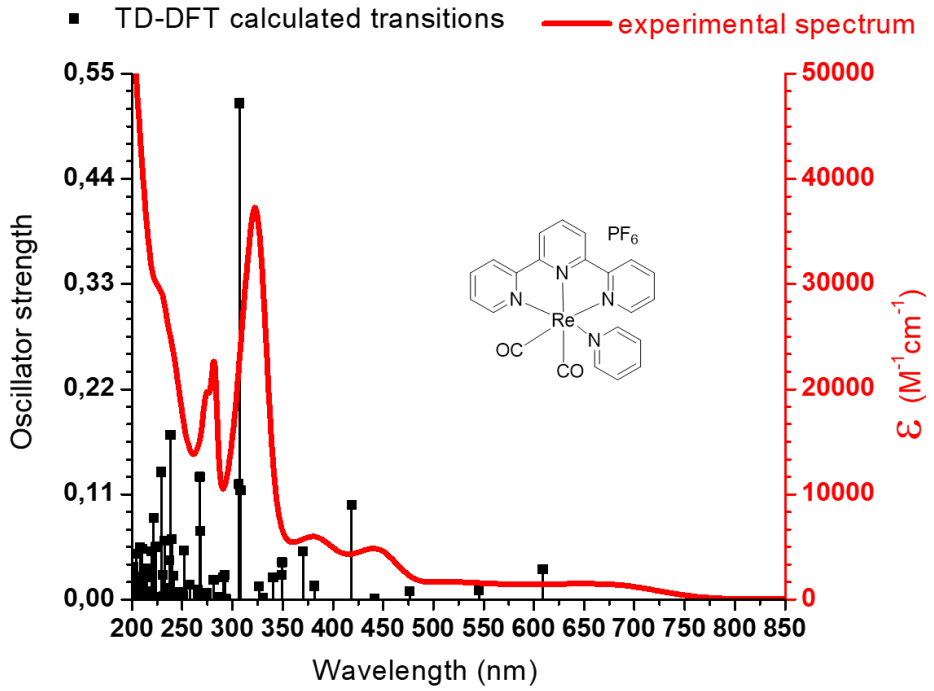


Figure S45. Theoretical and experimental absorption spectra for complex **3a**

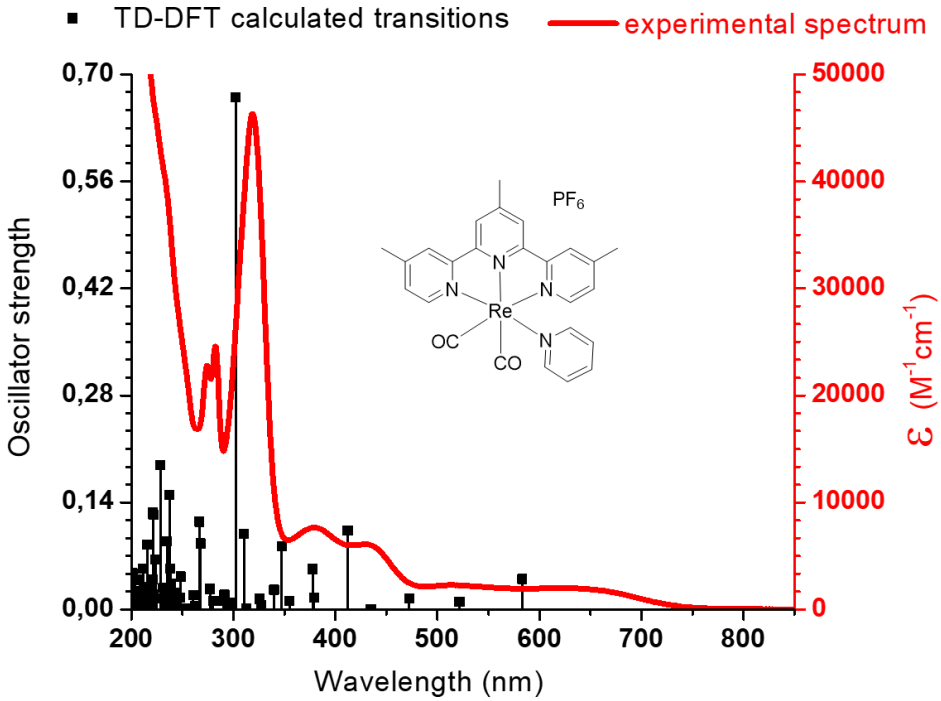


Figure S46. Theoretical and experimental absorption spectra for complex **3b**

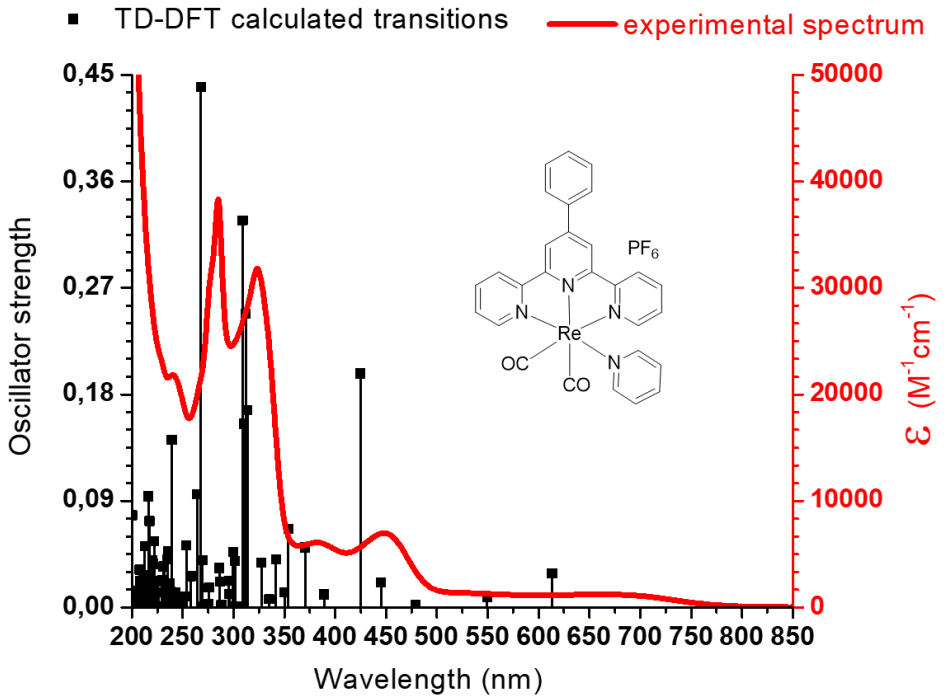


Figure S47. Theoretical and experimental absorption spectra for complex **3c**

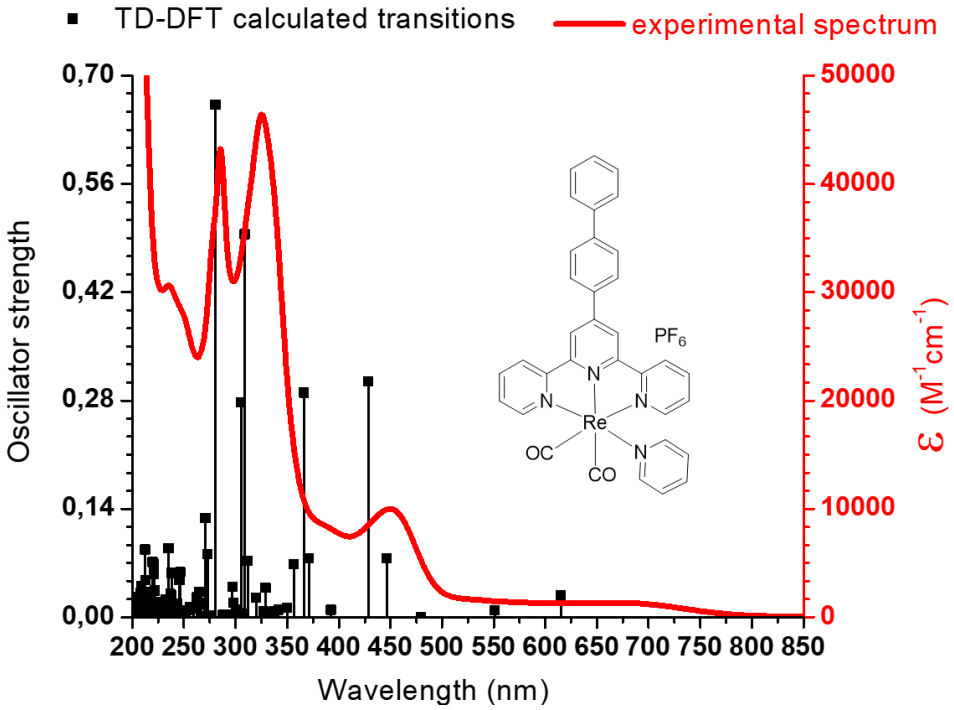


Figure S48. Theoretical and experimental absorption spectra for complex **3d**

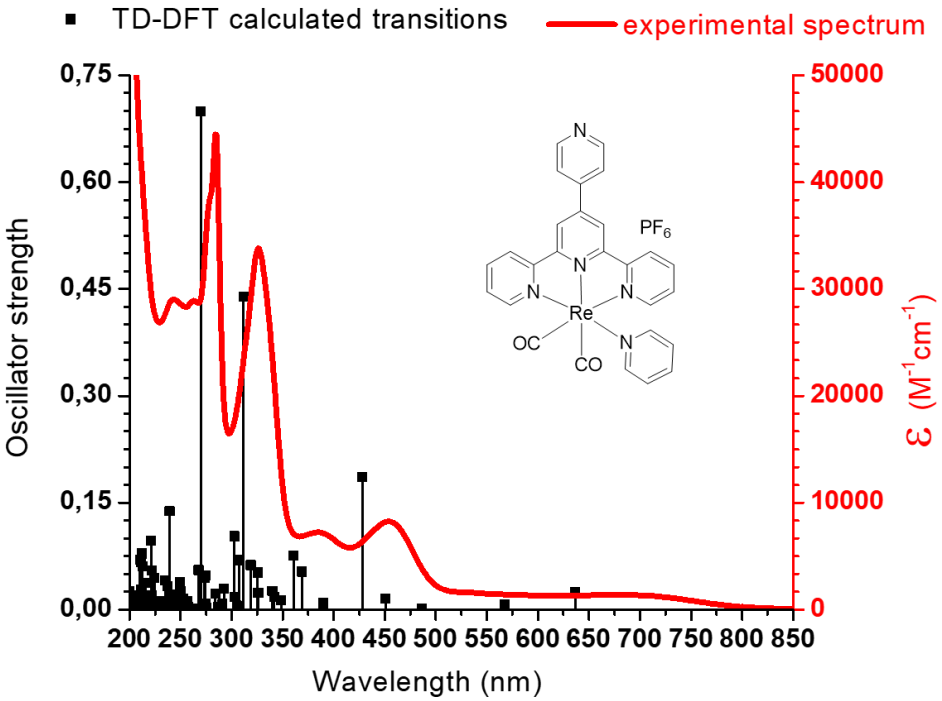


Figure S49. Theoretical and experimental absorption spectra for complex **3e**

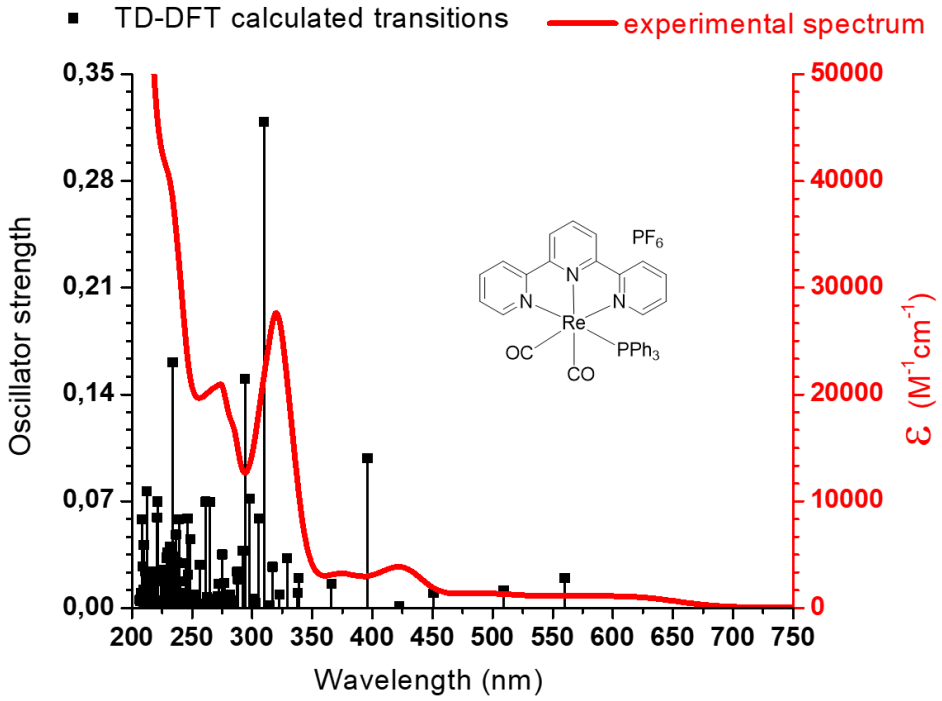


Figure S50. Theoretical and experimental absorption spectra for complex **4a**

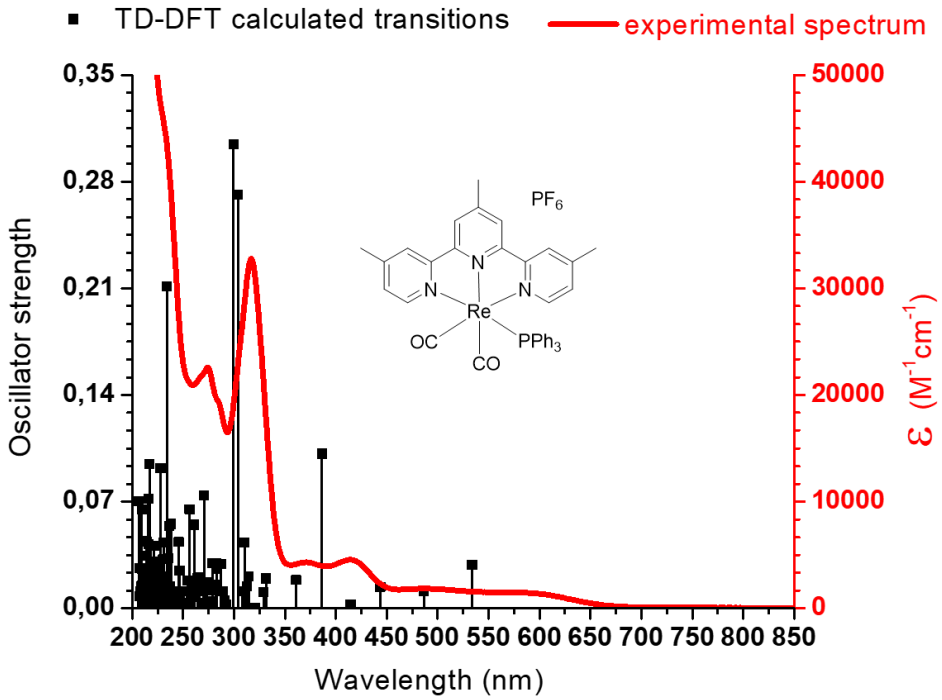


