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for

Polymerisation of Styrene using Pincer Type Amine Functionalized Azo Aromatic Complexes of Co(II) as Catalysts

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S1. Instrumentation and methods

General.

A Cary 8454 UV-vis spectrophotometer was used to record UV-vis spectra. IR spectroscopic data were obtained with the Bruker Platinum-ATR instrument. Cyclic voltammetry was conducted in 0.1 M Bu_4NClO_4 solutions by using a three-electrode configuration (Pt working electrode, Pt counter electrode, and Ag/AgCl reference electrode) and a PC-controlled PAR model 273A electrochemistry system. ^{1}H and ^{13}C NMR spectra were recorded either in 400 MHz JEOL ECS NMR spectrometer or 500 MHz Bruker AvanceIII NMR spectrometer, tetramethylsilane (TMS) was used as an internal reference. A Perkin-Elmer 240C elemental analyzer was used to collect microanalytical data (C, H, N). Powder X-ray diffraction (PXRD) data were collected using a Rigaku, Smart Lab with high-intensity rotating anode X-ray generator with the help of Control Win software in the 2θ range, 5-50◦C. Room-temperature magnetic moment measurements for the complexes **1-4** were performed with Gouy Balance (Sherwood Scientific, Cambridge, UK). The spectroscopic grade solvents were used for spectroscopic and electrochemical studies.

Molecular weight measurements.

The number-average molecular weight (M_n), weight-average molecular weight (M_w), and polydispersity indexes ($Đ$) were determined by gel permeable chromatography (GPC) in a size exclusion chromatography (SEC) instrument using DMF as eluent with a flow rate of 1.0 mL/min (nominal) at 35°C (nominal). The SEC instrument was equipped with Waters 2414 refractive index (RI) detector, a Waters 1515 HPLC pump, one PolarGel-M guard column (50 × 7.5 mm), and two PolarGel-M analytical columns (300 × 7.5 mm). The

instrument was calibrated with polystyrene standards, and molecular weights and Đ values were calculated from the calibration graph. DMF solution of synthesized polymers was filtered through a 0.45 μm syringe filter before injection to the instrument.

Thermal analysis

Thermogravimetric analysis (TGA) was performed with a 4−6 mg sample weight at 10^{o}C/min heating rate in N_2 atmosphere using the Mettler Toledo TGA/SDTA 851e instrument. The baseline was calibrated by scanning the temperature domain of the experiments with an empty crucible. The temperature calibration was performed, taking the onset of the endothermic melting peak at the heating rate of the measurements, using five calibration standards, and the enthalpy scale was calibrated using indium as standard reference material. Polystyrene samples with masses in the range of 4–6 mg were weighed in aluminium crucibles. All runs were performed under N_2 atmosphere to increase thermal contact between the crucible and the apparatus sensor, at a heating rate of 10°C/min. The differential scanning calorimetry (DSC) experiment was conducted on a Mettler Toledo DSC1/STARe instrument at various heating rates (5, 10, 15, 20, and 25 °C/min) in an N_2 atmosphere with sample weights of ∼4−5 mg.

Nanoindentation Studies

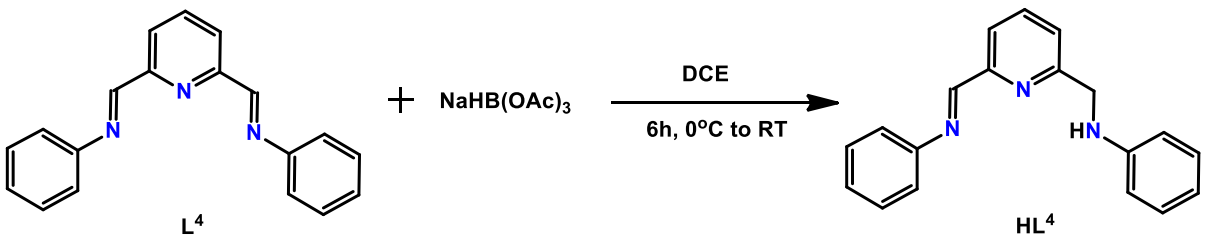
Nanoindentation experiments have been performed on the film state of our synthesized polystyrene using the TI Premier from Hysitron, Minneapolis, USA, equipped with an in-situ Scanning Probe Microscope (SPM). A Berkovich tip (three-sided pyramidal tip with a total included plane-edge angle of 142.3°) of radius ~150 nm was employed to determine the hardness (*H*) and elastic modulus (*E*) of the crystals. The *H* and *E* were extracted using

the standard Oliver-Pharr (O&P) method.[1] The complete details of the method can be found elsewhere.[2,3]

S2. Synthesis of Ligands

Preparation of Ligands, HL^4

The ligands, $\mathbf{L^4}$ was prepared and purified following literature procedure.[4] In 10 mL of DCE, 200 mg (1.09 mmol) of compound, $\mathbf{L^4}$ was dissolved in a 50 mL round bottom flask. 150 g (1.1 mmol) of Sodium triacetoxyborohydride was added to the solution under argon atmosphere at cold condition and stirred at room temperature for 4 h. The crude mass, obtained after DCE evaporation, was extracted using dichloromethane and loaded on a preparative silica gel TLC plate for purification. A solvent mixture of hexane: ethyl acetate (19:1) was used as an eluent to isolate ligand, $\mathbf{HL^4}$ in its pure state. It's yield and characterization data are as follows: yield: 71%, ESI-MS: m/z 288.1486 amu $[MH]^+$; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.64 (1 H, s), 8.11 (1 H, d, J=7.7), 7.77 (1 H, t, J=7.7), 7.45 – 7.40 (3 H, m), 7.33 – 7.28 (3 H, m), 7.22 – 7.17 (2 H, m), 6.76 – 6.67 (3 H, m), 4.81 (1 H, s), 4.54 (2 H, s); ^{13}C NMR (126 MHz, $CDCl_3$): δ 160.76, 158.68, 154.18, 151.02, 147.75, 137.27, 129.29, 129.21, 126.72, 123.02, 121.13, 120.19, 117.78, 113.10, 49.24; IR: 1597 cm^{-1} (CH=N); 3434 cm^{-1} (2° NH).



Scheme S1. Synthesis of ligand, $\mathbf{HL^4}$

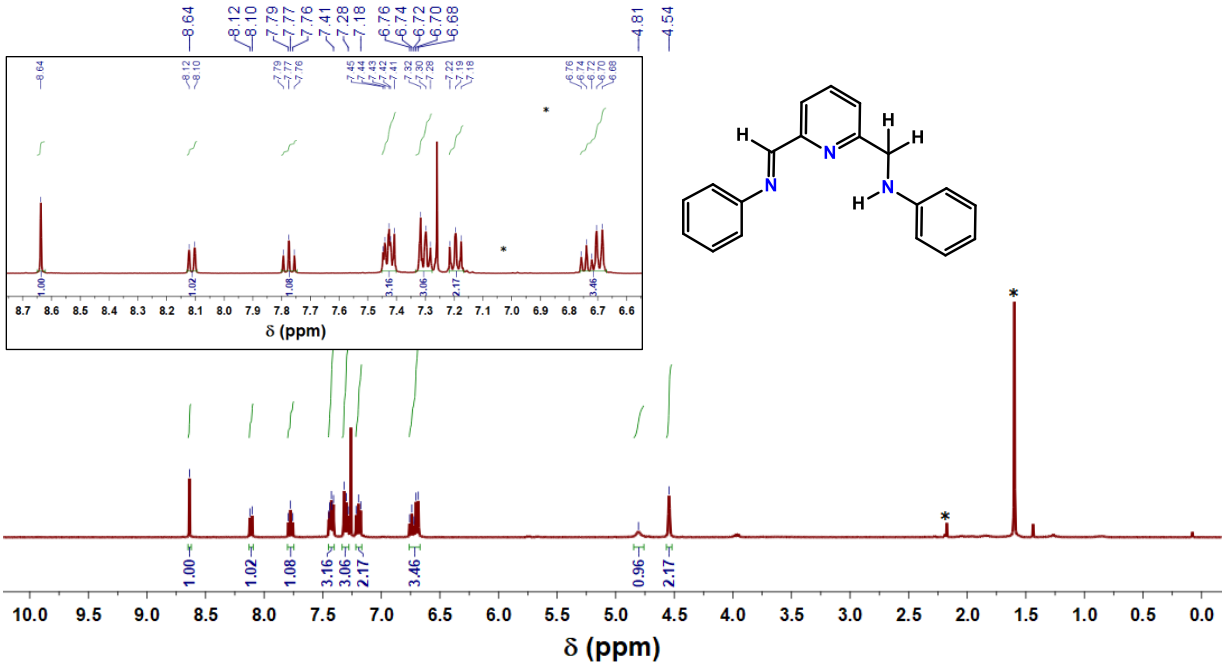


Figure S1. ^{1}H NMR spectrum of the ligand, **HL^{4}**

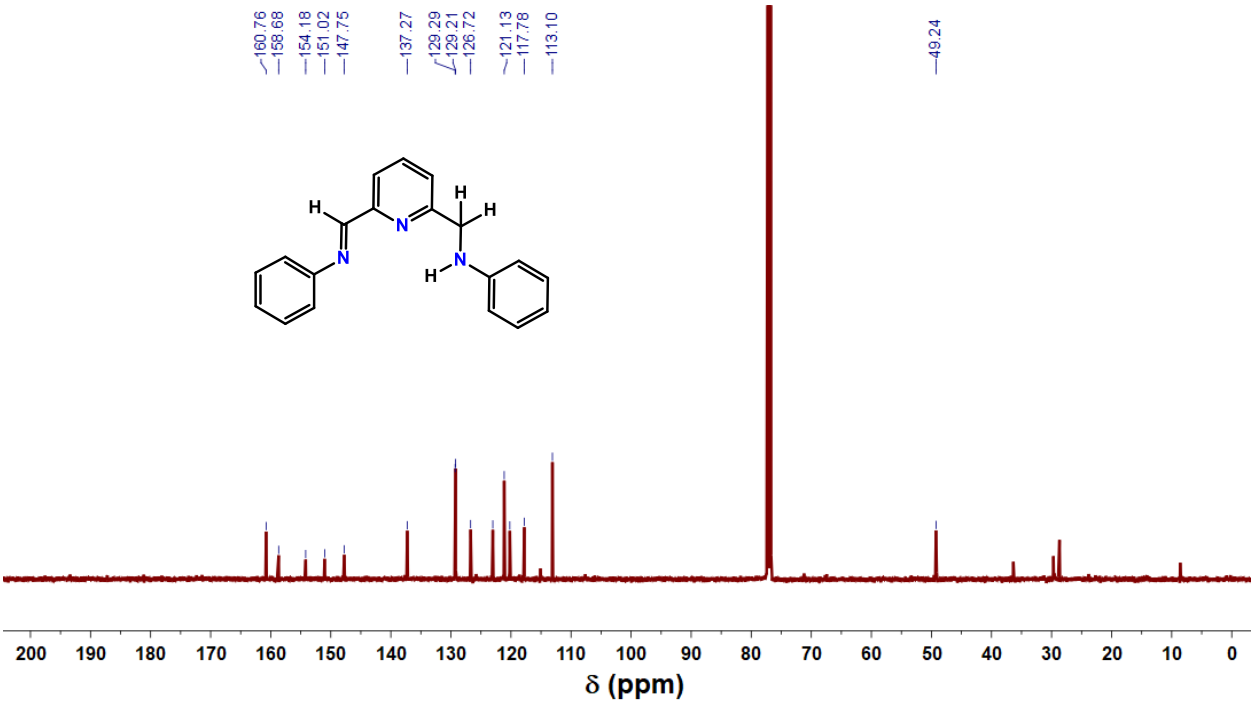


Figure S2. ^{13}C NMR spectrum of the ligand, **HL^{4}**

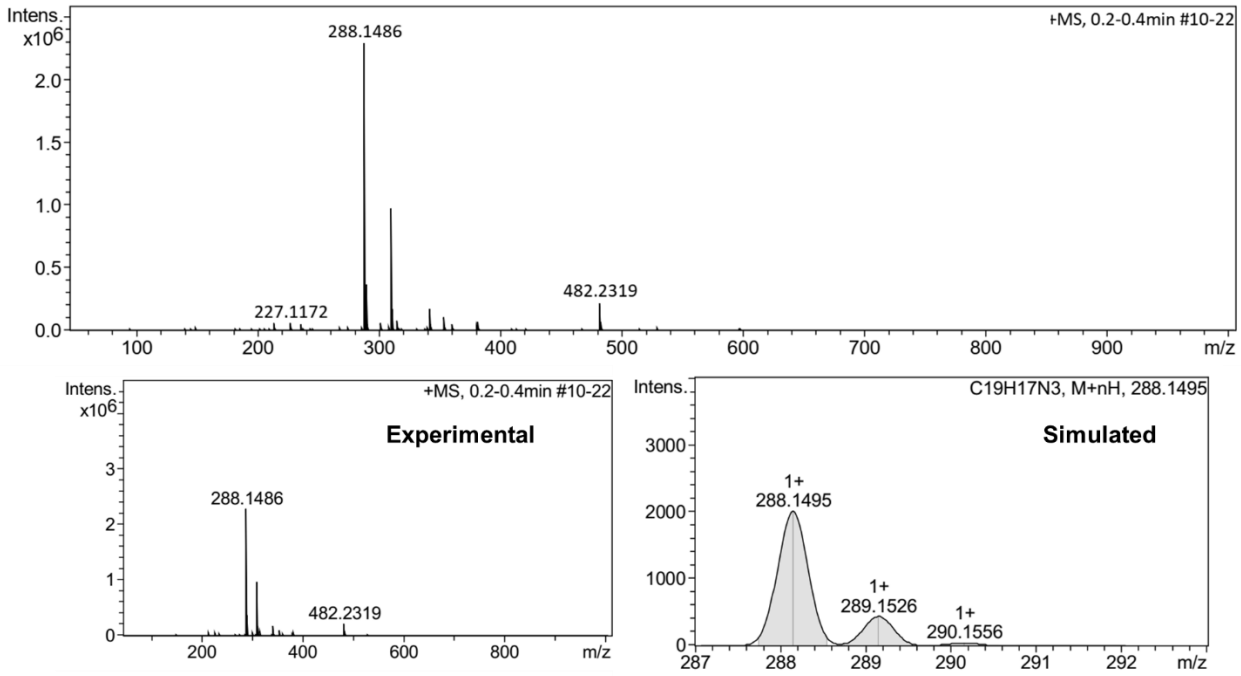


Figure S3. Full range ESI-MS spectrum of the ligand, **HL^4** in methanol (top); Experimental and simulated spectrum of the ligand, **HL^4** (bottom)