Figure S51. Theoretical and experimental absorption spectra for complex **4b**

D) Electrochemical data

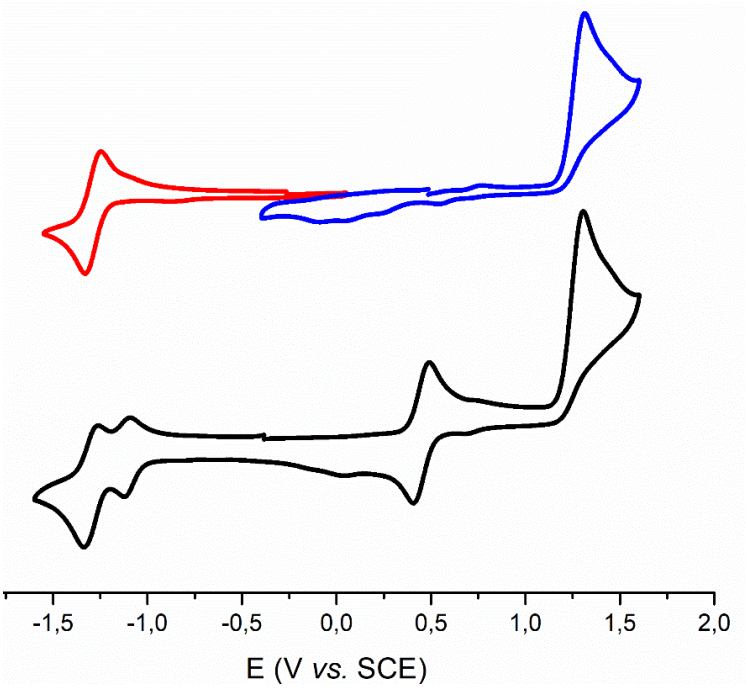


Figure S52 Cyclic voltammograms of **1a** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

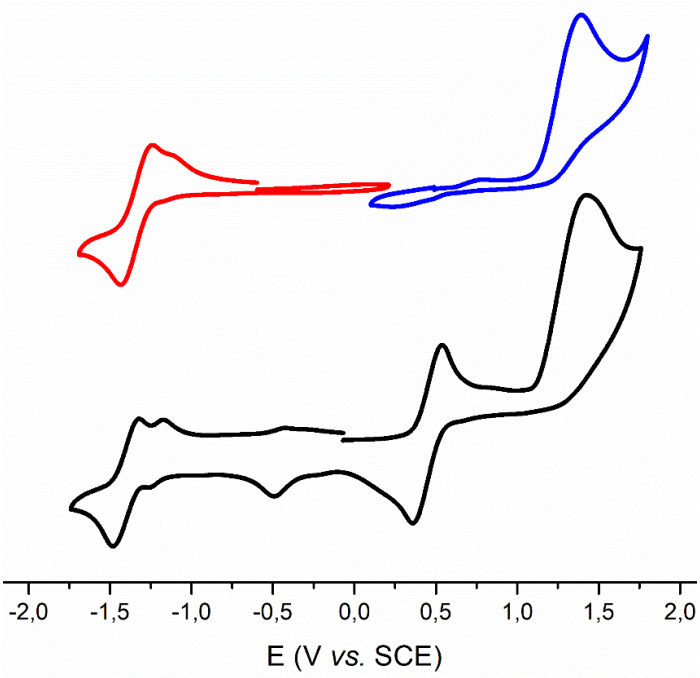


Figure S53 Cyclic voltammograms of **1b** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

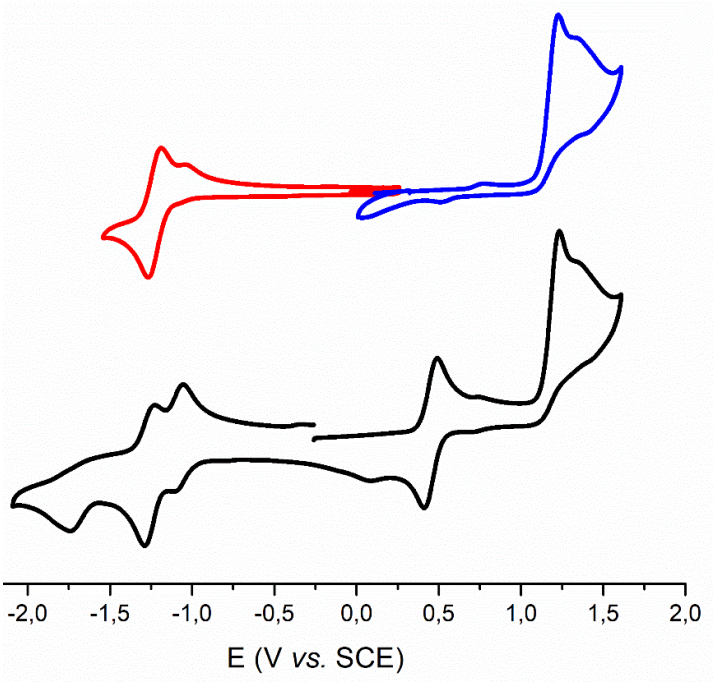


Figure S54 Cyclic voltammograms of **1c** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

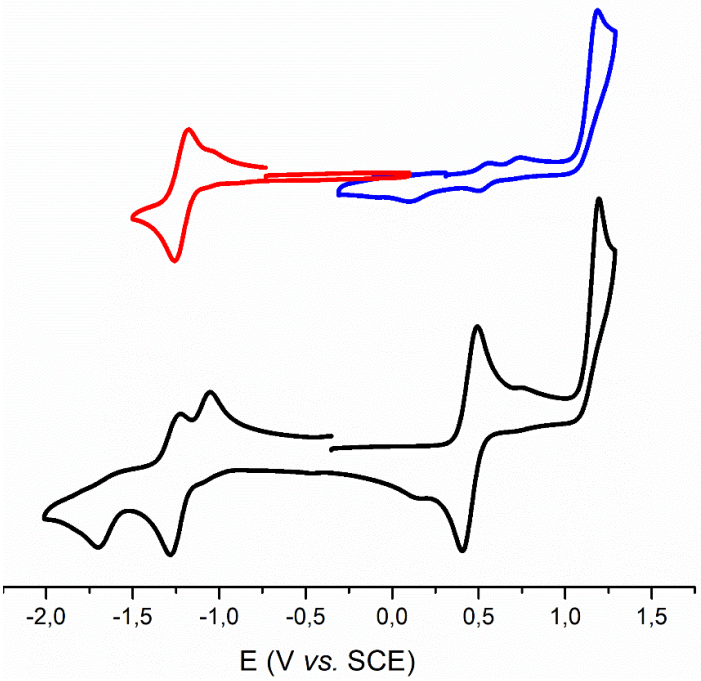


Figure S55 Cyclic voltammograms of **1d** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

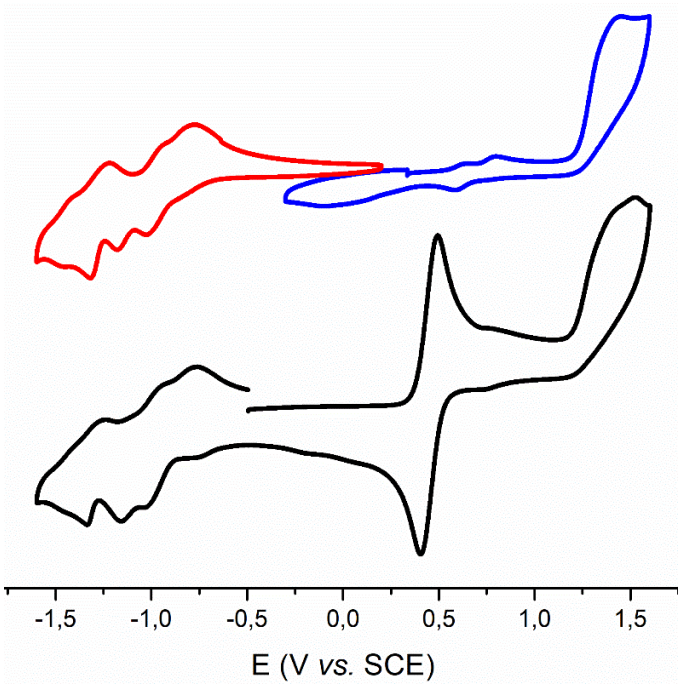


Figure S56 Cyclic voltammograms of **1e** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

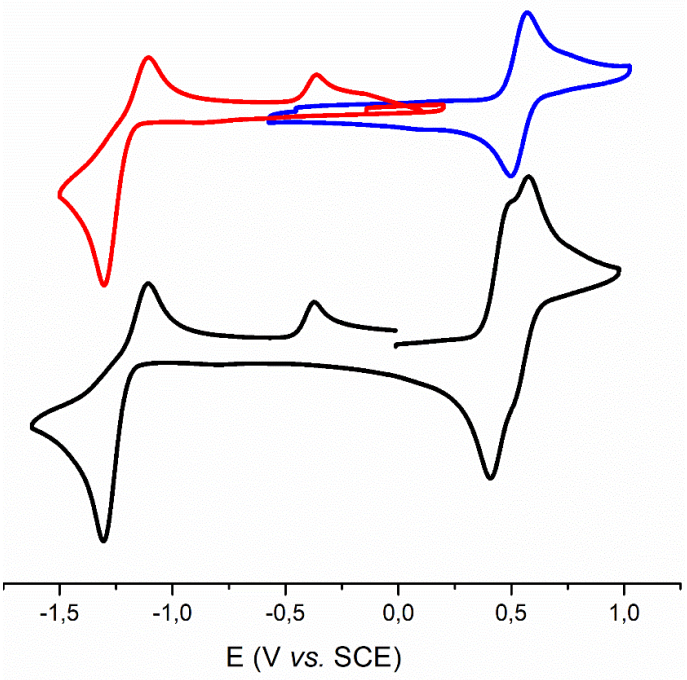


Figure S57 Cyclic voltammograms of **2a** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

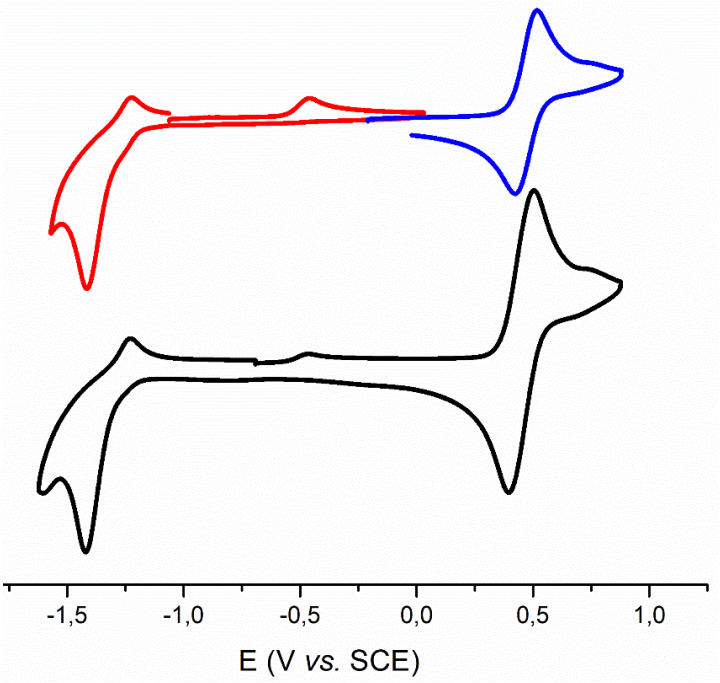


Figure S58 Cyclic voltammograms of **2b** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

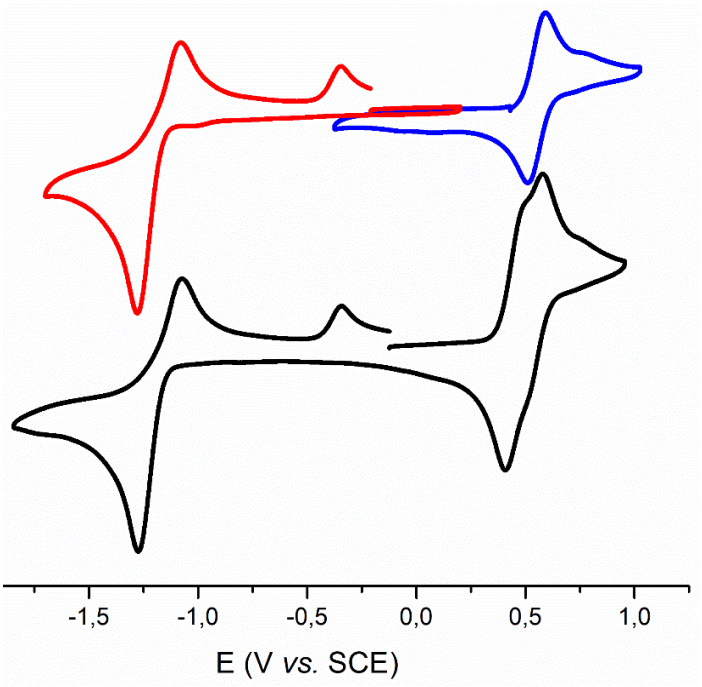


Figure S59 Cyclic voltammograms of **2c** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

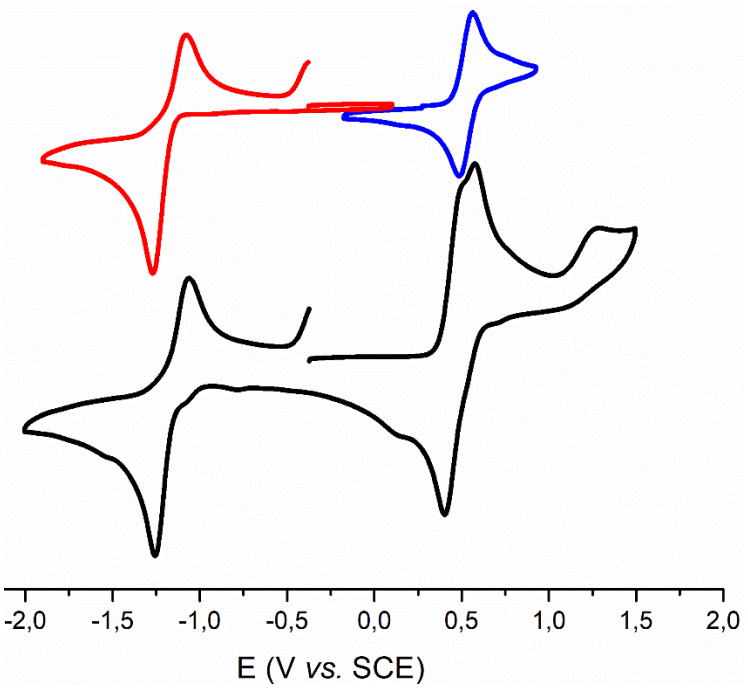


Figure S60 Cyclic voltammograms of **2d** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

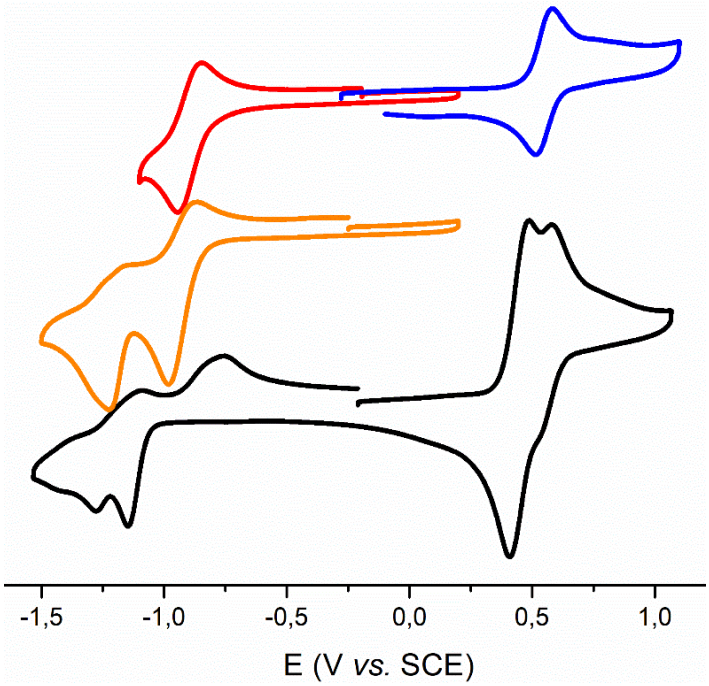


Figure S61 Cyclic voltammograms of **2e** at 200 mV/s in DMF/DMAP 0.1 M (red, orange and blue : without ferrocene, black : full range with ferrocene)

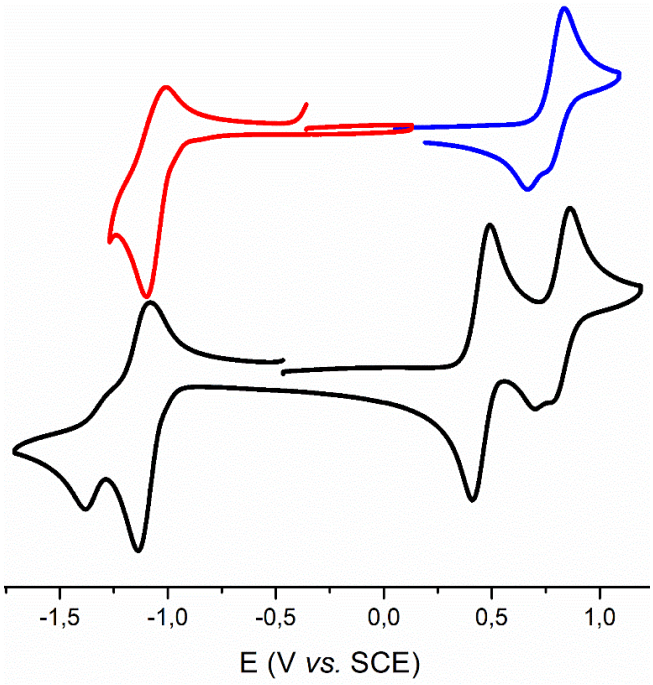


Figure S62 Cyclic voltammograms of **3a** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

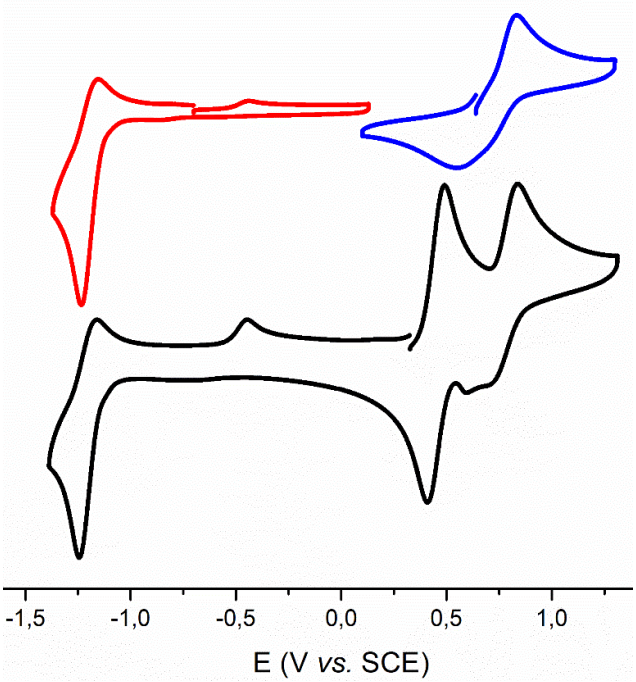


Figure S63 Cyclic voltammograms of **3b** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