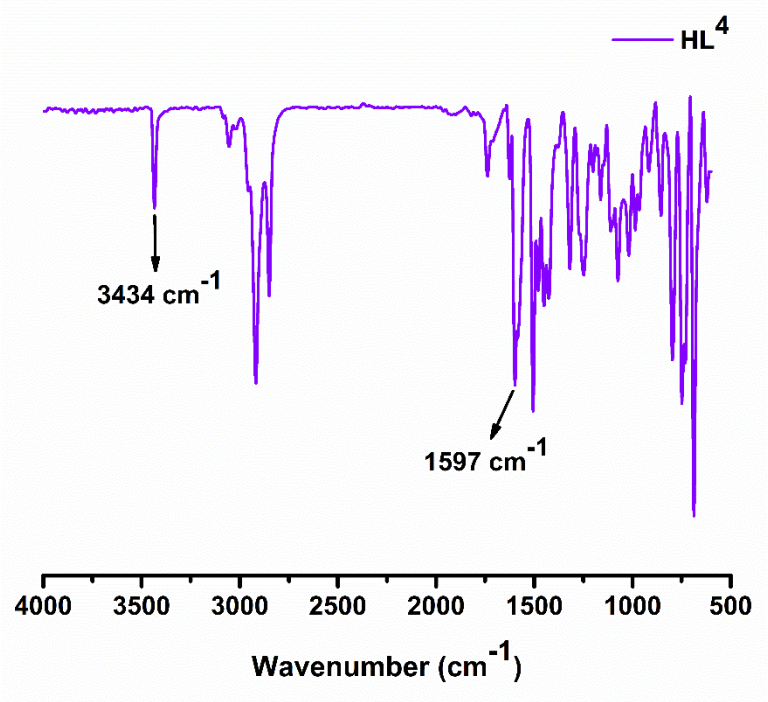


Figure S4. IR Spectrum of the ligands, **HL^4**

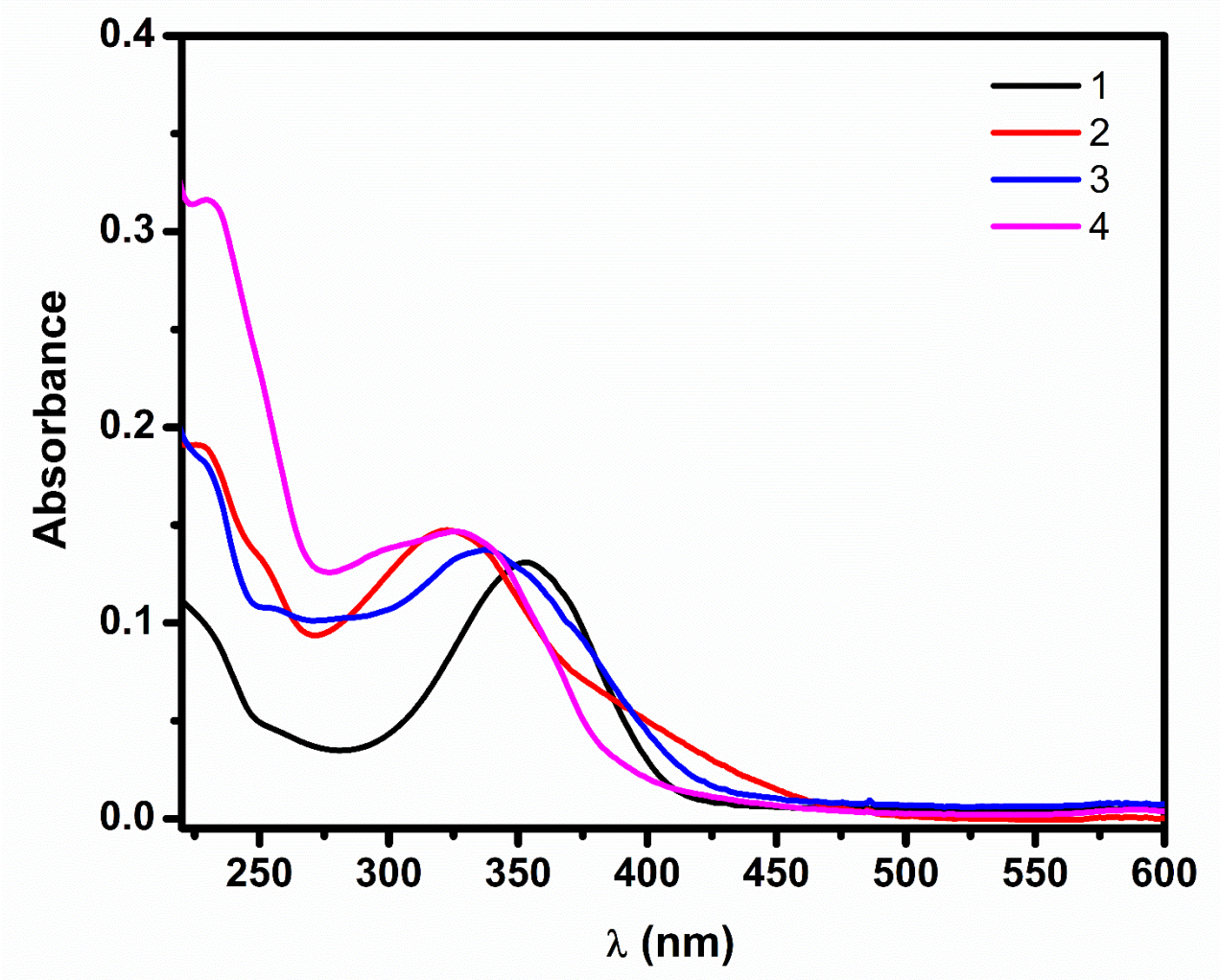


Figure S5. UV-*vis* spectra of the complexes **1-4**

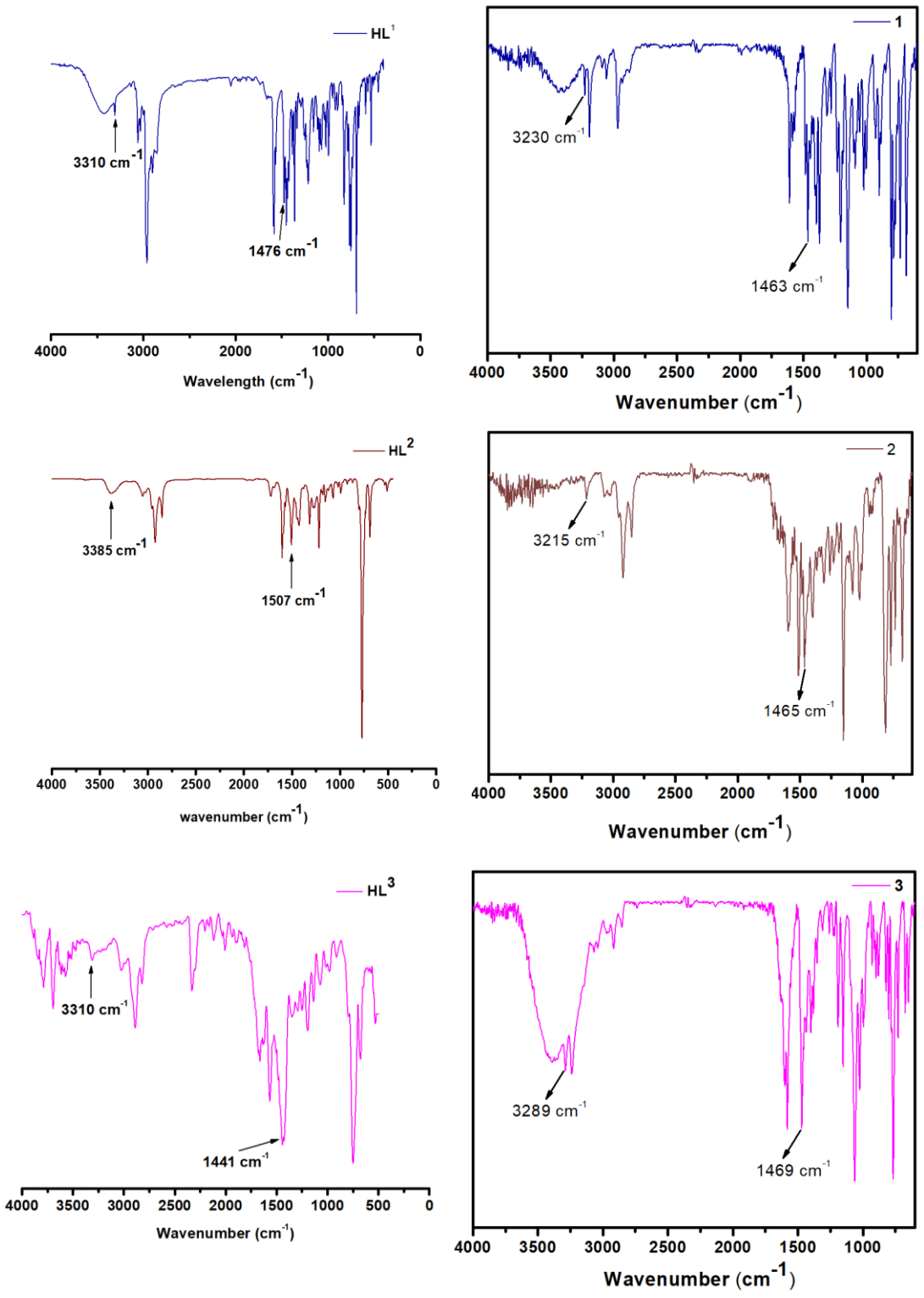


Figure S6. IR Spectrum of the ligands **HL^1-HL^3** and complexes **1-3**

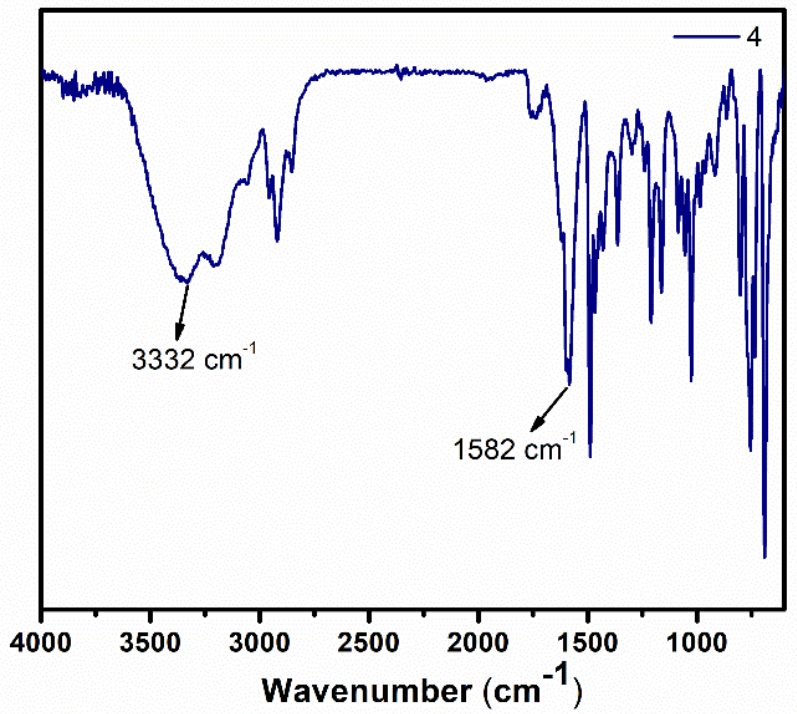


Figure S7. IR Spectrum of the complex **4**.

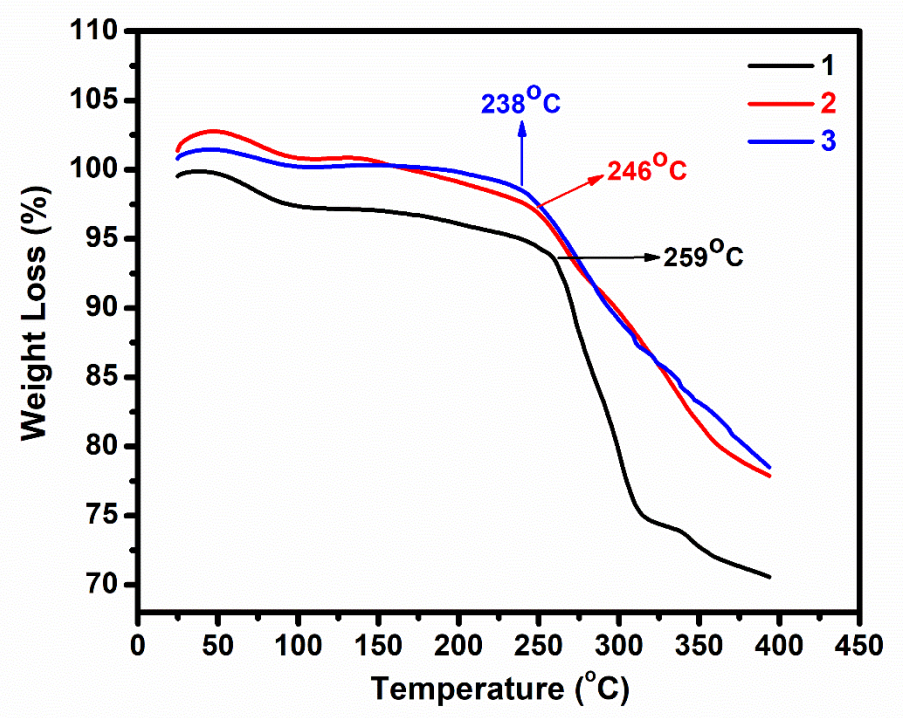


Figure S8. TGA data of the complexes **1-3**

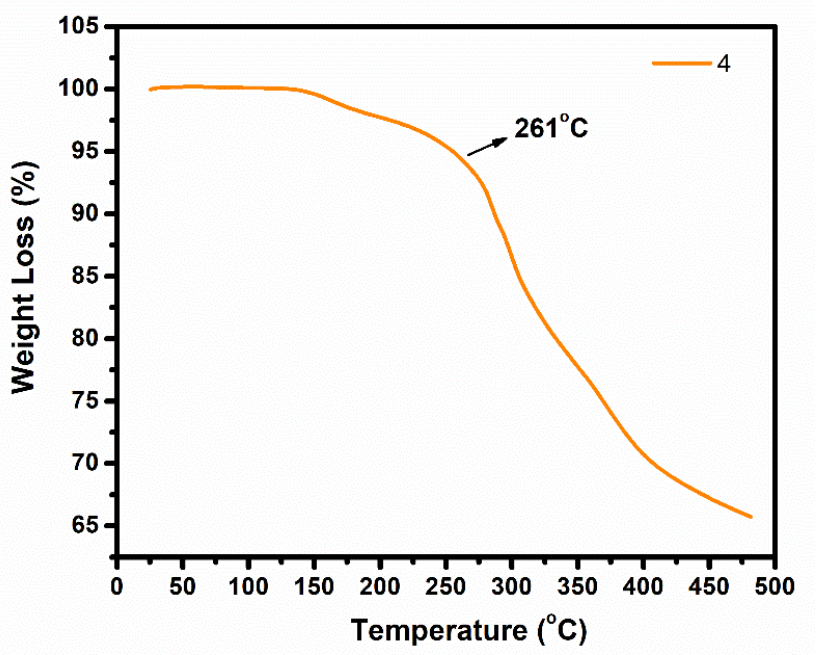


Figure S9. TGA data of the complex **4**

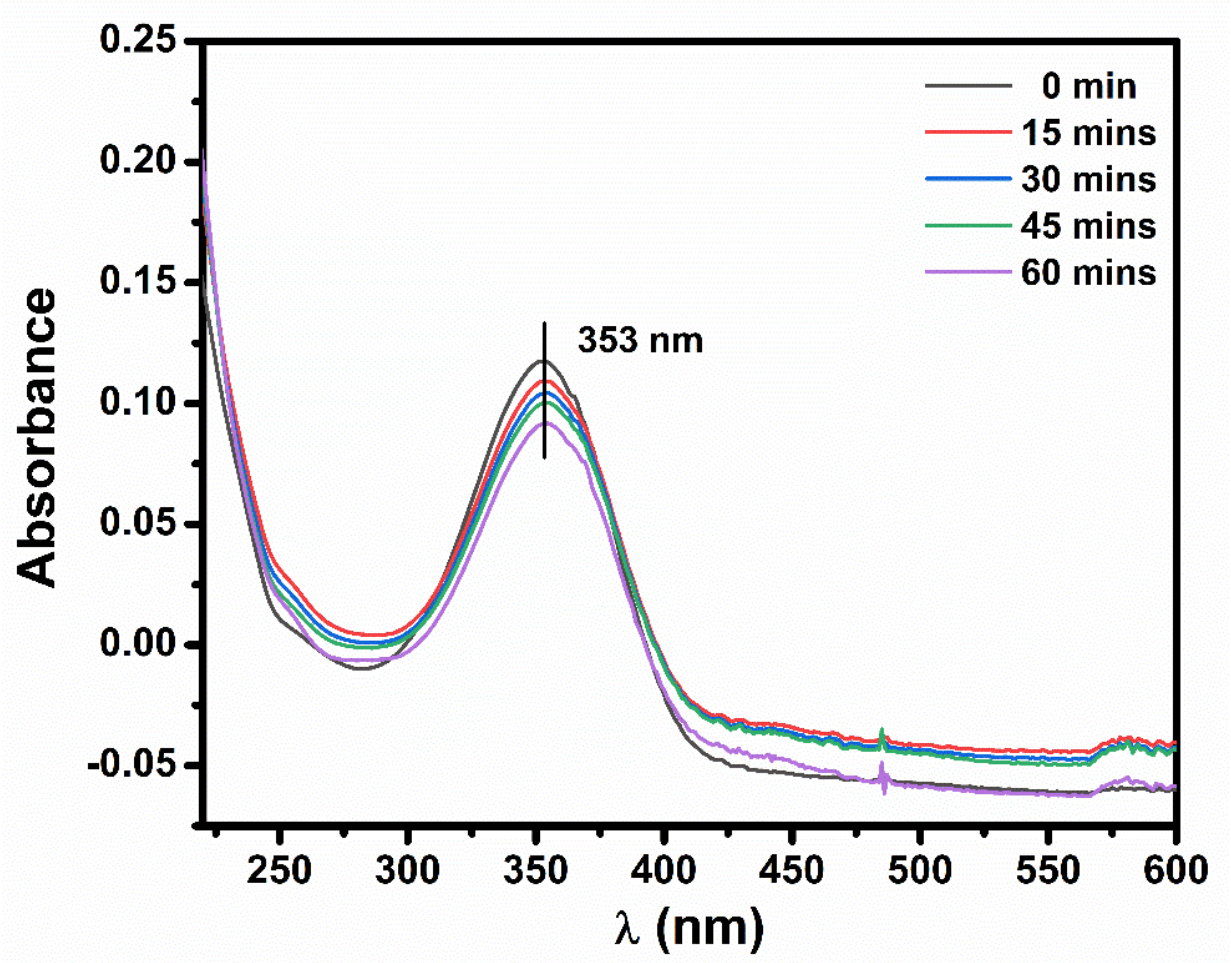


Figure S10. UV-*vis* spectral changes of the representative complex **1** (1 x 10^{-5} M) upon exposure with 365 nm UV light in acetonitrile solvent.