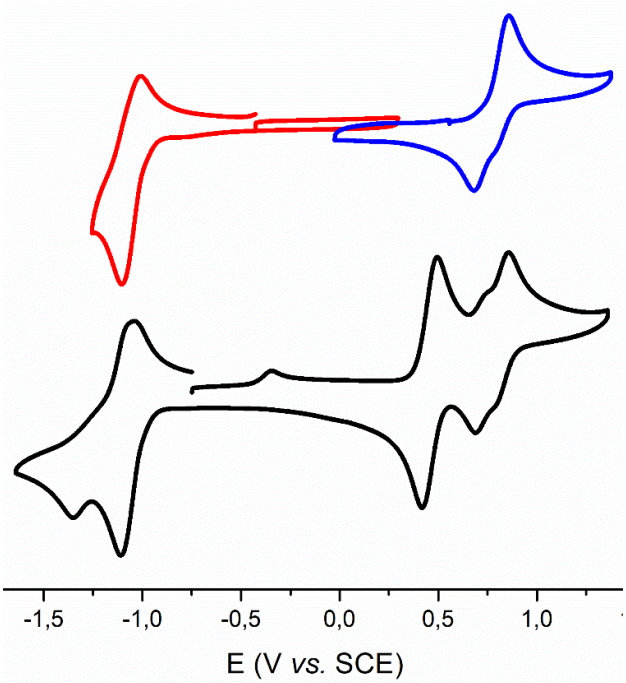


Figure S64 Cyclic voltammograms of **3c** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

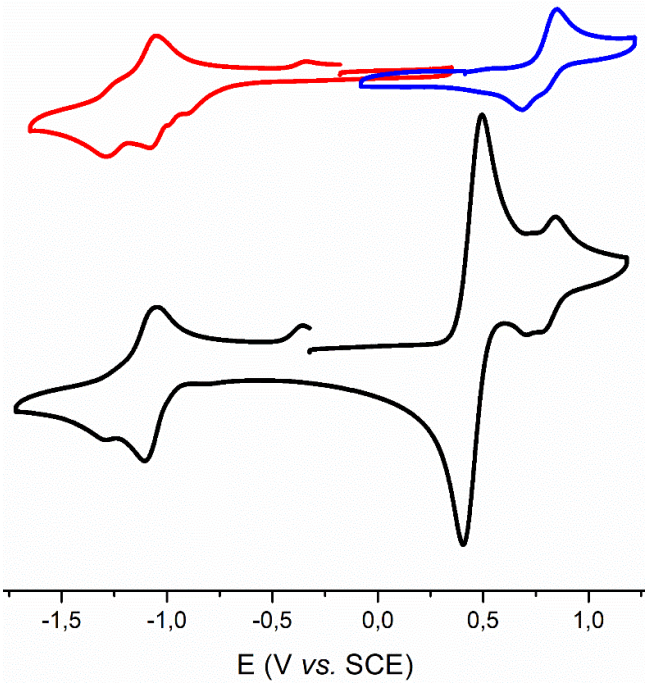


Figure S65 Cyclic voltammograms of **3d** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

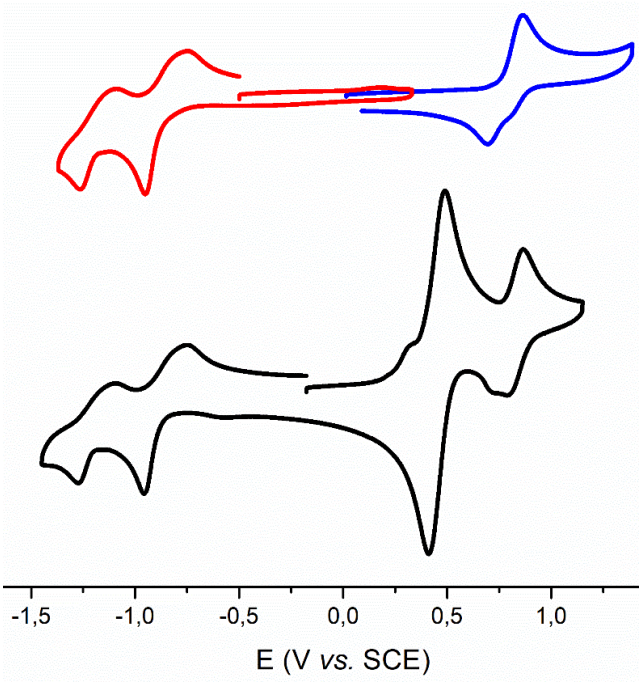


Figure S66 Cyclic voltammograms of **3e** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

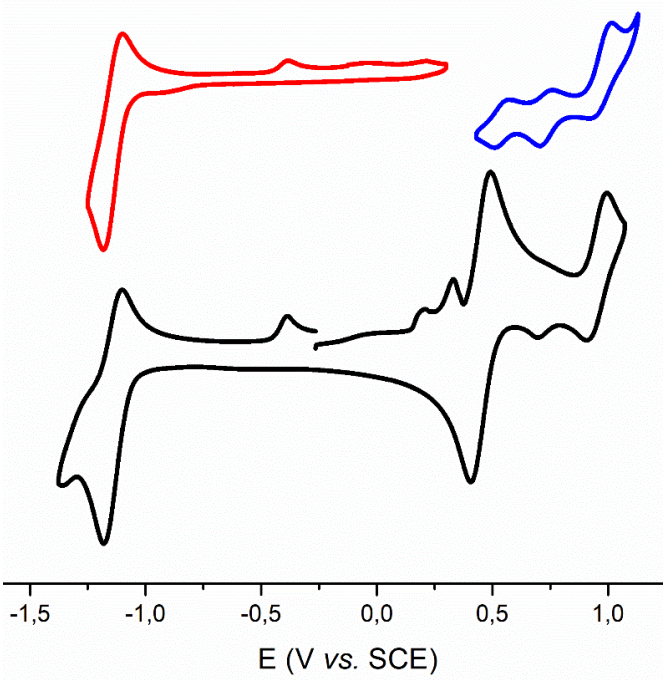


Figure S67 Cyclic voltammograms of **4a** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

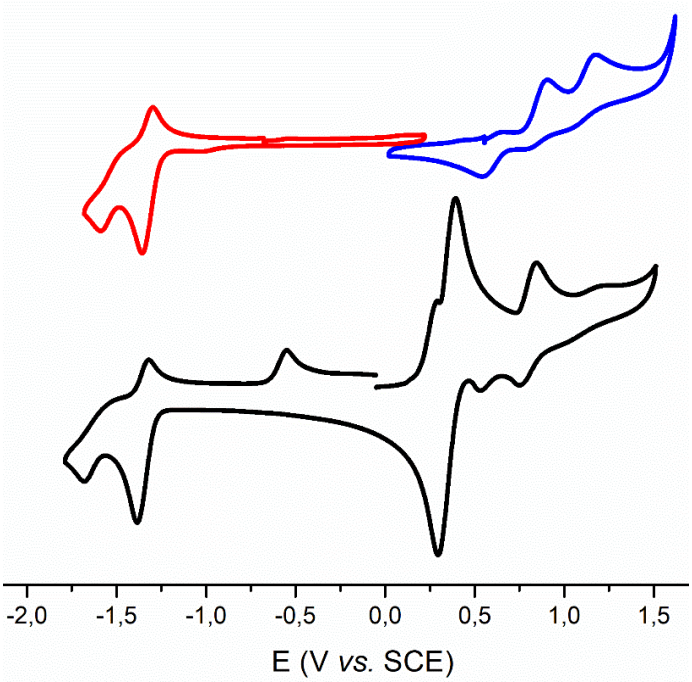


Figure S68 Cyclic voltammograms of **4b** at 200 mV/s in DMF/DMAP 0.1 M (red and blue : without ferrocene, black : full range with ferrocene)

E) Emission data

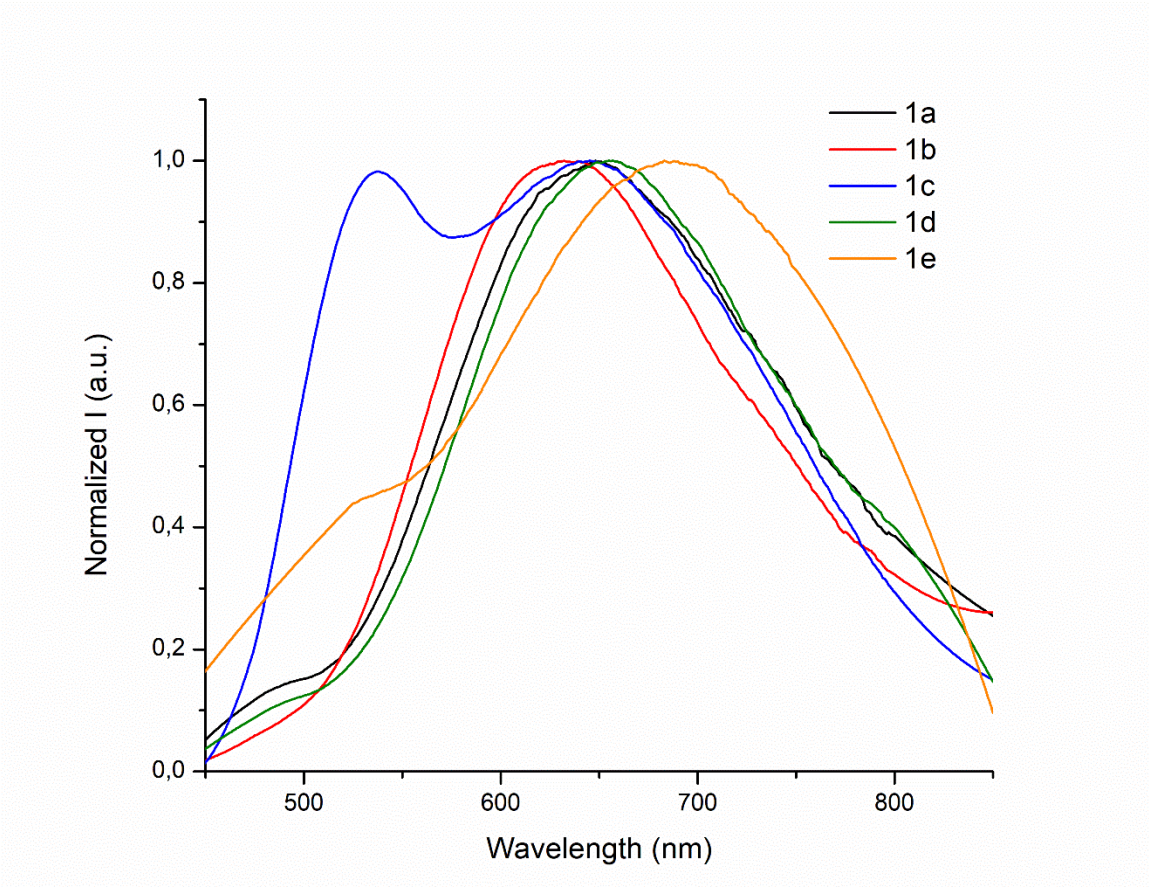
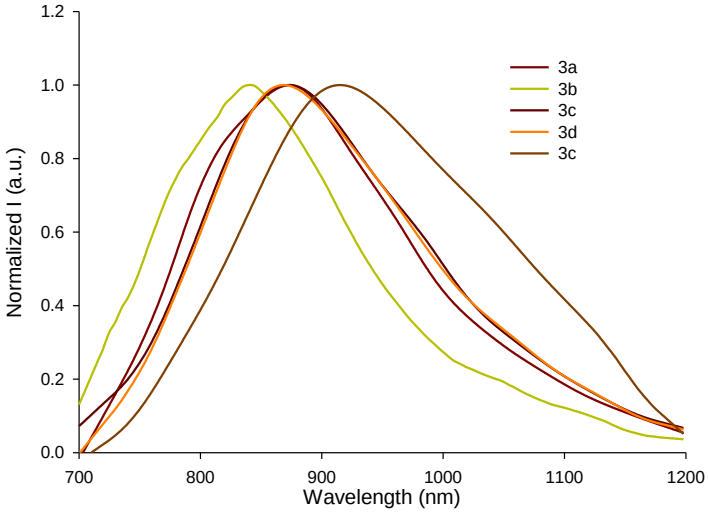


Figure S69. Emission spectra of **series 1** complexes ($2{,}5 \times 10^{-5}$ M, λ_{ex} 340 nm)



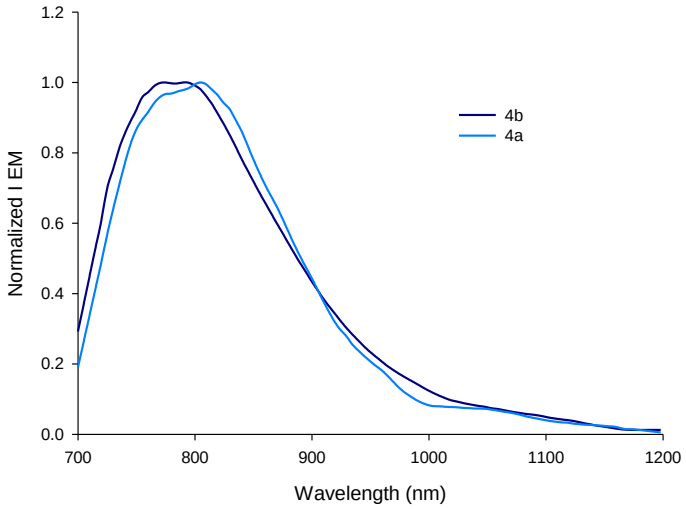


Figure S70. Emission spectra of **series 3** in acetonitrile ($5x10^{-5}$ M, λ_{ex} 440 nm)

Figure S71. Emission spectra of **series 4** in acetonitrile ($5x10^{-5}$ M, λ_{ex} 440 nm).

F) Coordinates of optimized geometries

Table S20. Coordinates of the optimized geometry of **1a**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	1.307778	0.225098	1.406016	20	6	0.237491	-4.820687	4.944150
2	7	0.233659	0.208298	4.003140	21	6	-1.061250	-2.625325	4.365493
3	6	1.117206	0.974312	2.093462	22	7	1.282710	-3.155260	4.066124
4	6	0.904927	1.416231	2.013471	23	6	1.037133	-4.396038	4.540432
5	6	0.376727	1.384140	3.308306	24	6	-1.305977	-3.918823	4.845543
6	6	0.549729	0.961570	3.376916	25	1	-1.869027	-1.912341	4.252483
7	1	1.380870	-1.926919	1.651920	26	1	1.888288	-5.067772	4.589190
8	1	1.021369	2.355284	1.489691	27	1	-2.310014	-4.215097	5.130271
9	6	0.060921	2.603459	4.004197	28	1	0.383650	-5.829928	5.312348
10	6	0.994915	4.774010	5.449568	29	75	0.113337	0.493781	6.148960
11	7	0.419255	2.439807	5.310958	30	35	2.507838	1.155211	6.151049
12	6	0.152093	3.857329	3.383747	31	6	0.360494	-1.240959	6.812556
13	6	0.619025	4.954946	4.111542	32	8	0.681497	-2.280686	7.278015
14	6	0.881105	3.504127	6.013902	33	6	0.245086	1.053249	7.962965
15	1	0.125681	3.982472	2.345691	34	8	0.312796	1.422686	9.087496
16	1	0.694012	5.929042	3.641700	35	6	-1.951012	0.068866	6.119429
17	1	-1.160931	3.326322	7.043192	36	8	-3.111130	0.195212	6.119677
18	1	-1.369113	5.594557	6.049290	37	1	1.743307	0.233016	0.413492
19	6	0.250016	-2.278404	3.998412					

Table S21. Coordinates of the optimized geometry of **1b**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	1.159452	0.193887	1.187805	24	1	-1.684733	-2.060751	4.281487
2	7	0.347322	0.070927	3.903286	25	1	2.075411	-5.209793	4.122596
3	6	1.041443	-1.025810	1.868209	26	1	0.095553	-5.995464	5.058250
4	6	0.797966	1.349357	1.896535	27	75	0.229614	0.279950	6.081330
5	6	0.405099	1.268257	3.234025	28	35	2.832728	0.979985	5.826293
6	6	0.612236	-1.068263	3.200959	29	6	0.785520	-1.470340	6.629884
7	1	1.262419	-1.962852	1.370895	30	8	1.160032	-2.522886	7.021862
8	1	0.844862	2.310746	1.401007	31	6	0.288626	0.780479	7.915717
9	6	0.024474	2.458347	4.012337	32	8	0.338614	1.114544	9.052838
10	6	0.777311	4.563529	5.607147	33	6	-1.594387	0.169885	6.236954
11	7	0.185433	2.244490	5.343014	34	8	-2.744988	0.451471	6.355219
12	6	0.155225	3.726741	3.447014	35	6	0.728534	6.187262	3.657812
13	6	0.556050	4.813447	4.239145	36	1	0.162969	6.795959	3.856171
14	6	0.584335	3.284113	6.118249	37	1	-1.581167	6.704321	4.108644
15	1	0.003632	3.878428	2.386678	38	1	0.872433	6.152255	2.574609
16	1	0.751191	3.076014	7.166434	39	6	1.650016	0.263872	0.229182
17	1	-1.099616	5.356373	6.272690	40	1	2.740378	0.390034	0.243246
18	6	0.390552	-2.411004	3.800548	41	1	1.214830	1.113661	0.763046
19	6	0.005236	-4.972327	4.710411	42	1	1.418817	0.653060	0.778368
20	6	0.871210	-2.777719	4.292462	43	6	-2.415722	-4.500655	5.330666
21	7	1.430461	-3.279161	3.727768	44	1	-2.572676	-5.579009	5.234167
22	6	1.228164	-4.534023	4.186056	45	1	-3.240623	-3.981154	4.833248
23	6	-1.084142	-4.084413	4.767811	46	1	-2.469899	-4.253052	6.398896

Table S22. Coordinates of the optimized geometry of **1c**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	0.139164	0.054416	1.100135	25	1	-2.107817	-1.920860	4.847599
2	7	0.150905	0.144669	3.924972	26	1	1.547383	-5.142644	4.178923
3	6	0.132165	-1.110860	1.883156	27	1	-2.295708	-4.184878	5.899149
4	6	0.064845	1.267379	1.780441	28	1	0.418670	-5.833654	5.565326
5	6	0.199913	1.289458	3.168279	29	6	0.330826	0.009207	0.365474
6	6	0.043755	-1.046875	3.269485	30	6	0.701419	0.076826	-3.165027
7	1	0.268559	-2.088551	1.438142	31	6	0.940761	1.086112	-1.043481
8	1	0.119357	2.192158	1.222192	32	6	0.089984	-1.111660	-1.112153
9	6	0.414460	2.541304	3.911584	33	6	0.091449	-1.152888	-2.500022
10	6	0.877484	4.775922	5.482467	34	6	1.126661	1.042153	-2.430726
11	7	0.374692	2.430351	5.271387	35	1	1.299048	1.948590	0.488881
12	6	0.682431	3.772773	3.297509	36	1	0.584973	-1.942525	0.618182
13	6	0.912266	4.902445	4.087141	37	1	0.247203	-2.018296	-3.061256
14	6	0.606466	3.525836	6.037104	38	1	1.607223	1.874350	-2.935780
15	1	0.724033	3.856776	2.219671	39	1	0.843749	0.109955	-4.240900
16	1	-1.120688	5.859525	3.622566	40	75	0.150823	0.509694	6.059961
17	1	0.572424	3.389050	7.109274	41	35	2.662740	1.123588	5.266154
18	1	-1.056332	5.622819	6.133419	42	6	0.782459	-1.210712	6.619982
19	6	0.161475	-2.339171	3.995696	43	8	1.215331	-2.241841	7.007660
20	6	0.376599	-4.839799	5.134065	44	6	0.565869	1.134456	7.809388
21	6	-1.310256	-2.646751	4.744132	45	8	0.836820	1.544425	8.888415
22	7	0.835627	-3.234971	3.788682	46	6	-1.616600	0.120112	6.591014
23	6	0.727005	-4.455009	4.358348	47	8	-2.727000	0.120918	6.944223
24	6	-1.416822	-3.919019	5.321349					

Table S23. Coordinates of the optimized geometry of **1d**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	2.006258	0.050785	0.340086	30	6	6.323610	0.076242	0.044509
2	7	0.833034	0.126267	0.442304	31	6	4.139979	-1.141052	0.241199
3	6	1.290477	1.254419	0.232690	32	6	4.266388	1.112927	0.626261
4	6	1.246053	-1.111032	0.562731	33	6	5.659015	1.069905	0.531157
5	6	0.146391	-1.051862	0.604582	34	6	5.532483	-1.179995	0.340043
6	6	0.105513	1.273439	0.316654	35	1	3.568348	-2.005907	0.564849
7	1	1.796759	2.198514	0.075088	36	1	3.796441	2.008864	1.020469
8	1	1.745221	-2.059988	0.704797	37	1	6.232158	1.944860	0.822432
9	6	0.971357	-2.248486	0.835029	38	1	6.007755	-2.085470	0.704794
10	6	-2.692469	-4.367247	1.308653	39	75	-2.960836	0.142935	0.015004
11	7	-2.317218	-2.068887	0.695735	40	35	-2.041364	0.939962	-2.401162
12	6	0.446454	-3.492976	1.210378	41	6	-3.382705	1.564346	0.746286
13	6	-1.311739	-4.564545	1.446105	42	8	-3.684540	2.585981	-1.262161
14	6	-3.156878	-3.107562	0.932799	43	6	-4.711228	0.700160	0.484078
15	1	0.619964	-3.630625	1.329321	44	8	-5.791117	-1.069806	0.805085
16	1	0.916404	-5.531089	1.737235	45	6	-3.584684	0.374076	1.718164
17	1	-4.215009	-2.916861	0.817039	46	8	-3.997840	0.694469	2.787015
18	1	-3.400272	-5.167140	1.487822	47	6	7.803234	0.119152	0.059957
19	6	0.763867	2.606945	0.314371	48	6	10.628710	0.200572	0.259780
20	6	-1.767685	5.173708	0.316338	49	6	8.435742	0.862506	-1.079951
21	6	-1.561471	3.022123	1.394078	50	6	8.614447	0.582673	0.857811
22	7	0.446296	3.429382	0.716361	51	6	10.011790	0.542614	0.759725
23	6	0.950681	4.682531	0.712760	52	6	9.832975	0.902938	-1.179428
24	6	-2.069890	4.327826	1.392465	53	1	7.836607	-1.391799	-1.815460
25	1	-1.754815	2.351400	2.222607	54	1	8.155737	1.142758	1.667695
26	1	0.683403	5.309418	-1.557540	55	1	10.617118	1.083536	1.481249
27	1	-2.683256	4.676199	2.216734	56	1	10.298842	-1.474481	-1.976869
28	1	-2.142561	6.190217	0.275376	57	1	11.711506	0.231698	0.336446
29	6	3.479098	0.007280	0.242821					