S3. X-ray crystallographic details

Suitable X-ray quality crystals of compounds **1**, **2, 3**, and **4** were obtained from the slow evaporation of a dichloromethane−hexane solution of the corresponding compounds. Data for the crystals of the compound **1** was collected by using a Bruker D8 venture diffractometer with monochromatic Cu\K$_\alpha$ radiation (λ = 1.54184 Å). Data for the crystals of the compounds **2**, **3**, and **4** were collected on Oxford Diffraction SuperNova (Dual, EOS) diffractometer with monochromatic equipped with Mo\K$_\alpha$ radiation (λ = 0.71073 Å) or Cu\K$_\alpha$ radiation (λ = 1.54184 Å). Data reduction was done with CrysAlis^{PRO}, Agilent Technologies, Version 1.171.37.34. Structures were solved by Olex 2[5], with the Superflip[6] or, ShelXT[7] structure solution programme using Charge flipping and refined with the ShelXL refinement package[8] using Least-squares minimization. All hydrogen atoms were added in calculated positions. Refinement details and relevant explanations (wherever applicable) are included in the individual CIFs. All the data were deposited in http://www.ccdc.cam.ac.uk. Crystallographic data for compounds **1**, **2**, **3**, and **4** are collected in Table **S1**. Selected bond lengths and bond angles are presented in Table **S2.**

Table S1. Crystallographic Data of the complexes **1–4**

	Complex 1	**Complex 2**	**Complex 3**	**Complex 4**
CCDC No.	2083747	2083749	2083750	2124862
empirical formula	$C_{32}H_{40}Cl_4Co_2N_8$	$C_{20}H_{19}Cl_2N_5Co$	$C_{20}H_{20}Cl_2CoN_4$	$C_{19}H_{17}N_3Cl_2Co$
formula wt.	796.38	459.23	446.25	453.236
crystal system	monoclinic	monoclinic	triclinic	monoclinic
space group	$P2_1/c$	$P2_1/n$	P-1	$P2_1/n$
a (Å)	15.242(6)	8.0005(4)	9.1251(6)	9.4655(2)
b (Å)	11.780(5)	22.9904(10)	9.7997(6)	13.2728(2)
c (Å)	19.686(18)	11.6606(7)	11.9466(6)	16.6662(3)
α (deg)	90.00	90.00	88.053(5)	90
β (deg)	93.34(4)	102.494(6)	75.080(5)	104.567(2)
γ (deg)	90.00	90.00	71.225(6)	90
Cell Volume	3531(4)	2094.00(19)	975.96(10)	2026.53(7)
Z	4	4	2	4
T (K)	100.00(10)	100.00(10)	100.01(10)	100.00(12)
μ (mm^{-1})	10.427	1.090	9.505	9.224
ρ_{calcd}($g\ cm^{-3}$)	1.498	1.457	1.518	1.486
F (000)	1640.0	940.0	458.0	928.5
2θ range (deg)	5.8 to 104.06	3.54 to 52.74	7.66 to 132.4	8.62 to 136.62
Data/restraints/ parameters	3929/0/421	4275/0/248	3396/0/246	3702/0/226
R_1, $wR_2[I > 4\sigma(I)]$	R_1 = 0.0315, wR_2 = 0.0853	R_1 = 0.0591, wR_2 = 0.1709	R_1 = 0.0890, wR_2 = 0.2411	R_1 = 0.0603, wR_2 = 0.1592
R_1, wR_2 (all data)	R_1 = 0.0324, wR_2 = 0.0859	R_1 = 0.0777, wR_2 = 0.1931	R_1 = 0.0962, wR_2 = 0.2543	R_1 = 0.0614, wR_2 = 0.1603
GOF on F^2	1.111	1.088	1.025	1.035
largest difference in peak and hole (e $Å^{-3}$)	0.51/-0.52	1.74/-1.37	2.37/-0.98	0.88/-1.01

Table S2. Summary of selected experimental and calculated bond lengths (Å) and bond angles (°) of Complex **1-4**

Bonds and Angles	**1**		**2**		**3**		Bonds and Angles	**4**	
	X-ray	DFT	X-ray	DFT	X-ray	DFT		X-ray	DFT
N1-N2	1.267(3)	1.259	1.259(5)	1.260	1.256(7)	1.259	C7-N1	1.280(5)	1.279
C12-N4	1.468(4)	1.475	1.444(6)	1.479	1.483(7)	1.477	C13-N3	1.425(5)	1.477
Co1-N1	2.351(3)	2.347	2.288(4)	2.306	2.252(5)	2.301	Co1-N1	2.208(3)	2.284
Co1-N3	2.023(3)	2.059	2.023(3)	2.061	2.018(5)	2.071	Co1-N2	2.022(3)	2.081
Co1-N4	2.207(3)	2.261	2.229(4)	2.289	2.261(5)	2.334	Co1-N3	2.280(3)	2.303
Co1-Cl1	2.272(10)	2.328	2.269(13)	2.318	2.242(15)	2.329	Co1-Cl1	2.2690(10)	2.305
Co1-Cl2	2.263(12)	2.295	2.239(14)	2.290	2.275(16)	2.279	Co1-Cl2	2.2703(9)	2.323
N1-Co1-N3	70.95(10)	71.31	72.28(14)	71.97	73.19(18)	72.30	N1-Co1-N2	76.73(11)	75.15
N3-Co1-N4	79.01(10)	78.39	75.80(15)	77.08	77.64(18)	76.53	N2-Co1-N3	75.35(12)	76.39
N2-N1-Co1	116.10(18)	115.60	116.2(3)	116.1	116.4(4)	116.0	C7-N1-Co1	112.2(2)	111.8
C12-N4-Co1	107.99(18)	108.29	108.1(3)	107.1	110.5(3)	109.3	C13-N3-Co1	107.6(2)	107.2
C11-C12-N4	112.76(2)	112.54	109.1(4)	111.7	111.7(5)	112.8	C12-C13-N3	111.4(3)	111.7
C7-N2-N1	112.83(2)	113.84	113.0(4)	113.8	113.4(5)	113.9	C8-C7-N1	118.7(3)	119.3

S4. Computational details

All computational calculations were performed in Gaussian 16 (G16) programme.[9] Complete geometry optimization of the complexes **1-4,** were carried out using the density functional theory method at the RB3LYP and UB3LYP levels of theory.[10] The 6-31+G* basis set for C, H, N, and Cl atoms was used, and the LANL2DZ basic set with effective core potential was used for Co-atom.[11-13] The vibrational frequency calculations were performed to ensure that the optimized geometries represent the local minima and there are only positive Eigenvalues. An isosurface value of 0.06 was used for the visualization of molecular orbitals. The 3D images of the optimized geometries and molecular orbitals were visualized using ChemCraft visualization software,[14] and GaussView software[15], respectively.

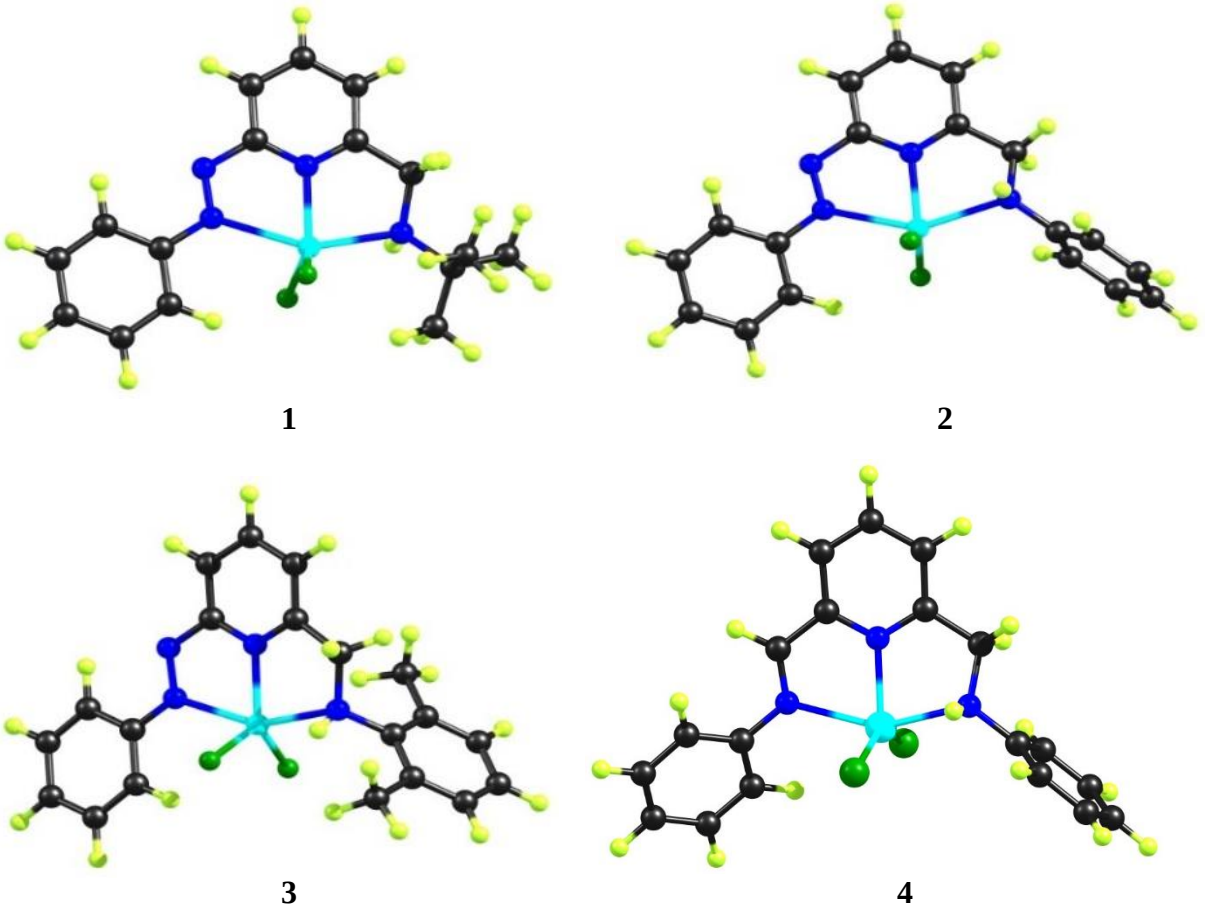


Figure S11. Optimized Structure of the complexes **1-4.**

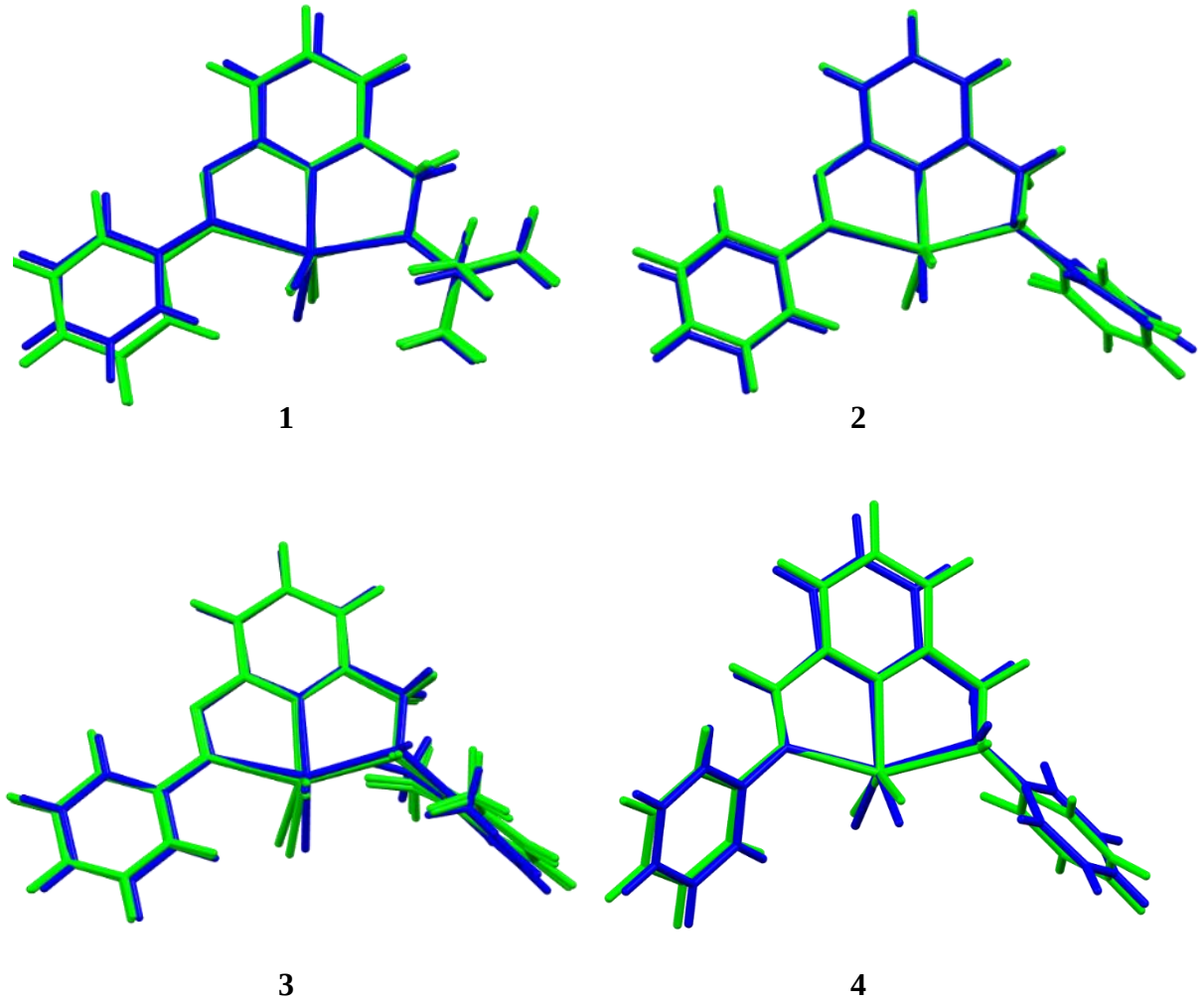


Figure S12. Overlay of X-ray crystal structure and DFT optimized structure of complexes **1-4** (Blue colour denotes X-ray crystal structure and Green colour denotes DFT optimized structure).

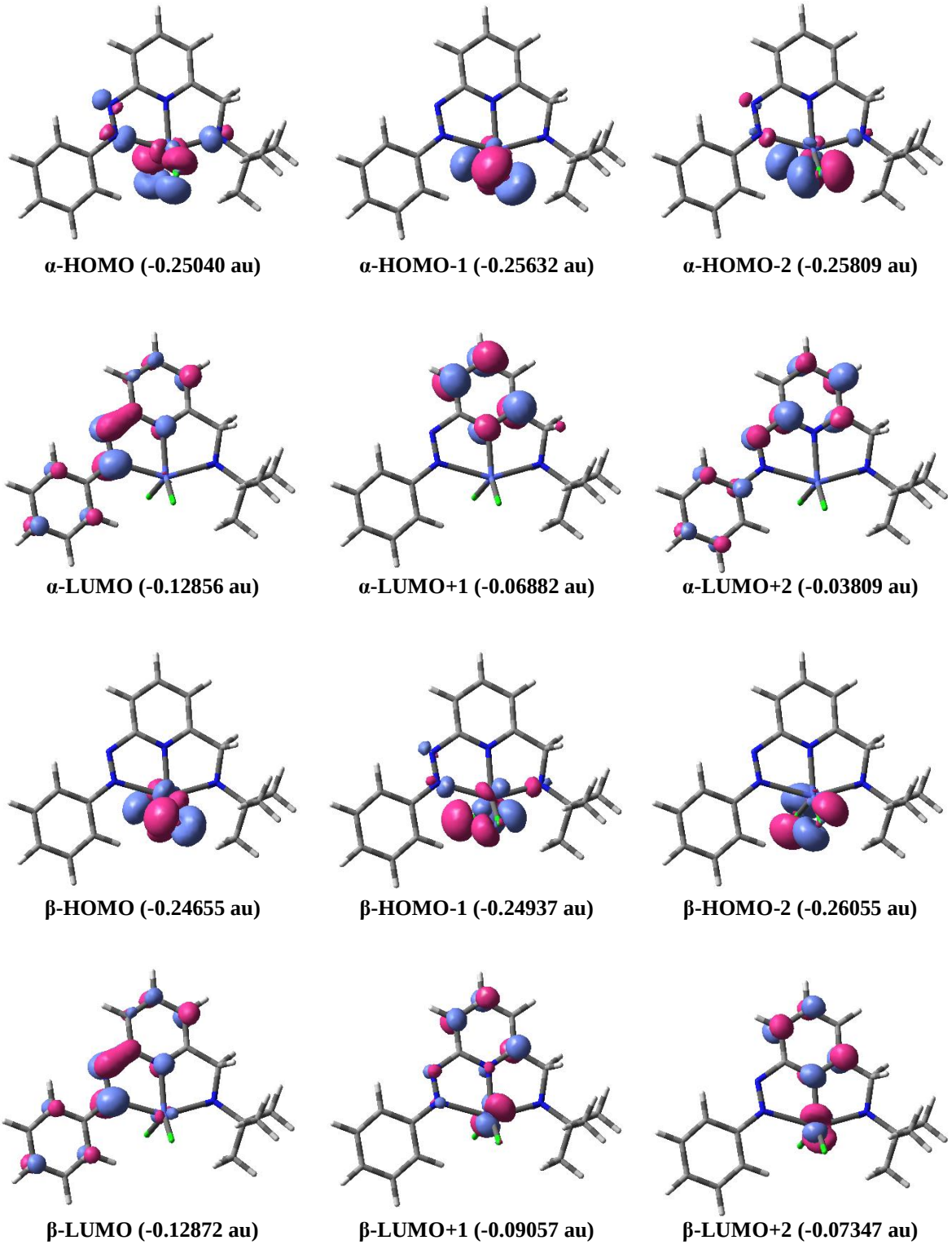


Figure S13. FMO's of the Complex **1** (isosuface value=0.06)

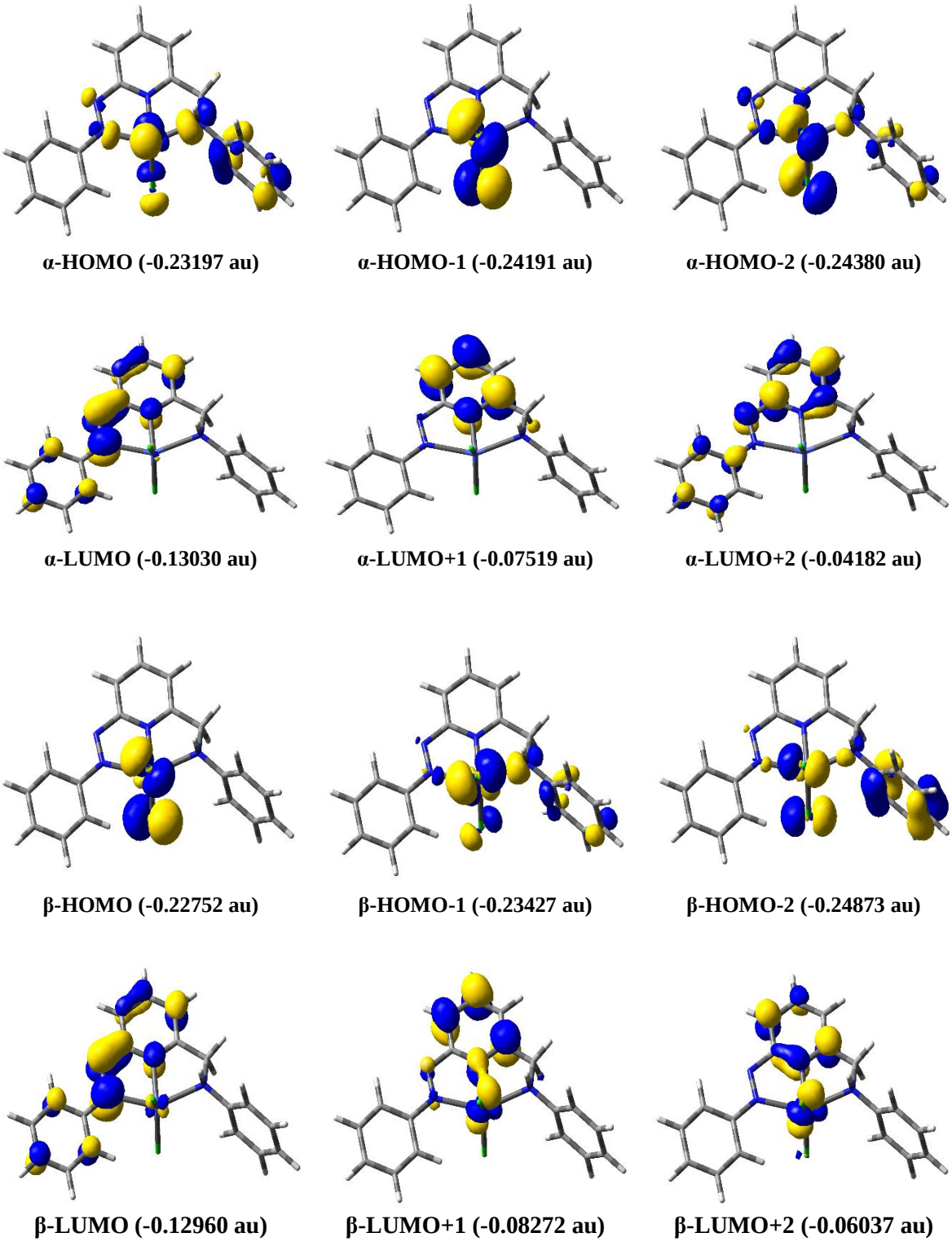


Figure S14. FMO's of the Complex **2** (isosurface value=0.06)

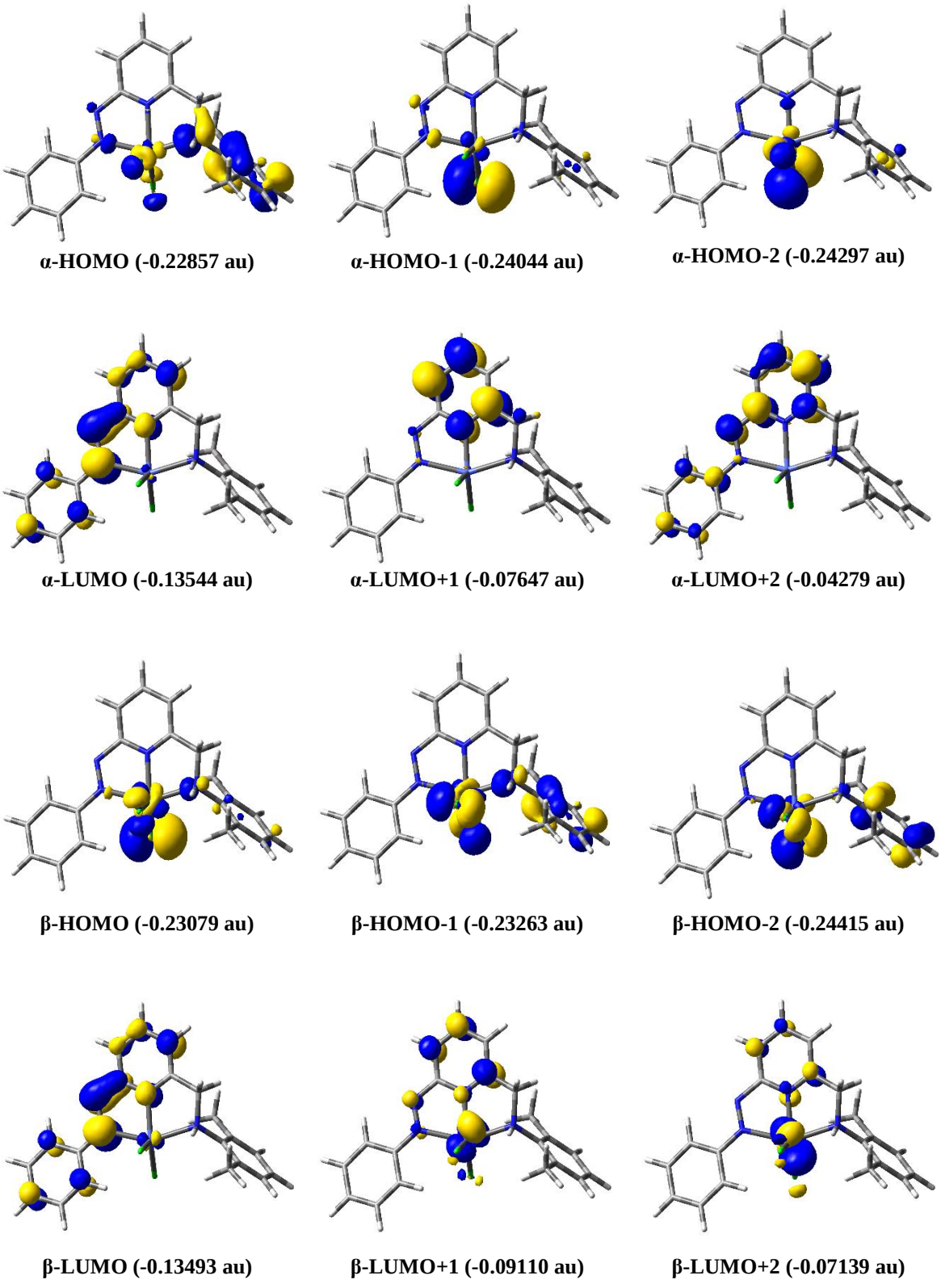


Figure S15. FMO's of the Complex **3** (isosurface value=0.06)

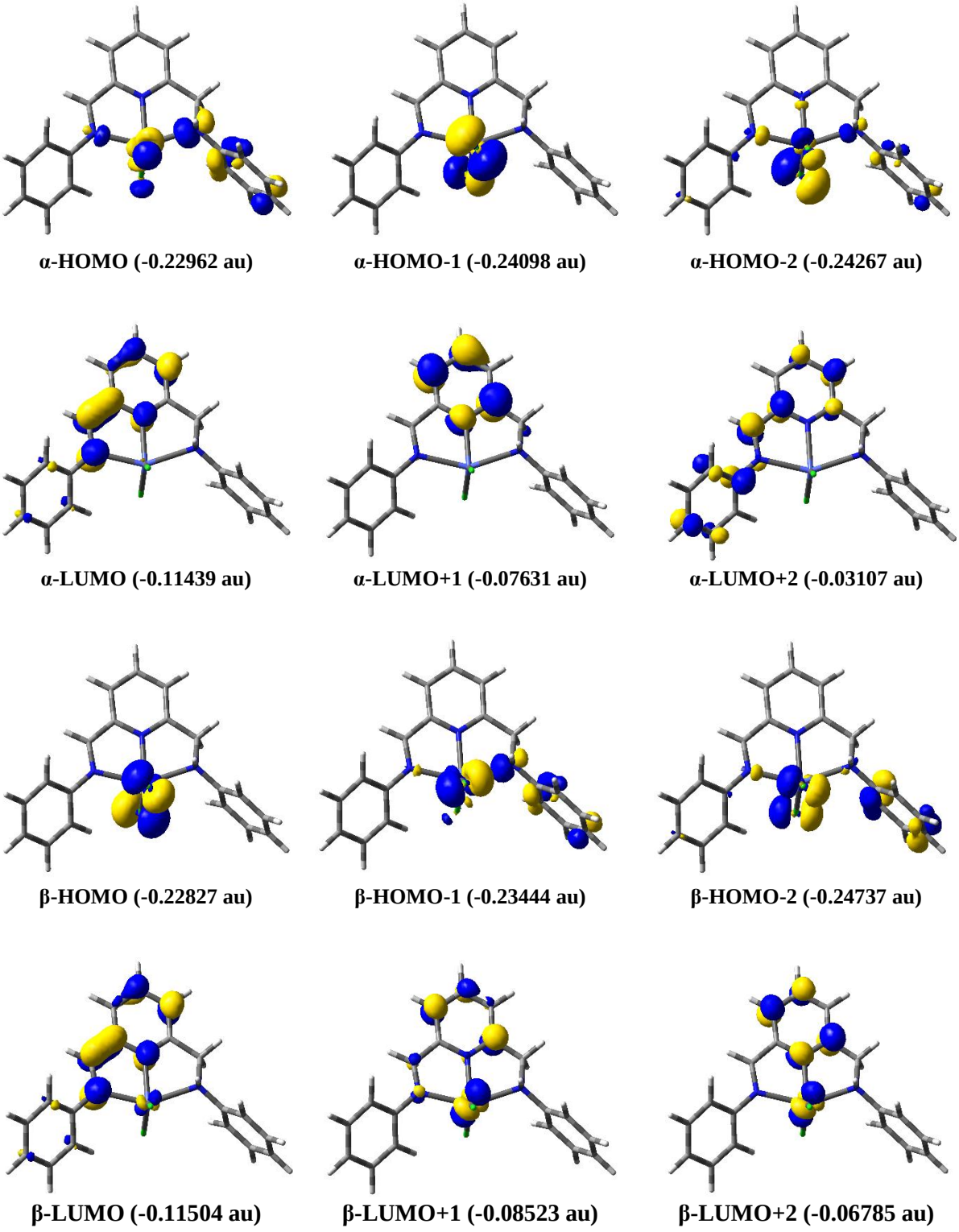


Figure S16. FMO's of the Complex **4** (isosurface value=0.06)

Figure S17. ^{1}H NMR monitoring of styrene polymerization by using the complex **1**

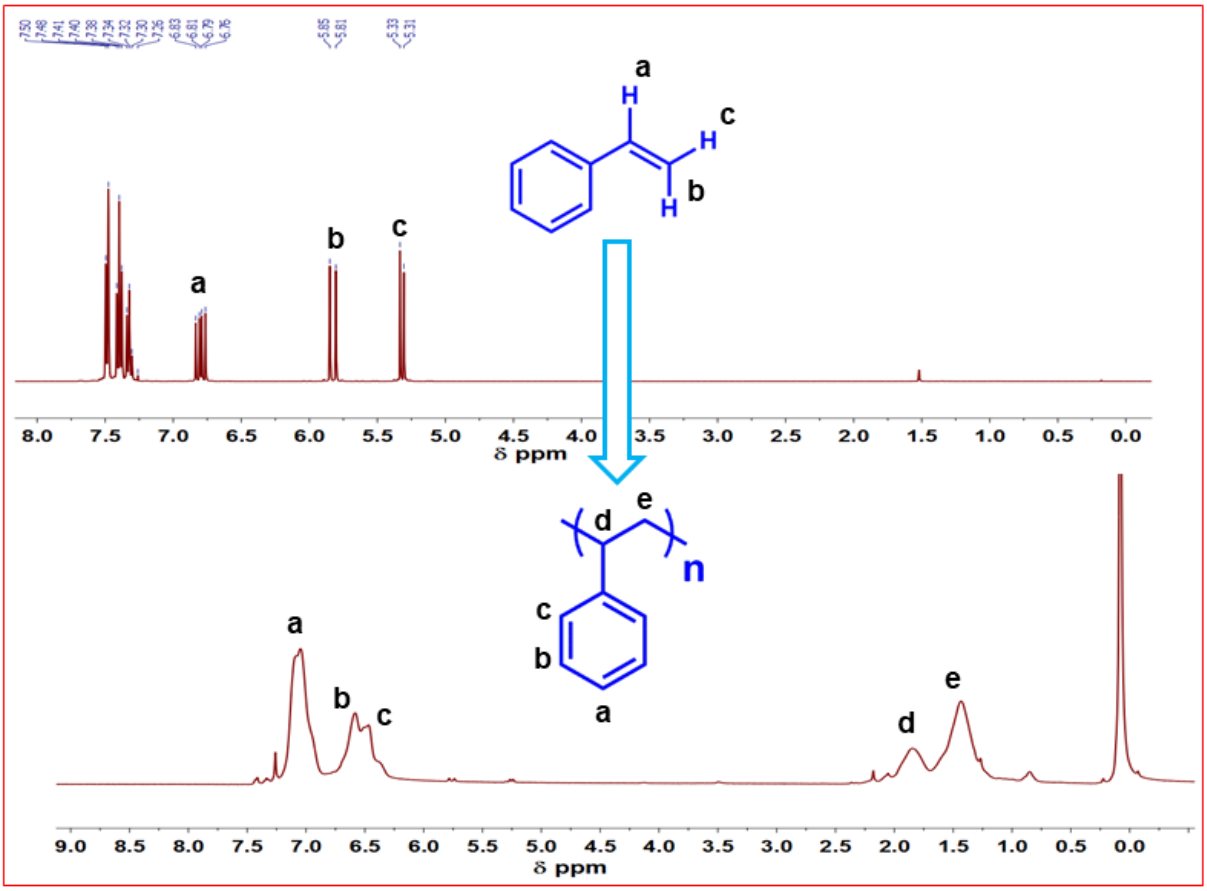
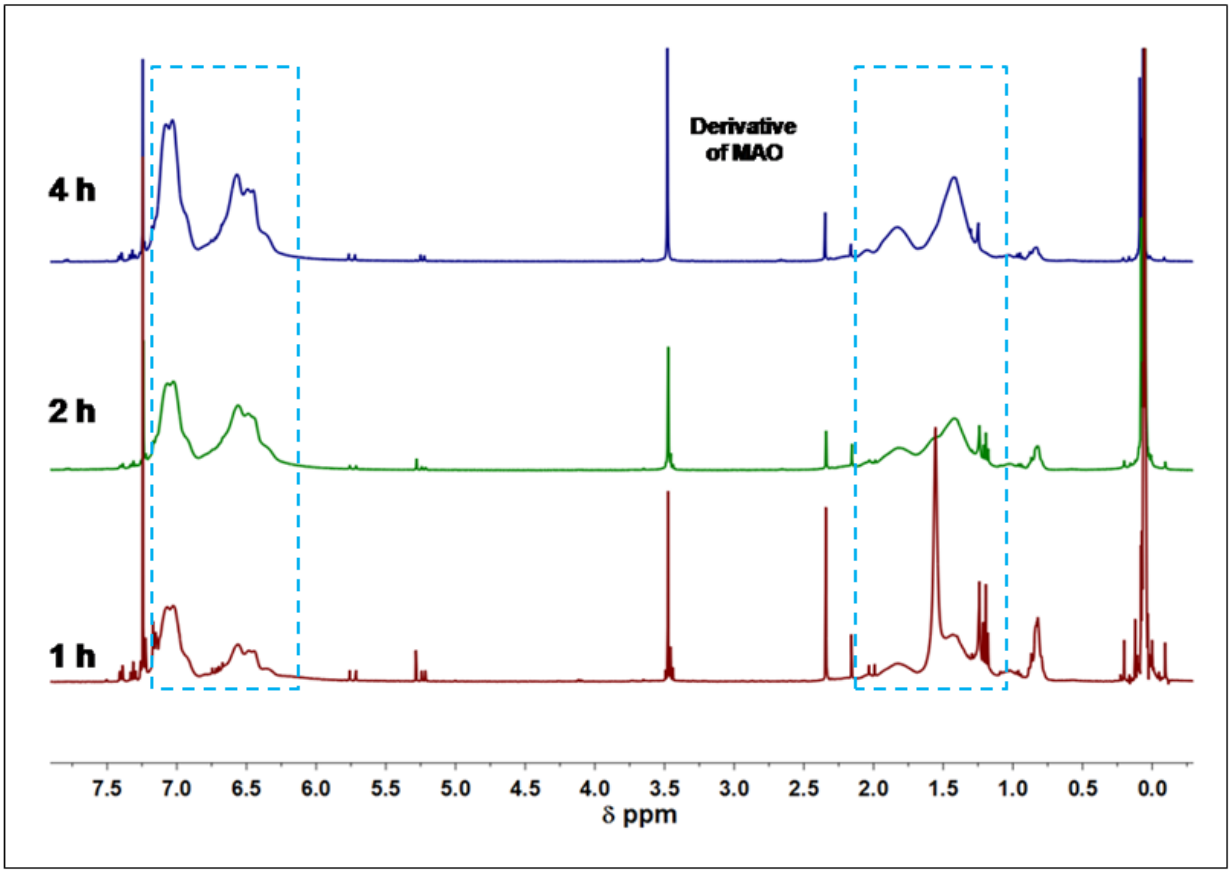
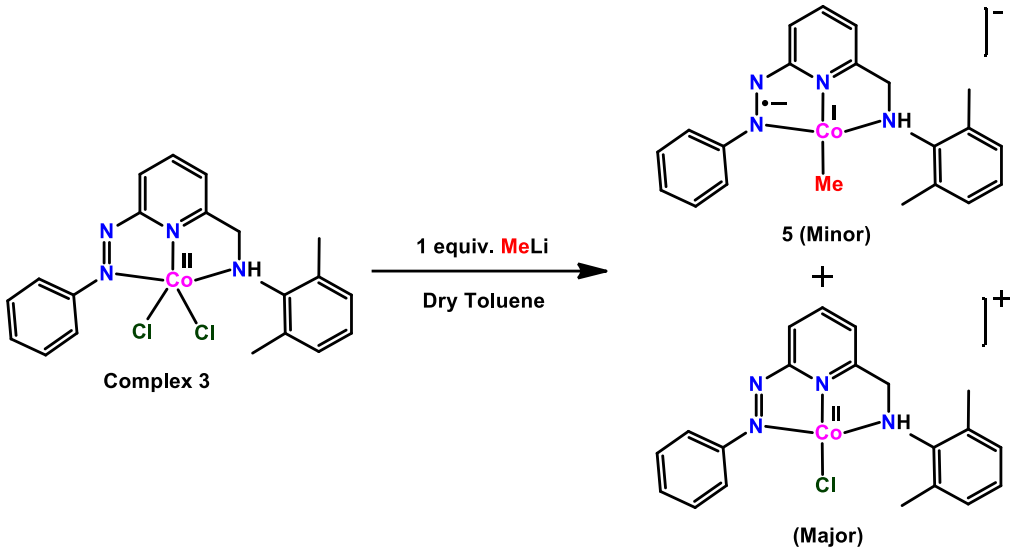