Table S24. Coordinates of the optimized geometry of **1e**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	0.199819	0.063083	1.116315	24	6	-1.384795	-3.933731	5.300513
2	7	0.137559	0.144688	3.927536	25	1	-2.087263	-1.940447	4.823146
3	6	0.191614	-1.105443	1.890359	26	1	1.603926	-5.129250	4.192061
4	6	0.025675	1.273974	1.788479	27	1	-2.268747	-4.208797	5.866066
5	6	0.186102	1.291581	3.174561	28	1	0.373484	-5.840212	5.552242
6	6	0.008173	-1.045508	3.274554	29	6	0.416305	0.021294	0.347294
7	1	0.344522	-2.080007	1.443649	30	6	1.053004	1.081155	-1.021649
8	1	0.076316	2.198578	1.229472	31	6	0.004187	-1.080675	-1.116650
9	6	0.425196	2.539186	3.916678	32	6	0.221624	-1.077635	-2.498142
10	6	0.937615	4.764523	5.483889	33	6	1.240186	0.997794	-2.406486
11	7	0.406993	2.424850	5.276621	34	1	1.424603	1.949403	0.488297
12	6	0.695318	3.768841	3.300381	35	1	0.520779	-1.920826	0.665658
13	6	0.950095	4.894272	4.088627	36	1	0.100914	-1.914638	-3.109006
14	6	0.663016	3.515921	6.040596	37	1	1.734641	1.801226	-2.942934
15	1	0.719817	3.855388	2.222201	38	75	0.126556	0.508228	6.068728
16	1	-1.160448	5.850257	3.622765	39	35	2.641743	1.147925	5.311814
17	1	0.645663	3.377314	7.112910	40	6	0.768004	-1.207298	6.634114
18	1	-1.136232	5.607930	6.133617	41	8	1.205753	-2.234841	7.025189
19	6	0.126009	-2.339964	3.996069	42	6	0.510460	1.133495	7.825136
20	6	0.334351	-4.844875	5.124200	43	8	0.761949	1.543896	8.908334
21	6	-1.281881	-2.658795	4.728316	44	6	-1.644441	0.099789	6.574708
22	7	0.880960	-3.226655	3.798259	45	8	-2.756749	0.152994	6.912445
23	6	0.775768	-4.448962	4.363246	46	7	0.834631	0.060013	-3.148569

Table S25. Coordinates of the optimized geometry of **2a**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	0.071313	0.219079	0.959170	19	6	0.033448	-2.099406	3.984647
2	7	0.002763	0.251015	3.704797	20	6	0.076135	-4.143585	5.850320
3	6	0.051590	0.990598	1.668113	21	6	0.040429	-3.428472	3.549208
4	6	0.079339	1.444633	1.640536	22	7	0.043884	-1.787475	5.329404
5	6	0.047660	1.433855	3.040825	23	6	0.068680	-2.800626	6.232490
6	6	0.020527	0.947398	3.067791	24	6	0.060829	-4.466750	4.486749
7	1	0.067854	-1.933457	1.136233	25	1	0.030156	-3.652656	2.489626
8	1	0.116942	2.374593	1.087449	26	1	0.081667	-2.510327	7.274059
9	6	0.087061	2.605734	3.931366	27	1	0.065807	-5.500471	4.160424
10	6	0.176791	4.690129	5.750287	28	1	0.094686	-4.912792	6.613124
11	7	0.090734	2.324175	5.282843	29	75	0.009386	0.274340	5.776837
12	6	0.124208	3.924096	3.465947	30	35	2.726108	0.240110	5.487701
13	6	0.168500	4.982601	4.379744	31	6	0.253171	0.292735	7.646547
14	6	0.138840	3.356686	6.162764	32	8	0.436789	0.304103	8.835204
15	1	0.118772	4.124407	2.401558	33	6	-1.834474	0.298243	6.032342
16	1	0.196943	6.008287	4.030098	34	8	-3.022415	0.313947	6.223777
17	1	0.145478	3.089825	7.210643	35	1	0.093780	0.206550	0.124615
18	1	0.213059	5.475788	6.495483					

Table S26. Coordinates of the optimized geometry of **2b**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	0.026659	0.131324	1.001953	23	6	0.229539	-4.485267	4.640004
2	7	0.023820	0.230089	3.773952	24	1	0.270356	-3.681035	2.639962
3	6	0.098887	-1.051225	1.763683	25	1	0.005803	-2.469214	7.390244
4	6	0.077856	1.362826	1.677491	26	1	0.164278	-4.868373	6.777289
5	6	0.082333	1.388310	3.075733	27	75	0.051665	0.298493	5.844589
6	6	0.090902	0.977835	3.160215	28	35	2.757841	0.087089	5.472816
7	1	0.151568	-2.009141	1.259926	29	6	0.353947	0.342747	7.703890
8	1	0.162462	2.280042	1.106783	30	8	0.574912	0.368824	8.887350
9	6	0.221580	2.577863	3.934960	31	6	-1.775443	0.443257	6.152485
10	6	0.491158	4.695391	5.681608	32	8	-2.955517	0.537701	6.377839
11	7	0.248544	2.326805	5.290665	33	6	0.597579	6.377927	3.782759
12	6	0.324282	3.878763	3.434942	34	1	1.651665	6.683901	3.780746
13	6	0.463061	4.974644	4.302244	35	1	0.055002	7.088327	4.414500
14	6	0.385366	3.381655	6.133971	36	1	0.224301	6.465594	2.758709
15	1	0.295305	4.045072	2.364106	37	6	0.067821	0.080713	0.499947
16	1	0.405437	3.147720	7.189694	38	1	0.351577	0.855071	0.880453
17	1	0.594455	5.494822	6.407277	39	1	0.481257	0.916163	0.943694
18	6	0.121712	-2.111010	4.102373	40	1	-1.105258	0.144069	0.852822
19	6	0.153957	-4.115933	5.996211	41	6	0.303278	-5.926470	4.222080
20	6	0.211935	-3.445170	3.696439	42	1	0.695063	-6.381883	4.247251
21	7	0.051475	-1.771013	5.436975	43	1	0.690652	-6.031327	3.204904
22	6	0.065171	-2.772037	6.353685	44	1	0.940133	-6.503765	4.899797

Table S27. Coordinates of the optimized geometry of **2c**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	0.070968	0.080361	0.963500	24	6	0.001376	-4.499837	4.643581
2	7	0.050881	0.193401	3.738019	25	1	0.097822	-3.742531	2.627167
3	6	0.075772	-1.101506	1.734957	26	1	0.140372	-2.466737	7.371693
4	6	0.027715	1.320213	1.635861	27	1	0.014195	-5.542219	4.346457
5	6	0.008903	1.351133	3.032107	28	1	0.110422	-4.886681	6.779047
6	6	0.062180	-1.018925	3.129018	29	6	0.096307	0.019306	0.516279
7	1	0.059269	-2.066894	1.244956	30	6	0.147816	0.098875	-3.339788
8	1	0.026042	2.243190	1.069844	31	6	0.564962	0.996990	-1.289442
9	6	0.068858	2.550720	3.883782	32	6	0.783526	-1.018766	-1.180499
10	6	0.234251	4.687451	5.636240	33	6	0.810652	-1.076012	-2.579689
11	7	0.115606	2.309424	5.242481	34	6	0.541016	0.937156	-2.688517
12	6	0.100629	3.854568	3.378846	35	1	1.124952	1.790591	0.803274
13	6	0.182711	4.939241	4.258620	36	1	-1.323524	-1.768425	0.609270
14	6	0.200687	3.367178	6.089089	37	1	-1.352767	-1.875885	-3.074692
15	1	0.061979	4.024495	2.309866	38	1	1.063795	1.691941	-3.267924
16	1	0.206954	5.953814	3.877642	39	1	0.167690	0.144225	-4.424432
17	1	0.240716	3.131176	7.143598	40	75	0.035948	0.275838	5.802771
18	1	0.300893	5.494381	6.356173	41	35	2.742017	0.206932	5.418076
19	6	0.024967	-2.147143	4.075696	42	6	0.349340	0.345703	7.661348
20	6	0.069848	-4.139016	5.995956	43	8	0.577173	0.389772	8.841689
21	6	0.045548	-3.487943	3.678602	44	6	-1.796531	0.323312	6.126525
22	7	0.037494	-1.798128	5.410101	45	8	-2.976224	0.354882	6.362483
23	6	0.087012	-2.785945	6.339908					

Table S28. Coordinates of the optimized geometry of **2d**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	1.951241	0.003689	0.164391	29	6	3.429835	0.000260	0.119371
2	7	0.824488	0.014253	0.275656	30	6	6.282230	0.002537	0.033418
3	6	1.229492	1.215927	0.110114	31	6	4.137875	-1.066227	0.472709
4	6	1.225955	-1.204365	0.248391	32	6	4.174434	1.065156	0.667915
5	6	0.169449	-1.173767	0.293795	33	6	5.570698	1.061891	0.626956
6	6	0.165611	1.195184	0.164216	34	6	5.534054	-1.065701	0.515827
7	1	1.756532	2.154756	0.004267	35	1	3.601110	-1.895511	0.923960
8	1	1.751449	-2.149758	0.294878	36	1	3.666857	1.895448	1.150139
9	6	-1.072853	-2.336361	0.348371	37	1	6.109958	1.905403	1.047210
10	6	-2.918580	-4.398305	0.429345	38	1	6.045252	-1.910221	0.967972
11	7	-2.421069	-2.038367	0.343706	39	75	-2.892323	0.018475	0.288477
12	6	0.624717	-3.660370	0.396089	40	35	-2.637805	0.137275	-2.430197
13	6	-1.551722	-4.707302	0.438635	41	6	-4.765480	0.008502	0.067667
14	6	-3.314016	-3.060241	0.379718	42	8	-5.956567	0.000481	0.100550
15	1	0.436855	-3.875212	0.400012	43	6	-3.127590	0.126840	2.131837
16	1	-1.214804	-5.736923	0.476834	44	8	-3.306512	0.197415	3.319833
17	1	-4.358491	-2.780537	0.368579	45	6	7.765633	0.003560	0.011965
18	1	-3.673736	-5.174687	0.458417	46	6	10.598213	0.005395	0.099230
19	6	-1.065544	2.358683	0.079196	47	6	8.456619	0.605015	-1.086105
20	6	-2.904306	4.421459	0.089201	48	6	8.522139	0.597101	1.017555
21	6	0.612953	3.677790	0.025966	49	6	9.922894	0.596433	0.975049
22	7	-2.414708	2.066289	0.104538	50	6	9.857317	0.606232	-1.129930
23	6	-3.304264	3.088059	0.017764	51	1	7.900234	-1.052673	-1.904701
24	6	-1.536465	4.725266	0.110764	52	1	8.017856	1.045733	1.868749
25	1	0.449373	3.888237	0.041906	53	1	10.485470	1.057369	1.781700
26	1	-4.349740	2.812465	0.036655	54	1	10.368540	-1.067778	-1.969728
27	1	-1.196136	5.751220	0.192525	55	1	11.683657	0.006062	0.132644
28	1	-3.656828	5.198191	0.154508					