Figure S18. ^{1}H NMR kinetics experiment of polymerisation reaction



Scheme S2.



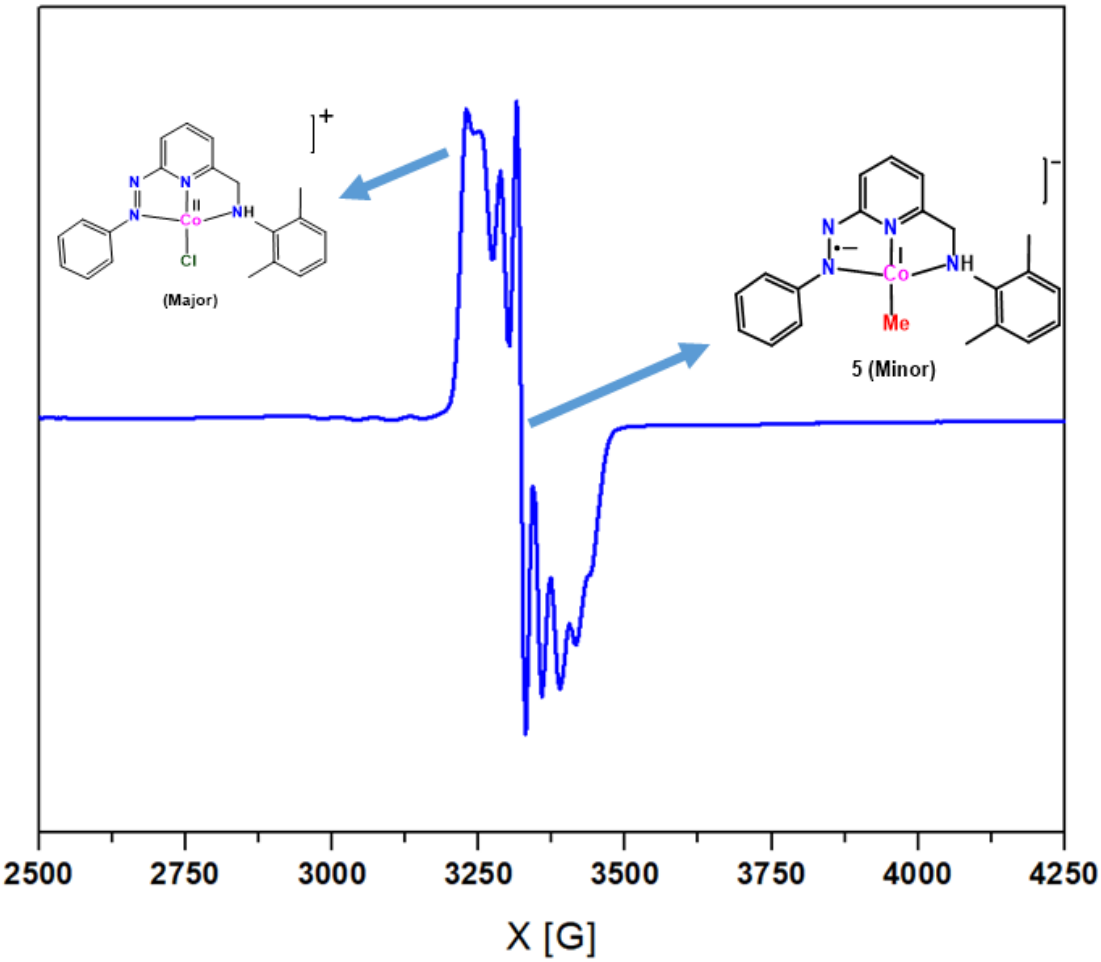
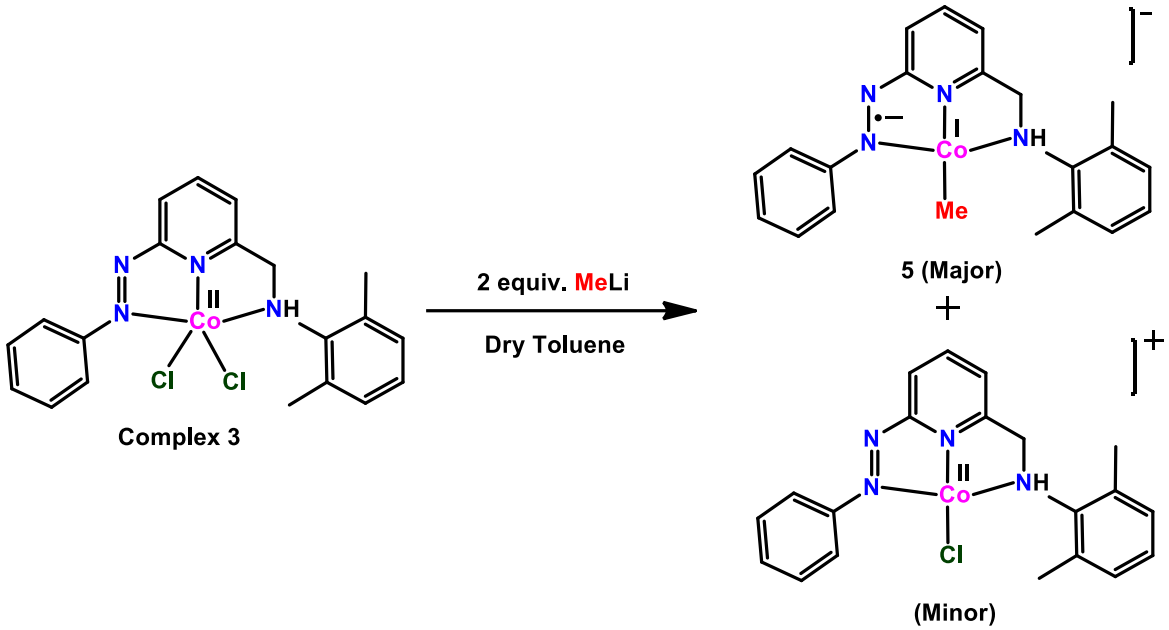


Figure S19. EPR spectrum of the Complex **3** upon treatment with 1 equiv. of MeLi.

Scheme S3.



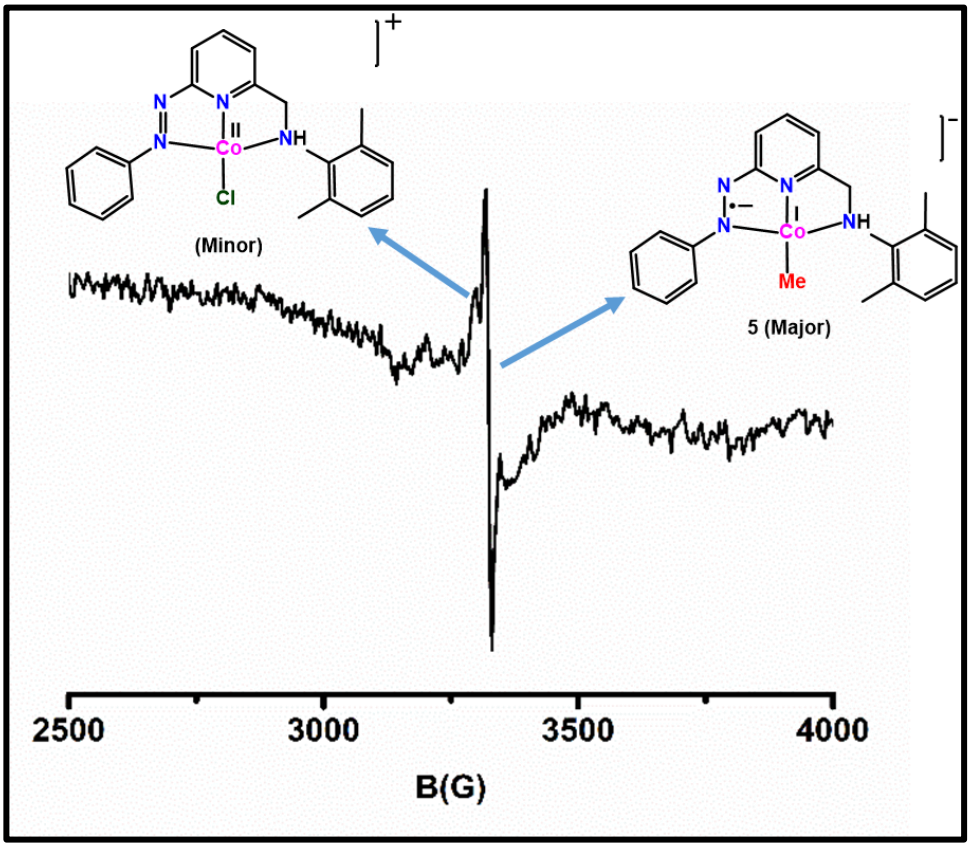
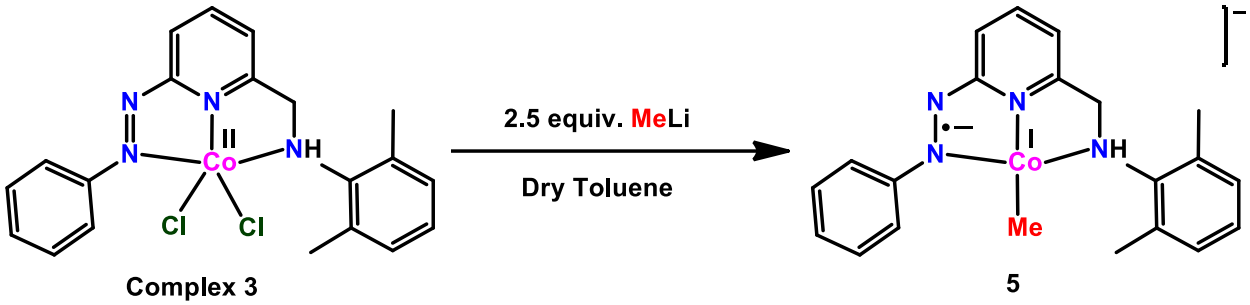


Figure S20. EPR spectrum of the Complex **3** upon treatment with 2 equiv. of MeLi.

Scheme S4.



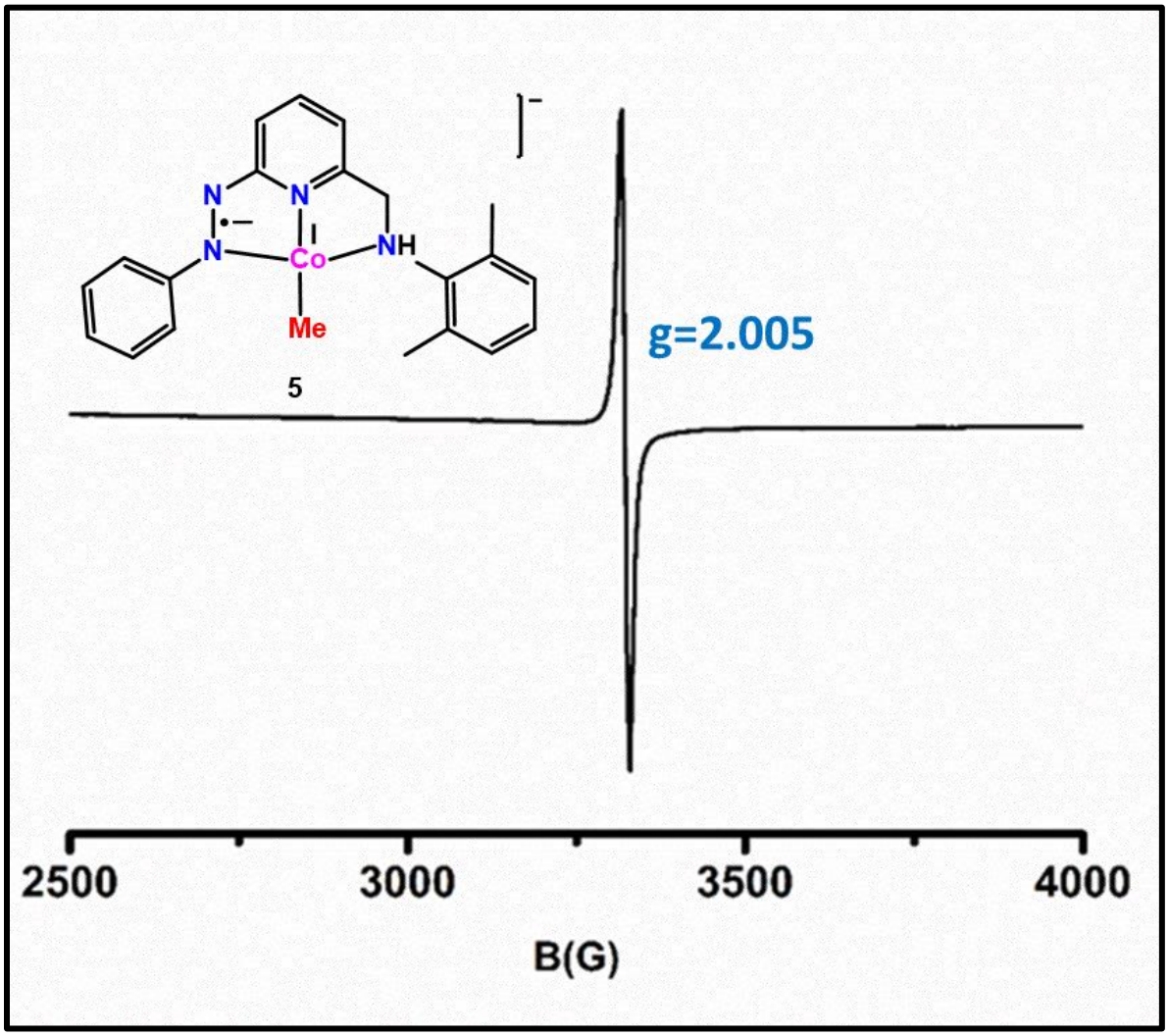
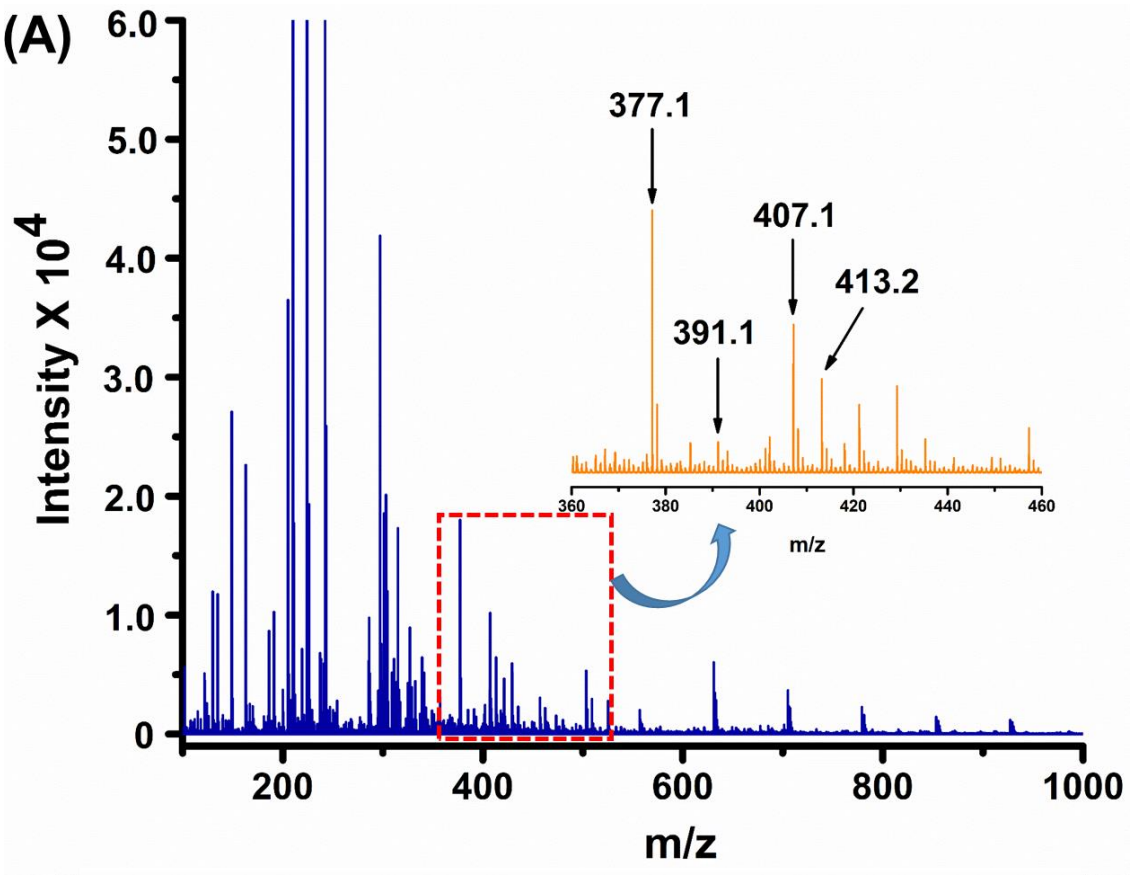
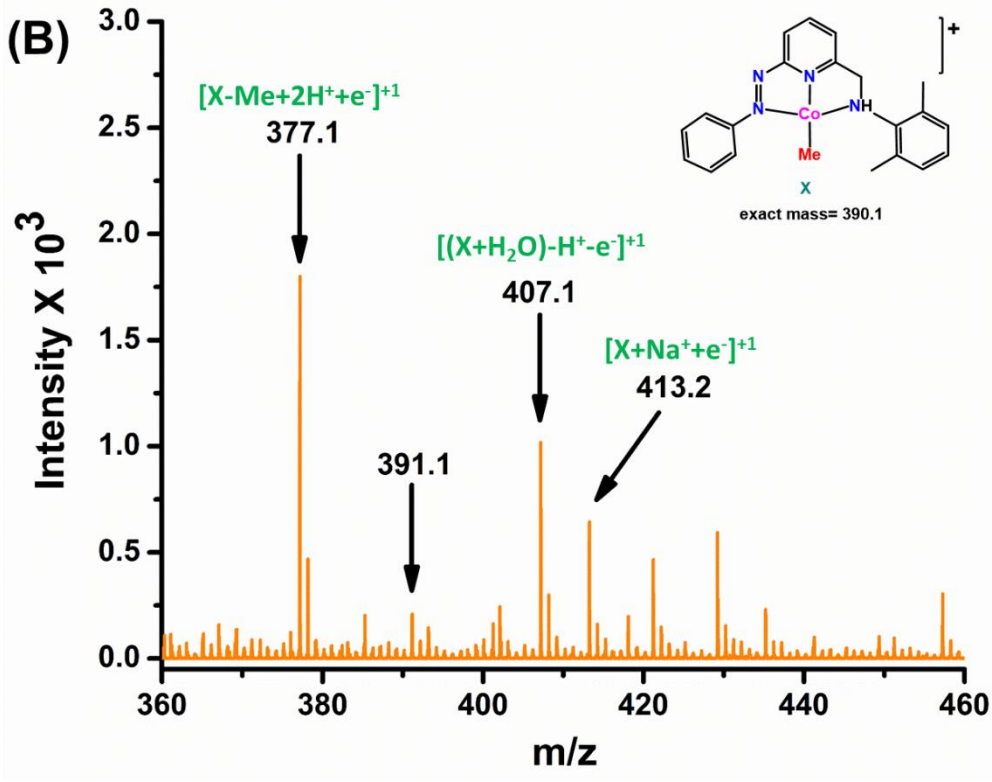


Figure S21. EPR spectrum of the Complex **3** upon treatment with 2.5 equiv. of MeLi.


(A)
Intensity X 10^4
6.0
5.0
4.0
3.0
2.0
1.0
0
200
400
600
800
1000
m/z
377.1
407.1
413.2
391.1
360
380
400
420
440
460
m/z


(B)
Intensity X 10^3
3.0
2.5
2.0
1.5
1.0
0.5
0.0
360
380
400
420
440
460
m/z
[X-Me+2H+ +e-]+1
377.1
[(X+H2O)-H+ -e-]+1
407.1
[X+Na+ +e-]+1
413.2
391.1
N
N
N
Co
NH
Me
+
X
exact mass= 390.1

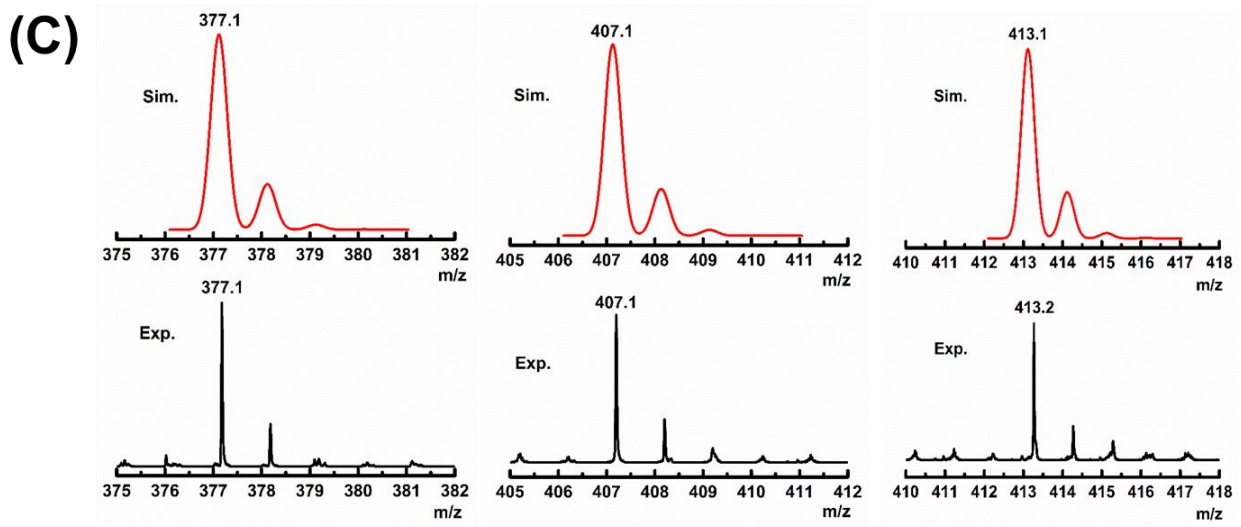


Figure S22. (A): Full range mass spectrum of the mixture of complex **3** and MMAO-12 (1000 equiv.) in acetonitrile solution. (Zoomed picture shown in the inset), (B): Zoomed spectrum highlighting the molecular ion peak with probable composition, (C): Experimental and simulated spectrum of the corresponding peaks.

Scheme S5. Plausible Mechanism

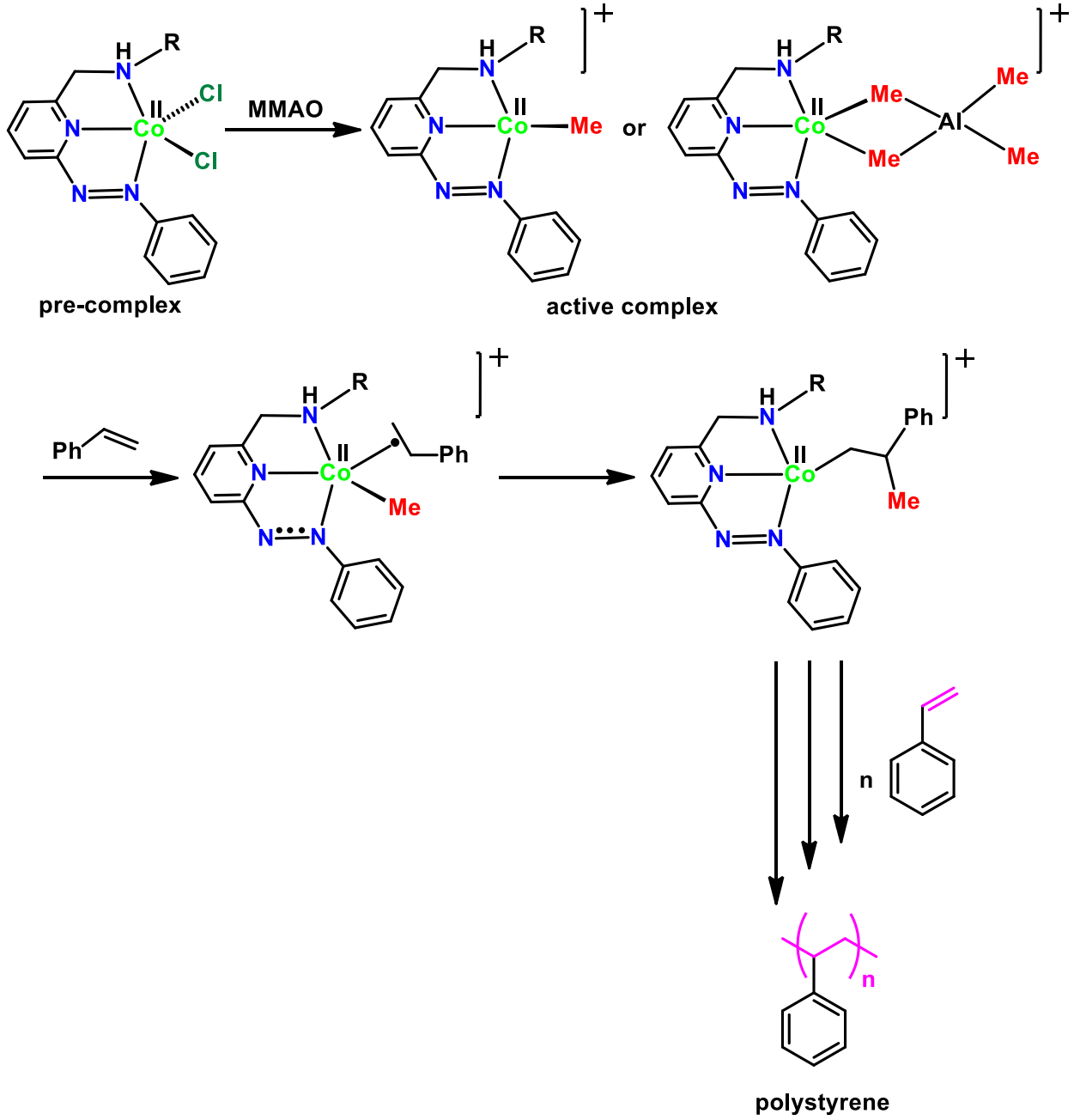
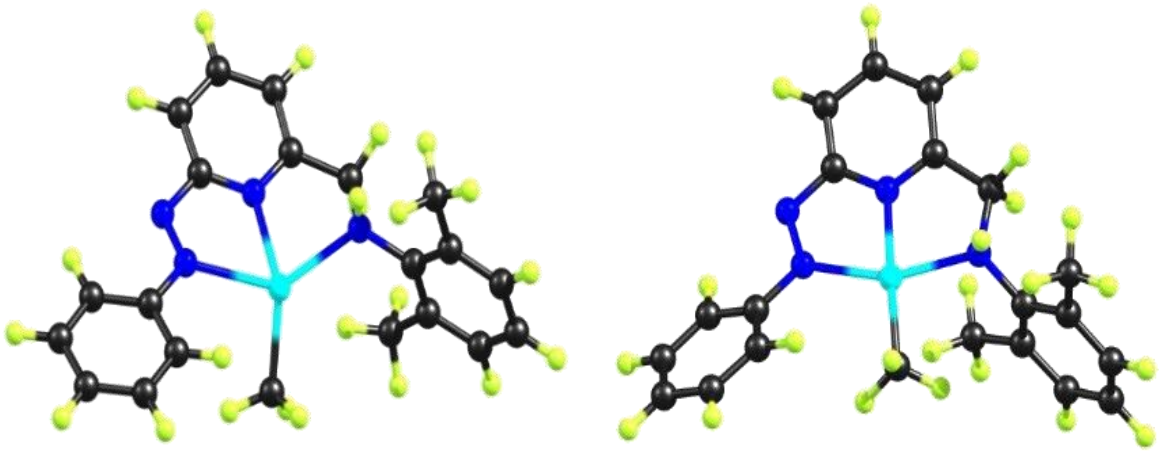


Figure S23. Optimized Structure of the cationic monomethylated intermediate, **[3.Me]**$^{+}$



[3.Me]$^{+}$ **(quartet)** **[3.Me]**$^{+}$ **(doublet)**

Table S3. Energy Comparison between doublet and quartet state of the cationic monomethylated intermediate, **[3.Me]**$^{+}$

Structure	**Quartet state**	**Doublet state**	Doublet-Quartet Gap (^{2}**6**–^{4}**6**) in kcal/mol
[3.Me]$^{+}$	-1177.893475 a.u.	-1177.891113 a.u.	1.482

We have undertaken benchmarking calculations to ascertain the energetic difference between the two lowest possible electronic configuration for the intermediate, **[3.Me]**$^{+}$ i.e. cationic Co(II)-alkyl complex. At b3lyp/6-311+g*(C, H, N)/lanl2dz(Co)/cpcm (solvent=toluene) level of theory, **[3.Me]**$^{+}$ (doublet) structure is found to be ~1.5 kcal/mol uphill respectively as compared to **[3.Me]**$^{+}$ (quartet).