Table S29. Coordinates of the optimized geometry of **2e**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	0.073492	0.082087	0.970749	23	6	0.118107	-2.784600	6.339748
2	7	0.045789	0.194156	3.738013	24	6	0.037583	-4.499102	4.643414
3	6	0.072283	-1.101456	1.735818	25	1	0.072344	-3.742840	2.627383
4	6	0.032106	1.322890	1.637077	26	1	0.172890	-2.465335	7.371414
5	6	0.011977	1.353562	3.033919	27	1	0.027580	-5.541539	4.346377
6	6	0.051861	-1.019153	3.130363	28	1	0.155843	-4.885171	6.778372
7	1	0.056886	-2.065924	1.243895	29	6	0.103477	0.020914	0.509570
8	1	0.032621	2.245165	1.069839	30	6	0.559335	0.982668	-1.296632
9	6	0.061051	2.552718	3.885496	31	6	0.797379	-1.002878	-1.183563
10	6	0.217349	4.688710	5.638613	32	6	0.801670	-1.022590	-2.583303
11	7	0.113042	2.310334	5.243774	33	6	0.503821	0.883749	-2.691894
12	6	0.082799	3.856887	3.380983	34	1	1.133612	1.784288	0.845125
13	6	0.160351	4.941342	4.261398	35	1	-1.349749	-1.762590	0.641211
14	6	0.193574	3.367972	6.090871	36	1	-1.336357	-1.800100	-3.119465
15	1	0.039739	4.027768	2.312321	37	1	1.013879	1.611999	-3.314280
16	1	0.176867	5.956329	3.881219	38	75	0.047612	0.276329	5.801625
17	1	0.237982	3.131721	7.145121	39	35	2.750162	0.223099	5.410185
18	1	0.280713	5.495552	6.358923	40	6	0.366327	0.347497	7.659996
19	6	0.005074	-2.146891	4.076165	41	8	0.597402	0.392615	8.839041
20	6	0.108116	-4.137726	5.995492	42	6	-1.785105	0.312941	6.131672
21	6	0.018595	-3.487575	3.678578	43	8	-2.963605	0.337524	6.371385
22	7	0.059526	-1.797124	5.410213	44	7	0.164013	0.099233	-3.341644

Table S30. Coordinates of the optimized geometry of **3a**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	0.030697	0.301535	0.961187	24	6	0.145060	-4.432597	4.422429
2	7	0.051714	0.297927	3.706575	25	1	0.181502	-3.588241	2.438808
3	6	0.083061	0.916382	1.654190	26	1	0.030019	-2.525056	7.238896
4	6	0.000573	1.518680	1.656762	27	1	0.168825	-5.460485	4.079313
5	6	0.018667	1.490432	3.056664	28	1	0.082199	-4.913711	6.540037
6	6	0.092905	0.891994	3.054398	29	75	0.050438	0.291592	5.781840
7	1	0.114129	-1.850740	1.108497	30	6	0.171649	0.305534	7.667214
8	1	0.029226	2.454894	1.114059	31	8	0.257466	0.322891	8.865620
9	6	0.029850	2.652729	3.963348	32	6	-1.825334	0.317458	5.963013
10	6	0.110179	4.711568	5.812572	33	8	-3.013204	0.328404	6.108079
11	7	0.104861	2.351032	5.311101	34	1	0.018647	0.302027	0.122720
12	6	0.019467	3.976964	3.520059	35	7	2.258377	0.207824	5.653907
13	6	0.017421	5.022667	4.450055	36	6	5.064434	0.036737	5.556478
14	6	0.152890	3.371717	6.204840	37	6	2.980951	1.015510	4.834072
15	1	0.083874	4.194124	2.461067	38	6	2.933788	0.688888	6.424064
16	1	0.022165	6.053314	4.116804	39	6	4.323852	0.800650	6.402827
17	1	0.218708	3.091040	7.246947	40	6	4.374090	0.959642	4.759769
18	1	0.147956	5.487204	6.567909	41	1	2.435312	1.726395	4.229546
19	6	0.123099	-2.057598	3.955832	42	1	2.338370	-1.321139	7.069168
20	6	0.098729	-4.132597	5.789631	43	1	4.808751	-1.530851	7.039771
21	6	0.154123	-3.378980	3.501011	44	1	4.898358	1.629676	4.088827
22	7	0.091474	-1.767175	5.306098	45	1	6.146408	0.028202	5.519621
23	6	0.074604	-2.795652	6.192487					

Table S31. Coordinates of the optimized geometry of **3b**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	0.194597	3.934055	0.397778	28	6	0.054533	-2.673811	0.873540
2	7	0.088713	1.220662	0.163504	29	8	0.086487	-3.865205	-1.037417
3	6	1.044027	3.276839	0.249452	30	6	0.110974	0.597188	-2.469083
4	6	-1.376942	3.182661	0.264231	31	8	0.170613	0.493540	-3.661571
5	6	-1.299749	1.813476	0.013003	32	7	0.174945	-1.131729	1.582287
6	6	1.074235	1.909223	0.032750	33	6	0.473084	-1.605695	4.339252
7	1	1.962485	3.842270	0.354185	34	6	0.632769	0.521864	2.488947
8	1	-2.337043	3.670057	0.383190	35	6	1.135029	-1.976357	2.049227
9	6	-2.430426	0.875054	0.149030	36	6	1.310831	-2.236246	3.408333
10	6	-4.419817	-1.022566	0.373236	37	6	0.514928	0.733221	3.864190
11	7	-2.077051	0.444023	0.367623	38	1	-1.394326	0.143309	2.106891
12	6	-3.767217	1.261719	0.054369	39	1	1.765901	-2.451094	1.309497
13	6	-4.801464	0.315143	0.171137	40	1	2.089990	-2.920353	3.722962
14	6	-3.070044	-1.362980	0.465017	41	1	-1.188381	0.220839	4.540961
15	1	-4.014028	2.304000	0.113689	42	1	0.586994	-1.789473	5.402051
16	1	-2.759819	-2.386407	0.626016	43	6	6.086286	1.273448	0.308436
17	1	-5.165261	-1.805065	0.461173	44	1	6.193321	2.202813	0.878350
18	6	2.275399	1.076281	0.236388	45	1	6.815012	0.550623	0.683792
19	6	4.414887	0.600619	0.714295	46	1	6.342390	1.502710	0.733439
20	6	3.575664	1.575761	0.164428	47	6	0.240046	5.403657	0.708853
21	7	2.032717	0.251075	0.533822	48	1	-1.256050	5.799625	0.638767
22	6	3.097605	-1.057270	0.769857	49	1	0.400800	5.969471	0.024159
23	6	4.684494	0.741911	0.399720	50	1	0.127763	5.591620	1.724988
24	1	3.737566	2.621280	0.072596	51	6	-6.244087	0.726310	0.099097
25	1	2.873083	-2.086028	-1.018679	52	1	-6.892873	0.125531	0.121193
26	1	5.220707	-1.297142	0.916762	53	1	-6.566412	1.152146	-1.057984
27	75	0.006645	0.806862	0.602162	54	1	-6.401828	1.493451	0.665589

Table S32. Coordinates of the optimized geometry of **3c**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	3.258249	0.057966	0.100586	29	75	-1.567937	0.071094	0.541809
2	7	0.492893	0.017584	0.340161	30	6	-3.455164	0.137847	0.604875
3	6	2.502906	-1.249925	0.142888	31	8	-4.655507	0.188248	0.637312
4	6	2.572724	1.173810	0.170768	32	6	-1.565732	0.133160	-2.425448
5	6	1.181364	1.186386	0.282810	33	8	-1.595361	0.168238	-3.621448
6	6	1.113620	-1.186766	0.266234	34	7	-1.660898	0.055577	1.665916
7	1	3.000658	-2.207536	0.057647	35	6	-1.843445	0.279928	4.464066
8	1	3.126925	2.103598	0.154908	36	6	0.883170	0.703636	2.481359
9	6	0.312762	2.376915	0.336958	37	6	-2.528732	0.930599	2.244504
10	6	-1.475849	4.489245	0.396520	38	6	-2.647045	-1.067630	3.627430
11	7	-1.044040	2.114769	0.399936	39	6	0.946832	0.620385	3.873704
12	6	0.796186	3.687781	0.316302	40	1	0.200093	1.397349	2.011706
13	6	0.102455	4.760501	0.349546	41	1	-3.138275	-1.523879	1.575902
14	6	-1.908487	3.161491	0.418794	42	1	-3.357040	-1.778652	4.032819
15	1	1.862243	3.873847	0.273031	43	1	0.303233	1.252271	4.474130
16	1	0.262308	5.781075	0.335856	44	1	-1.914707	0.365499	5.542869
17	1	-2.959735	2.911946	0.460154	45	6	4.733309	0.098833	0.019683
18	1	-2.209047	5.286529	0.417088	46	6	7.548775	0.176206	0.246880
19	6	0.184389	-2.329199	0.341403	47	6	5.427188	0.916921	0.711045
20	6	-1.693321	-4.352306	0.568588	48	6	5.472467	-1.153936	0.556135
21	6	0.599505	-3.662912	0.293184	49	6	6.868029	-1.190713	0.445435
22	7	-1.149370	-2.001201	0.491554	50	6	6.822289	0.877024	0.825611
23	6	-2.057197	-3.004536	0.605427	51	1	4.880595	1.725529	1.187563
24	6	0.344184	-4.690544	0.405042	52	1	4.965852	-1.933233	-1.118078
25	1	1.648885	-3.901991	0.173255	53	1	7.422449	-2.003841	0.903653
26	1	-3.087956	-2.704371	0.738120	54	1	7.339647	1.660908	1.370044
27	1	0.031446	-5.727744	0.369078	55	1	8.630587	0.205900	0.333969
28	1	-2.459381	-5.112019	0.666266					

Table S33. Coordinates of the optimized geometry of **3d**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	2.031956	0.010401	0.225395	34	7	-2.821762	0.087923	1.701922
2	7	0.741451	0.036576	0.377026	35	6	-2.901949	0.333068	4.503207
3	6	1.296492	-1.194981	0.251220	36	6	-2.031746	0.682176	2.495120
4	6	1.321584	1.229900	0.267480	37	6	-3.650885	0.984113	2.304419
5	6	0.072387	1.217376	0.334929	38	6	-3.717944	-1.132028	3.689627
6	6	0.096527	-1.156488	0.330754	39	6	-2.045176	0.589188	3.888187
7	1	1.812701	-2.144289	0.186161	40	1	-1.379681	1.392766	2.007036
8	1	1.858063	2.170140	0.264793	41	1	-4.271435	-1.585644	1.653526
9	6	0.963826	2.391979	0.353563	42	1	-4.398678	-1.860037	4.114616
10	6	-2.791035	4.471659	0.339634	43	1	-1.394167	1.230605	4.470233
11	7	-2.317021	2.105455	0.371353	44	1	-2.933747	0.426712	5.583223
12	6	0.503683	3.711234	0.342465	45	6	3.508353	0.004181	0.151268
13	6	-1.421942	4.767670	0.338784	46	6	6.357928	0.031576	0.010689
14	6	-3.200250	3.136436	0.354489	47	6	4.213608	1.030778	0.497797
15	1	0.559760	3.916091	0.334835	48	6	4.254002	-1.053386	0.728298
16	1	-1.075433	5.794665	0.332149	49	6	5.649063	-1.063730	0.662127
17	1	-4.247645	2.868006	0.360972	50	6	5.608286	1.014396	0.569187
18	1	-3.538745	5.255564	0.330295	51	1	3.675076	1.837413	0.986463
19	6	-1.006692	-2.315397	0.383569	52	1	3.750621	-1.850066	-1.268107
20	6	-2.853309	-4.371449	0.563642	53	1	6.191281	-1.868205	-1.149481
21	6	0.565553	-3.641416	0.360945	54	1	6.115226	1.808811	1.108284
22	7	-2.350594	-2.011217	0.485712	55	6	7.839921	0.045533	0.062032
23	6	-3.243047	-3.030544	0.576799	56	6	10.669793	0.071964	0.201258
24	6	-1.493331	-4.685657	0.449090	57	6	8.575417	1.159384	0.072104
25	1	0.491661	-3.861487	0.279240	58	6	8.550257	-1.263954	0.122988
26	1	-4.283140	-2.748772	0.671471	59	6	9.949802	-1.277740	0.192040
27	1	-1.160512	-5.717078	0.432534	60	6	9.974981	1.147018	0.140787
28	1	-3.608196	-5.144541	0.641403	61	1	8.056592	2.111173	0.001135
29	75	-2.808464	0.053360	0.507156	62	1	8.009355	-2.205864	0.141684
30	6	-4.697748	0.086606	0.503626	63	1	10.476195	-2.226196	0.246227
31	8	-5.899167	0.115899	0.493965	64	1	10.521765	2.085429	0.139343
32	6	-2.873165	0.125779	-2.389230	65	1	11.754376	0.082102	0.254595
33	8	-2.945609	0.166529	-3.583228					

Table S34. Coordinates of the optimized geometry of **3e**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	3.255671	0.061977	0.097788	28	1	-2.474806	-5.022295	-1.119388
2	7	0.498809	0.044614	0.334167	29	75	-1.560348	0.124708	0.537476
3	6	2.502523	-1.244164	0.244092	30	6	-3.447555	0.206406	0.609168
4	6	2.581497	1.175049	0.061000	31	8	-4.646589	0.266315	0.648357
5	6	1.190192	1.202900	0.177784	32	6	-1.543776	0.355142	-2.409012
6	6	1.112541	-1.165458	0.359770	33	8	-1.564482	0.496429	-3.596725
7	1	3.002520	-2.203239	0.291459	34	7	-1.671642	0.197098	1.648348
8	1	3.136938	2.092696	0.085771	35	6	-1.874634	0.669451	4.413879
9	6	0.325892	2.395676	0.122022	36	6	0.884995	0.470977	2.532370
10	6	-1.454634	4.510153	0.014474	37	6	-2.558699	-1.104529	2.141918
11	7	-1.031609	2.144844	0.209250	38	6	-2.687653	-1.363177	3.506255
12	6	0.814485	3.696982	0.019038	39	6	0.958240	0.263513	3.911113
13	6	0.080430	4.771266	0.085774	40	1	0.186927	1.191765	2.130276
14	6	-1.892259	3.191746	0.131223	41	1	-3.175283	-1.623743	1.420181
15	1	1.881251	3.874494	0.077989	42	1	-3.412973	-2.094319	3.842860
16	1	0.287765	5.784936	0.193627	43	1	0.306761	0.826124	4.569150
17	1	-2.944328	2.950867	0.195853	44	1	-1.953638	0.850713	5.480223
18	1	-2.184941	5.308510	0.068311	45	6	4.731562	0.118015	0.019706
19	6	0.179683	-2.292023	0.541786	46	7	7.554596	0.222768	0.244173
20	6	-1.705778	-4.277791	0.952641	47	6	5.544512	0.905890	0.503890
21	6	0.588605	-3.626862	0.606790	48	6	5.374033	-1.196091	0.658618
22	7	-1.151674	-1.945067	0.669437	49	6	6.771053	-1.205800	0.747960
23	6	-2.063371	-2.930052	0.874193	50	6	6.935000	0.812173	0.371448
24	6	0.359325	-4.635989	0.812193	51	1	5.118489	1.753077	-1.030382
25	1	1.635700	-3.881890	0.500507	52	1	4.809056	-2.006657	1.105863
26	1	-3.092132	-2.614796	0.985048	53	1	7.283614	-2.024516	1.242647
27	1	0.051752	-5.674013	0.864160	54	1	7.578109	1.587999	0.774234

Table S35. Coordinates of the optimized geometry of **4a**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	-1.121222	-3.454584	2.769150	35	15	0.466785	1.217583	0.334856
2	7	0.682175	-1.915147	0.532340	36	6	0.602764	2.754797	0.224715
3	6	-2.146774	-2.636614	2.275338	37	6	-2.234809	5.045364	0.003812
4	6	0.124941	-3.496090	2.129269	38	6	-1.953001	2.710884	0.624291
5	6	0.325179	-2.699313	0.995817	39	6	0.079759	3.953689	0.292856
6	6	-1.901062	-1.866714	1.131854	40	6	0.893531	5.091511	0.404333
7	1	-3.108126	-2.610033	2.772320	41	6	-2.761202	3.851446	0.520298
8	1	0.913202	-4.130287	2.514158	42	1	-2.385117	1.799283	1.023874
9	6	1.557791	-2.607119	0.196958	43	1	0.956792	4.010325	0.608679
10	6	3.775231	-2.346708	-1.438639	44	1	0.476690	6.009850	0.806777
11	7	1.511082	-1.731175	0.870460	45	1	-3.798007	3.802486	0.838936
12	6	2.706700	-3.355297	0.470388	46	1	-2.862287	5.927521	0.080127
13	6	3.832478	-3.226533	0.350690	47	6	2.183836	1.875804	0.038176
14	6	2.604805	-1.619680	-1.666203	48	6	4.725592	2.945600	0.618052
15	1	2.723924	-4.034844	1.313392	49	6	2.952928	2.471716	0.979457
16	1	4.727715	-3.802810	0.147440	50	6	2.690361	1.832706	-1.348299
17	1	2.521367	0.940943	-2.502633	51	6	3.956466	2.364622	-1.637045
18	1	4.617307	-2.218530	-2.107963	52	6	4.218901	3.000339	0.690288
19	6	-2.858976	0.987532	0.444581	53	1	2.571715	2.526637	1.994301
20	6	-4.550363	0.628616	-1.035845	54	1	2.102311	1.402686	-2.150625
21	6	-4.188787	0.830239	0.847736	55	1	4.335611	2.324465	-2.653577
22	7	-2.368111	0.336060	0.671171	56	1	4.803738	3.456174	1.483458
23	6	-3.210952	0.452613	-1.387616	57	1	5.706784	3.354325	0.840210
24	6	-5.049455	0.015182	0.103803	58	6	0.595361	0.826941	2.168552
25	1	-4.553453	-1.345053	1.727926	59	6	0.875056	0.113493	4.882098
26	1	-2.788421	0.943119	-2.253340	60	6	1.597225	0.079778	2.569555
27	1	-6.082864	0.109890	0.405697	61	6	0.257934	1.379541	3.137222
28	1	-5.179106	1.265499	-1.646163	62	6	0.117722	1.022208	4.488178
29	75	0.359612	0.762931	-1.166197	63	6	1.737454	0.432312	3.917771
30	6	0.122496	0.380103	-2.651218	64	1	2.292450	0.487690	1.841297
31	8	0.017087	1.108312	-3.601866	65	1	-1.017685	2.102350	2.861950
32	6	0.890458	-2.097903	-2.386622	66	1	0.780438	1.460890	5.228054
33	8	-1.210266	-2.914447	-3.196286	67	1	2.518768	-1.126610	4.211976
34	1	-1.293788	-4.060049	3.651553	68	1	0.982462	0.159232	5.927614

Table S36. Coordinates of the optimized geometry of **4b**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	6	0.090002	-3.939329	1.806917	40	1	-1.289652	3.201979	2.572312
2	7	0.095275	-1.854558	0.027841	41	1	-2.922925	5.047414	2.425999
3	6	-1.117844	-3.420887	1.302514	42	1	-3.366249	4.335164	-1.806322
4	6	1.300199	-3.375408	1.362387	43	1	-3.976931	5.625507	0.239177
5	6	1.279104	-2.321415	0.444562	44	6	1.425559	2.394411	0.941424
6	6	-1.092125	-2.370081	0.381630	45	6	3.620005	4.102307	1.383239
7	1	-2.058679	-3.843549	1.633936	46	6	1.774682	2.772230	2.250134
8	1	2.239517	-3.761252	1.739933	47	6	2.170861	2.887383	0.144032
9	6	2.448482	-1.622548	0.113771	48	6	3.263060	3.739511	0.075350
10	6	4.530441	0.274942	-1.317673	49	6	2.872483	3.617864	2.468170
11	7	2.159995	0.620899	-1.017919	50	1	1.202540	2.417314	3.101675
12	6	3.766543	-1.948088	0.215491	51	1	1.893788	2.624403	-1.160248
13	6	4.845840	-1.272743	0.377378	52	1	3.830072	4.116094	0.770603
14	6	3.200564	0.021927	-1.607380	53	1	3.137217	3.901339	3.482441
15	1	3.960031	-2.736915	0.933113	54	1	4.468003	4.758448	1.555241
16	1	2.946373	0.778949	-2.335799	55	6	0.500304	0.475677	2.158667
17	1	5.313479	0.274980	-1.828018	56	6	-1.135797	-1.000767	4.472832
18	6	-2.258516	-1.735175	0.256095	57	6	0.518229	0.140078	2.910613
19	6	-4.329157	0.509932	-1.604067	58	6	-1.840301	0.328365	2.561396
20	6	-3.575874	-2.127035	0.005912	59	6	-2.154841	0.402908	3.716075
21	7	-1.967447	0.730445	-1.155765	60	6	0.200880	0.869455	4.064822
22	6	-3.000894	0.147938	-1.816040	61	1	1.558775	0.049215	2.611177
23	6	-4.649237	-1.517639	0.675838	62	1	-2.640768	0.785585	1.987073
24	1	-3.773799	-2.915096	0.711249	63	1	-3.192348	0.503603	4.020239
25	1	-2.740544	0.614985	-2.535772	64	1	0.996281	-1.332895	4.640683
26	1	-5.107106	0.003545	-2.164680	65	1	-1.379594	-1.563421	5.369033
27	75	0.101994	0.320464	-1.433194	66	6	-6.069607	-1.943090	0.437427
28	6	0.161589	1.125451	-2.644626	67	1	-6.182669	-2.449000	0.525242
29	8	0.230870	2.034459	-3.431242	68	1	-6.393362	-2.640937	-1.220348
30	6	0.185883	-1.461969	-2.928091	69	1	-6.750038	-1.086401	0.465009
31	8	0.231164	-2.148527	-3.904968	70	6	0.084551	-5.048783	2.819930
32	15	0.093361	1.358009	0.559197	71	1	1.006498	-5.635289	2.777740
33	6	-1.403358	2.701804	0.460755	72	1	0.765322	-5.721389	2.672218
34	6	-3.259471	4.812644	0.300297	73	1	0.002683	-4.633239	3.832794
35	6	-1.991258	3.034506	0.768937	74	6	6.268353	-1.591109	0.016426
36	6	-1.740092	3.439416	1.612733	75	1	6.646672	0.863964	0.713561
37	6	-2.667005	4.486517	1.532183	76	1	6.921006	-1.539655	0.893448
38	6	-2.917741	4.086674	0.849261	77	1	6.358348	-2.585627	0.428879
39	1	-1.724777	2.489151	-1.666512					

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