Figure S24. IR spectrum of the polystyrene obtained from the complex **1-4**

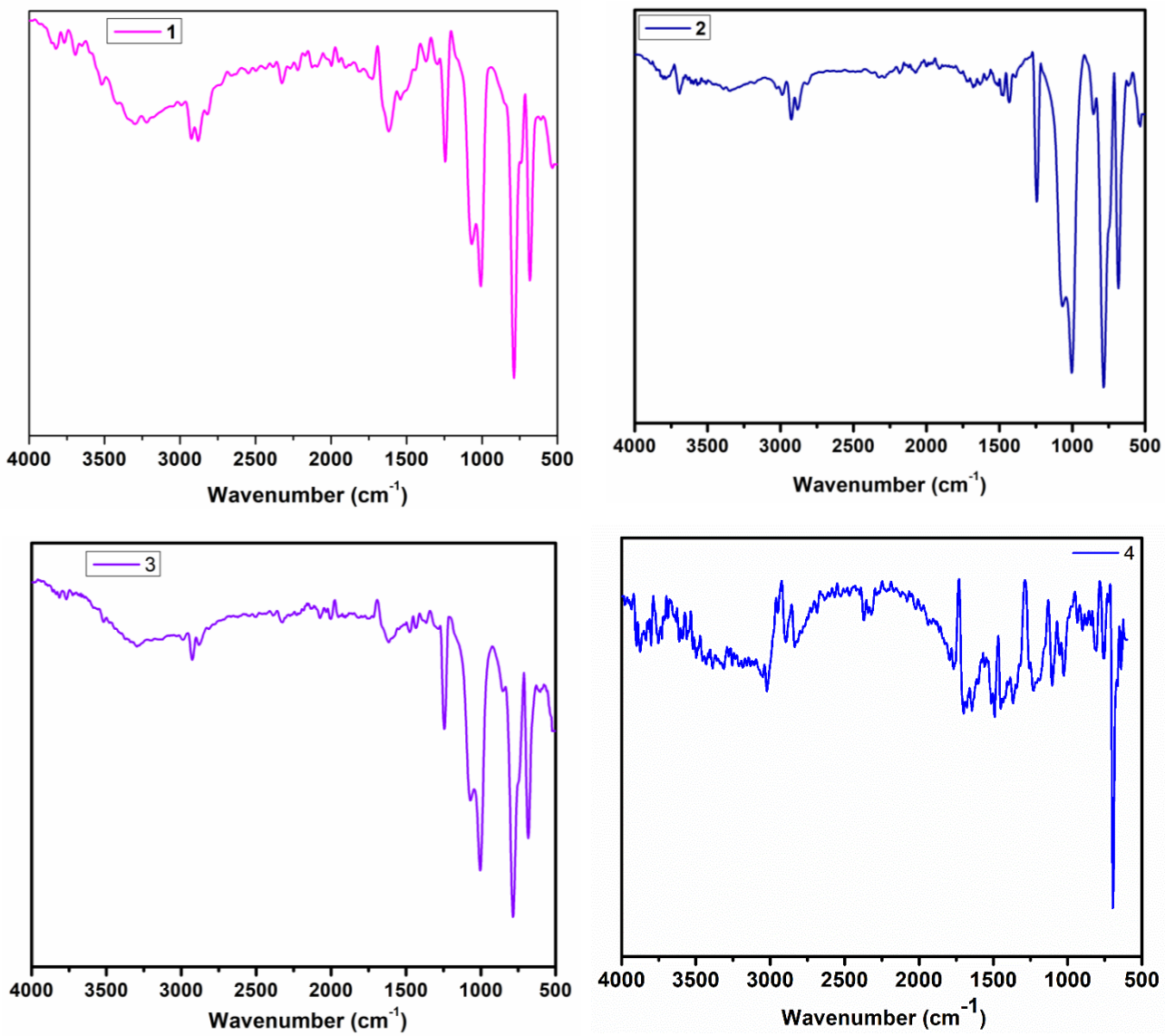


Figure S25. ^{13}C NMR spectrum of polystyrene obtained from the complex **2**

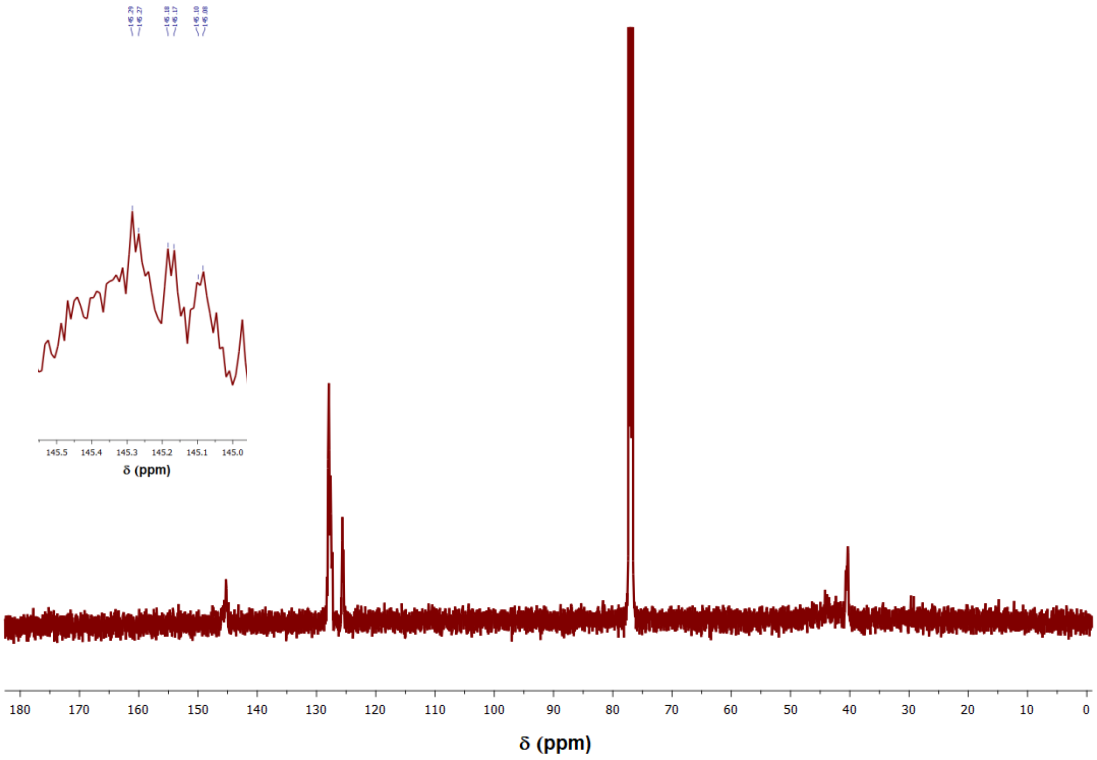


Figure S26. ^{13}C NMR spectrum of polystyrene obtained from the complex **3**

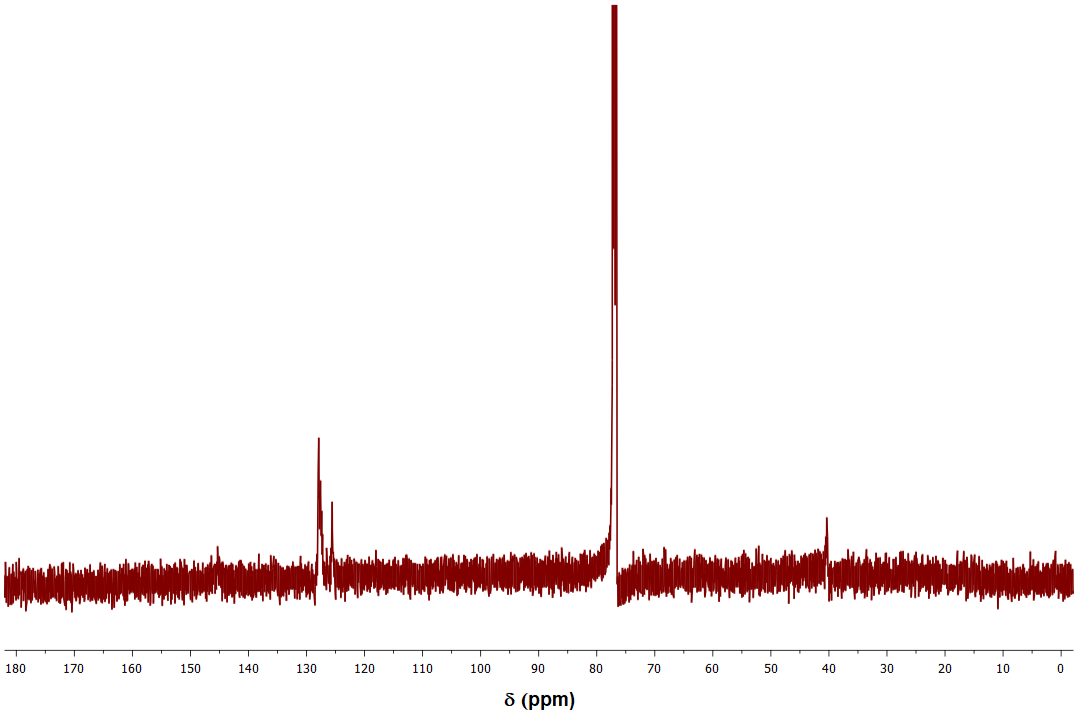


Figure S27. ^{13}C NMR spectrum of polystyrene obtained from the complex **4.**

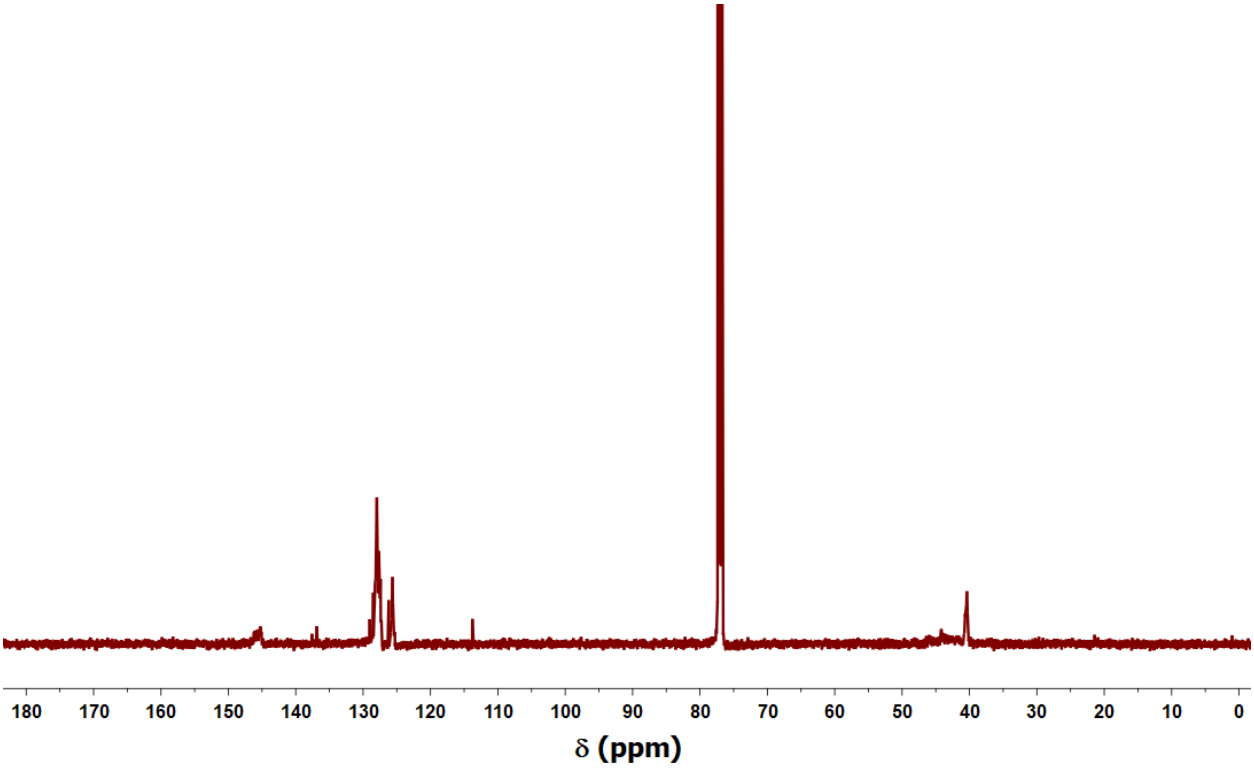


Figure S28. Powder XRD analysis of the polystyrene obtained from the complex **1-4**

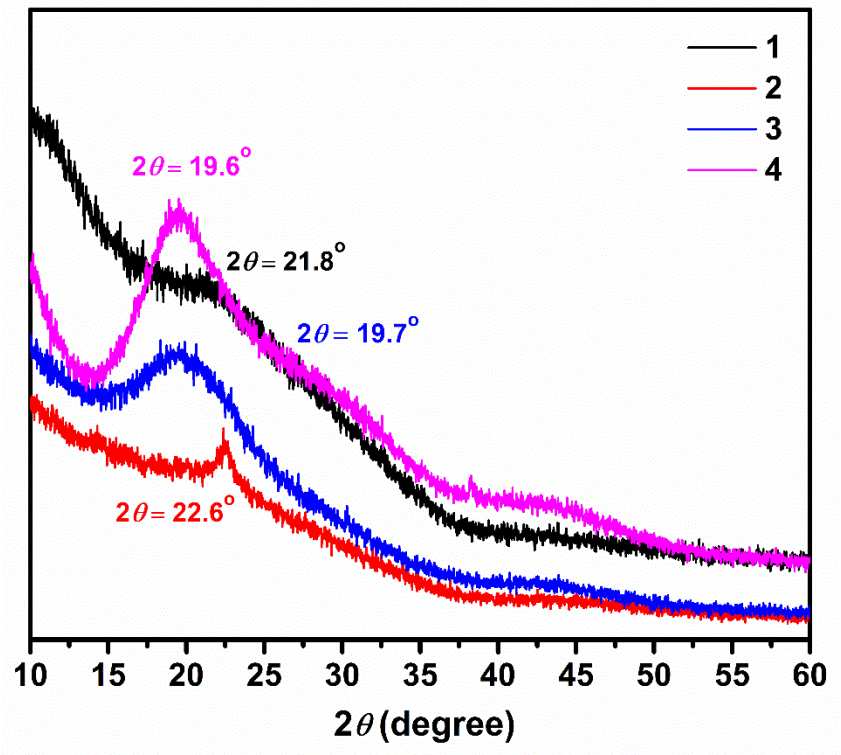


Figure S29. TGA analysis of the polystyrene obtained from the complex **3**

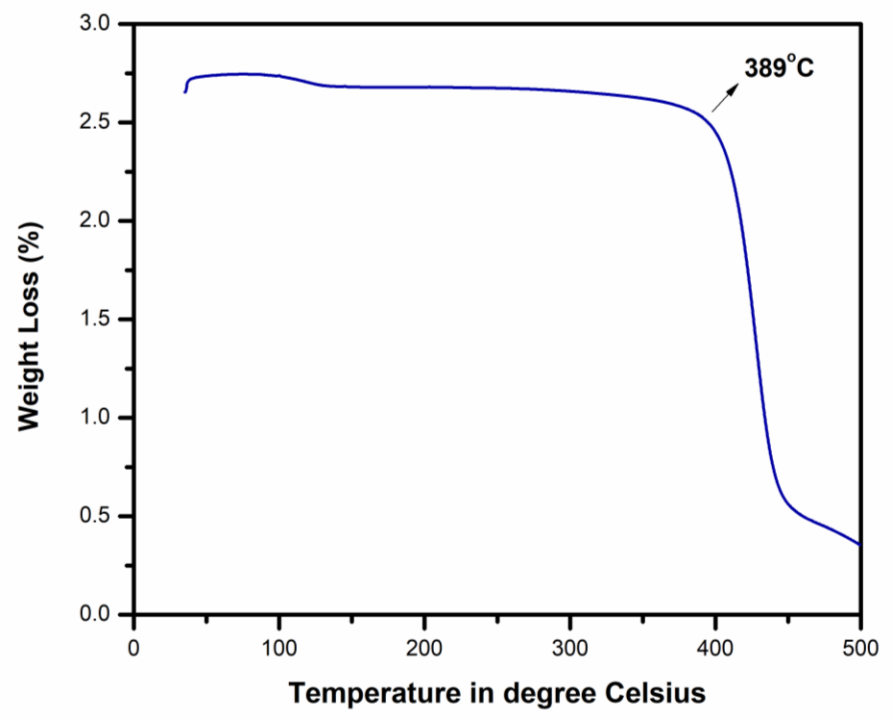


Figure S30. Load (*P*) – displacement (*h*) curves on film state of the polystyrene obtained from the complex **2**

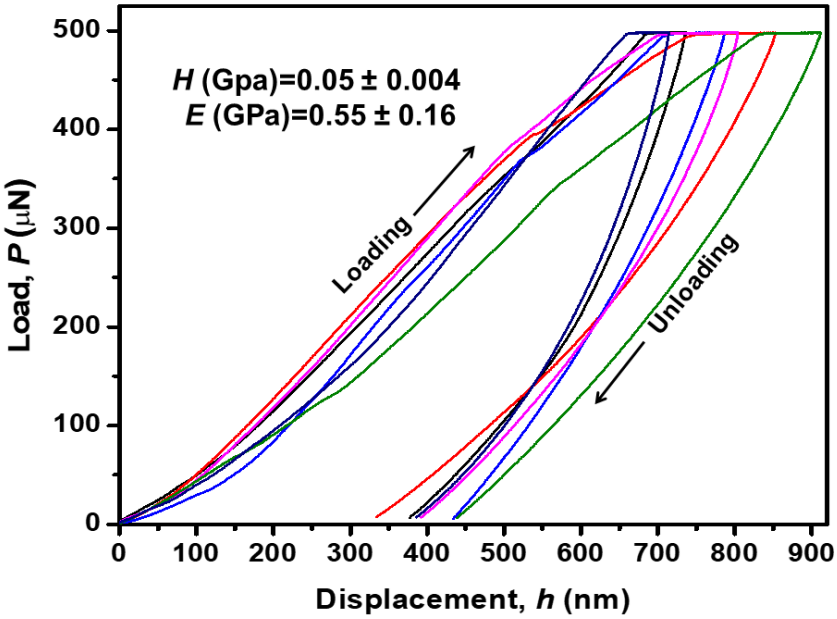


Figure S31. Load (*P*) – displacement (*h*) curves on film state of the polystyrene obtained from the complex **3**

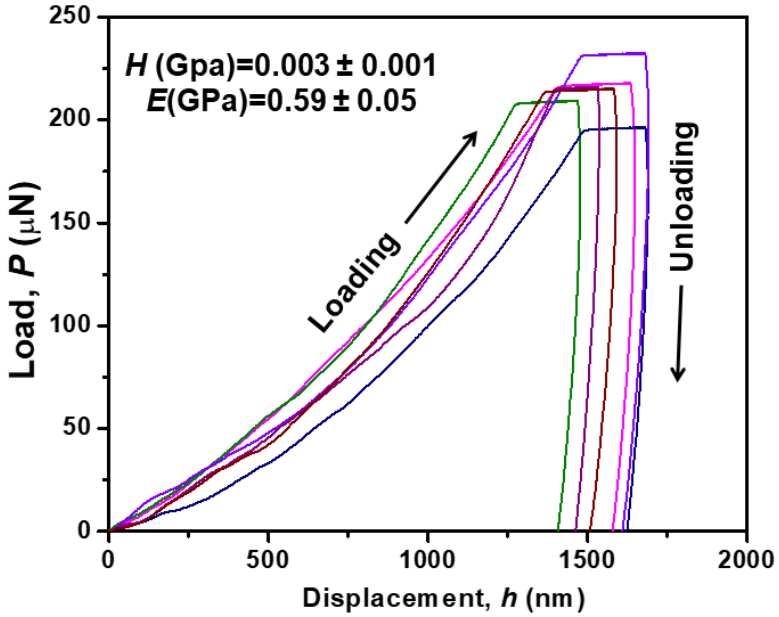


Figure S32. Comparison of LUMO energies between the azo-aromatic ligand, **HL^2** and imine based ligand, **HL^4**.

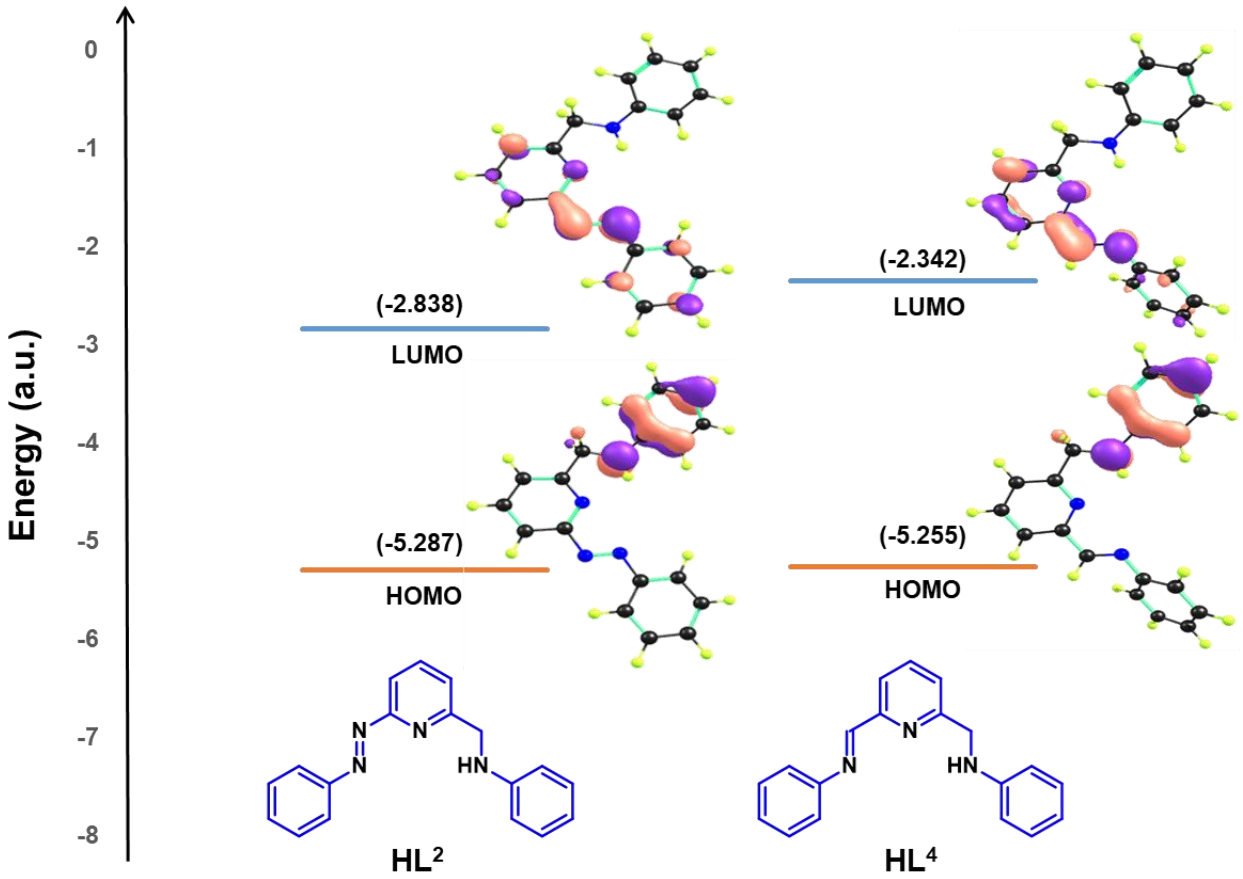


Table S4. Optimized Cartesian coordinates (Å) of the complexes **1-4**, and **[3.Me]**$^{+}$

****

Complex **1**

****

Co	3.271654000	9.003907000	9.468077000
Cl	3.428568000	10.910284000	8.141052000
Cl	1.486900000	7.683152000	10.048402000
N	4.992087000	8.872673000	10.592392000
N	4.628156000	7.832144000	8.089056000
H	4.913510000	8.687088000	7.609399000
C	1.816236000	11.771955000	13.002453000
H	2.642164000	11.715454000	13.699561000
C	7.366344000	8.877338000	11.981523000
H	8.305537000	8.878099000	12.524072000
N	3.023119000	10.339840000	11.381708000
C	7.239011000	8.141611000	10.806604000
H	8.070805000	7.564817000	10.418036000
N	4.014322000	10.368707000	12.157650000
C	0.840080000	11.150560000	10.858536000
H	0.923250000	10.622796000	9.918483000
C	-0.298691000	11.884813000	11.170345000
H	-1.118491000	11.929991000	10.462140000
C	1.901165000	11.095210000	11.771923000
C	5.106855000	9.598138000	11.714329000
C	6.016522000	8.155303000	10.129163000
C	5.771147000	7.334009000	8.877239000
H	6.698157000	7.285645000	8.294305000
H	5.547652000	6.312559000	9.195045000
C	6.287035000	9.620010000	12.452577000
H	6.340953000	10.214974000	13.355398000
C	-0.384308000	12.555454000	12.388174000
H	-1.275347000	13.125157000	12.631874000
C	0.674293000	12.495277000	13.303450000
H	0.599939000	13.016101000	14.252351000
C	4.100070000	6.892915000	7.028493000
C	2.941501000	7.628286000	6.340955000
H	2.121764000	7.807851000	7.038711000
H	2.556789000	7.025994000	5.513941000
H	3.257730000	8.594240000	5.939159000
C	5.195909000	6.571731000	5.995793000
H	5.587000000	7.483757000	5.533081000
H	4.789798000	5.947460000	5.195857000
H	6.034453000	6.023815000	6.435041000
C	3.576156000	5.603861000	7.674744000
H	4.376470000	4.975260000	8.076354000
H	3.060903000	5.006257000	6.918568000
H	2.864832000	5.824504000	8.471988000

****

Complex **2**

****

Co	2.790503000	10.581893000	8.196284000
Cl	1.183071000	11.286329000	6.682650000
Cl	3.197061000	10.800968000	10.439301000
N	1.761164000	8.529444000	8.406469000
N	4.010321000	9.164872000	7.330292000
N	2.358124000	7.553508000	7.878915000
C	0.516543000	8.257163000	9.004154000
C	3.592493000	7.892543000	7.291491000
C	5.168386000	9.528841000	6.777586000
C	-0.118914000	9.334407000	9.636137000
H	0.360220000	10.304293000	9.641036000
C	-0.084323000	6.985136000	8.990614000
H	0.417708000	6.163986000	8.495755000

C	-1.348729000	9.141203000	10.254956000
H	-1.839244000	9.974351000	10.745657000
C	4.348606000	6.895551000	6.679537000
H	3.980915000	5.877388000	6.666767000
N	4.373093000	11.849373000	7.133952000
H	3.828433000	11.898332000	6.274198000
C	-1.945468000	7.882591000	10.241588000
H	-2.906696000	7.733457000	10.722821000
C	5.976585000	8.588010000	6.135627000
H	6.911434000	8.891921000	5.678485000
C	5.556569000	10.986438000	6.929158000
H	6.196078000	11.083710000	7.810072000
H	6.152907000	11.311967000	6.068048000
C	-1.311116000	6.806638000	9.607554000
H	-1.782270000	5.829385000	9.598705000
C	5.558135000	7.259719000	6.094563000
H	6.170815000	6.512146000	5.602558000
C	4.671522000	13.191976000	7.569076000
C	4.372728000	14.274180000	6.739835000
H	3.918725000	14.102847000	5.767994000
C	4.637717000	15.574479000	7.165711000
H	4.392675000	16.409616000	6.517729000
C	5.213072000	15.799044000	8.413923000
H	5.421142000	16.810843000	8.745544000
C	5.505448000	14.714979000	9.241649000
H	5.928736000	14.881324000	10.226760000
C	5.229992000	13.414264000	8.829826000
H	5.395844000	12.581886000	9.504019000

****

Complex **3**

****

Co	-0.238155000	-0.263491000	-0.078746000
Cl	-0.376814000	-1.232649000	2.034114000
Cl	-0.492597000	-1.204131000	-2.139352000
N	-2.667796000	1.607446000	0.065242000
N	-0.298802000	1.789169000	0.186525000
N	-2.449982000	0.371151000	-0.034209000
N	1.988427000	0.296053000	0.343303000
H	1.785455000	0.023670000	1.303100000
C	0.814408000	2.495691000	0.392456000
C	-1.504312000	2.380755000	0.236815000
C	-3.579615000	-0.451333000	-0.205760000
C	0.751881000	3.868380000	0.652512000
H	1.663397000	4.429518000	0.825676000
C	4.975126000	-1.942488000	0.413742000
H	5.527213000	-2.535617000	1.136349000
C	-3.368259000	-1.833222000	-0.108904000
H	-2.372031000	-2.205029000	0.087748000
C	-4.866699000	0.056245000	-0.459058000
H	-5.010881000	1.125655000	-0.542365000
C	3.870355000	-1.206404000	0.845602000
C	-0.489455000	4.494797000	0.682477000
H	-0.558654000	5.559421000	0.877664000
C	-5.926991000	-0.822147000	-0.607838000
H	-6.921084000	-0.438425000	-0.811858000
C	-5.718425000	-2.202992000	-0.501587000
H	-6.554521000	-2.884689000	-0.620244000
C	3.470541000	-1.249203000	2.303424000
H	4.174258000	-1.859003000	2.872024000
H	3.469703000	-0.253943000	2.763815000
H	2.473886000	-1.675244000	2.452424000
C	-4.442945000	-2.703708000	-0.250402000
H	-4.281101000	-3.772784000	-0.169970000
C	5.374573000	-1.924849000	-0.917711000
H	6.234231000	-2.504102000	-1.238747000

C	2.139507000	1.764928000	0.301043000
H	2.807526000	2.121972000	1.095264000
H	2.615106000	2.038410000	-0.641171000
C	2.794672000	0.356823000	-2.514833000
H	3.172325000	1.382901000	-2.609326000
H	2.927068000	-0.114480000	-3.490310000
H	1.722099000	0.397010000	-2.330251000
C	4.657251000	-1.169424000	-1.835626000
H	4.954134000	-1.166321000	-2.880166000
C	3.536706000	-0.423411000	-1.455632000
C	3.153655000	-0.445850000	-0.101621000
C	-1.643690000	3.745123000	0.472413000
H	-2.633749000	4.182045000	0.499429000

****

Complex **4**

****

Co	2.636257000	6.809699000	5.662399000
Cl	2.829653000	7.721586000	3.554521000
Cl	3.845462000	6.178833000	7.542699000
N	0.658219000	6.213958000	5.913371000
N	2.583754000	4.639861000	4.952076000
N	1.705381000	8.524249000	6.885907000
H	1.931715000	8.068320000	7.768582000
C	-0.240547000	7.072532000	6.389873000
C	0.323208000	4.949859000	5.599782000
C	2.285472000	9.843474000	6.883639000
C	3.680205000	3.864386000	4.516522000
C	1.421826000	4.122212000	5.088670000
H	1.205297000	3.084517000	4.825943000
C	-0.982519000	4.492470000	5.760938000
H	-1.243707000	3.472153000	5.503961000
C	-1.567477000	6.677949000	6.588568000
H	-2.291789000	7.378484000	6.988827000
C	2.897122000	10.333683000	8.038974000
H	2.930778000	9.720768000	8.935030000
C	-1.935728000	5.376249000	6.264999000
H	-2.959745000	5.048778000	6.408577000
C	0.247083000	8.483001000	6.655401000
H	0.029527000	9.092241000	5.774579000
H	-0.310082000	8.924504000	7.491191000
C	4.626704000	4.477154000	3.686178000
H	4.484142000	5.513040000	3.401600000
C	2.270112000	10.619797000	5.722308000
H	1.862063000	10.213881000	4.803978000
C	3.483616000	11.597787000	8.036585000
H	3.965020000	11.964977000	8.937091000
C	5.707301000	3.740244000	3.214314000
H	6.428976000	4.213735000	2.557125000
C	3.856921000	2.531654000	4.915136000
H	3.169681000	2.080206000	5.622777000
C	3.451842000	12.383227000	6.886901000
H	3.906601000	13.368235000	6.884991000
C	5.875935000	2.409084000	3.595821000
H	6.731847000	1.844686000	3.240567000
C	4.953731000	1.811083000	4.454973000
H	5.098665000	0.786810000	4.782639000
C	2.845012000	11.887446000	5.732954000
H	2.838771000	12.480292000	4.824135000

Complex [**3.Me**]$^{+}$ (quartet state)

Co	7.509246000	6.046605000	3.334491000
N	6.149129000	3.686130000	4.853982000
N	7.793154000	4.000964000	3.171472000
N	5.898599000	4.908881000	4.682737000
N	8.491587000	5.803273000	1.328788000

H	7.645947000	5.561581000	0.818310000
C	8.654226000	3.527926000	2.266077000
C	7.128946000	3.165164000	3.987153000
C	4.893030000	5.466018000	5.498074000
C	8.917210000	2.158634000	2.174085000
H	9.611548000	1.785295000	1.430788000
C	9.011904000	8.489904000	-1.210978000
H	8.533402000	8.851687000	-2.115244000
C	4.496328000	6.776289000	5.193618000
H	4.988184000	7.307593000	4.387883000
C	4.278933000	4.766861000	6.553516000
H	4.595858000	3.758414000	6.785030000
C	8.467118000	7.388607000	-0.548281000
C	8.272551000	1.291181000	3.050672000
H	8.468332000	0.226195000	3.004381000
C	3.275755000	5.383557000	7.283549000
H	2.801301000	4.852314000	8.101065000
C	2.872006000	6.687829000	6.970942000
H	2.084950000	7.161101000	7.547773000
C	7.222259000	6.729712000	-1.101319000
H	6.922747000	7.206795000	-2.034585000
H	7.370717000	5.667447000	-1.325546000
H	6.365285000	6.809290000	-0.421920000
C	3.481256000	7.381170000	5.925734000
H	3.170599000	8.391759000	5.686561000
C	10.154789000	9.121042000	-0.731635000
H	10.568774000	9.974579000	-1.257344000
C	9.312299000	4.558622000	1.374921000
H	9.466127000	4.151603000	0.371055000
H	10.297679000	4.800439000	1.771556000
C	10.960450000	7.125326000	2.392985000
H	11.751435000	6.398473000	2.177506000
H	11.443844000	7.980631000	2.867992000
H	10.295142000	6.681462000	3.133583000
C	10.757477000	8.656188000	0.429828000
H	11.642513000	9.154272000	0.813053000
C	10.244683000	7.561704000	1.135708000
C	9.096378000	6.928622000	0.627220000
C	7.356084000	1.793543000	3.974312000
H	6.812764000	1.151358000	4.655436000
C	7.862251000	7.588079000	4.558768000
H	7.520155000	8.499066000	4.049364000
H	7.342928000	7.511102000	5.516334000
H	8.933973000	7.694988000	4.754084000

Complex [**3.Me**]$^{+}$ (doublet state)

Co	7.080525000	5.702294000	2.955490000
N	6.393400000	3.704158000	4.859687000
N	7.701828000	3.873943000	2.943755000
N	6.124854000	4.917310000	4.588428000
N	8.194953000	5.759143000	1.199970000
H	7.416712000	5.724090000	0.545481000
C	8.518870000	3.417292000	1.999542000
C	7.250637000	3.093855000	3.938188000
C	5.278482000	5.548156000	5.539673000
C	8.921071000	2.077623000	2.013154000
H	9.581478000	1.691995000	1.245650000
C	9.590627000	8.632424000	-0.752400000
H	9.448832000	9.111739000	-1.715475000
C	4.349825000	6.493653000	5.089370000
H	4.291945000	6.731807000	4.036889000
C	5.353312000	5.213911000	6.901183000
H	6.089252000	4.494334000	7.236786000
C	8.797354000	7.530830000	-0.417490000

C	8.460342000	1.251844000	3.037245000
H	8.762922000	0.211691000	3.066959000
C	4.500807000	5.834532000	7.803072000
H	4.569867000	5.595954000	8.858470000
C	3.559091000	6.765300000	7.354774000
H	2.892200000	7.243820000	8.063497000
C	7.750612000	7.034292000	-1.389580000
H	7.780147000	7.615975000	-2.311068000
H	7.898968000	5.987032000	-1.672989000
H	6.733936000	7.130738000	-0.991351000
C	3.480660000	7.085267000	5.999142000
H	2.744959000	7.800714000	5.649682000
C	10.555345000	9.114288000	0.125000000
H	11.166475000	9.966066000	-0.153068000
C	8.966068000	4.468958000	1.014279000
H	8.866197000	4.116834000	-0.015677000
H	10.025352000	4.680985000	1.163993000
C	10.105887000	6.829704000	3.130496000
H	10.355042000	5.765456000	3.131779000
H	10.896546000	7.344164000	3.677731000
H	9.183853000	6.954800000	3.711959000
C	10.727677000	8.507949000	1.364975000
H	11.467824000	8.896137000	2.057099000
C	9.949108000	7.412640000	1.748543000
C	8.998496000	6.928000000	0.835218000
C	7.612359000	1.755770000	4.027934000
H	7.241570000	1.139008000	4.836359000
C	6.482147000	7.574515000	2.907959000
H	5.525305000	7.648757000	2.372455000
H	6.340953000	7.994084000	3.908321000
H	7.207182000	8.195441000	2.372444000

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