Supporting Information

Versatility of the bis(iminopyrrolylmethyl)amine ligand: tautomerism, protonation, helical chirality, and secondary coordination sphere with halogen bonds in the formation of copper(II) and nickel(II) complexes

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[§]*These authors have equal contribution to this work.*

Contents

1. NMR and IR Spectra

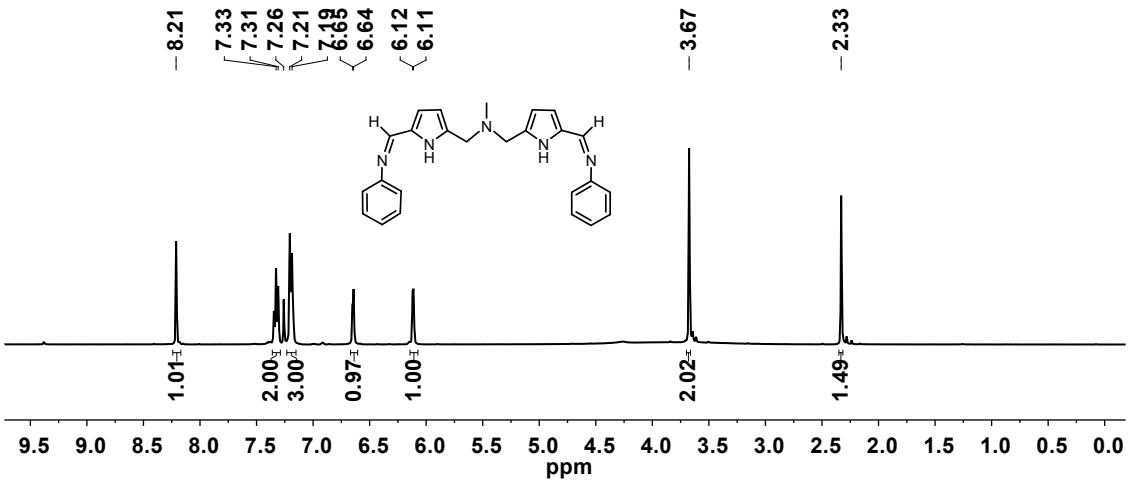

Figure S1: ^{1}H NMR spectrum of **H_2L2** in $CDCl_3$.

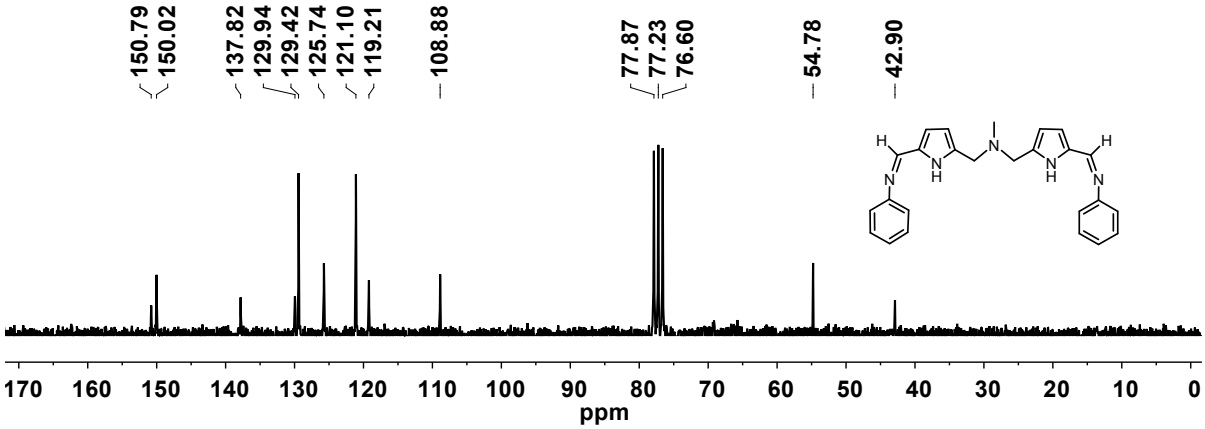

Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of **H_2L2** in $CDCl_3$.

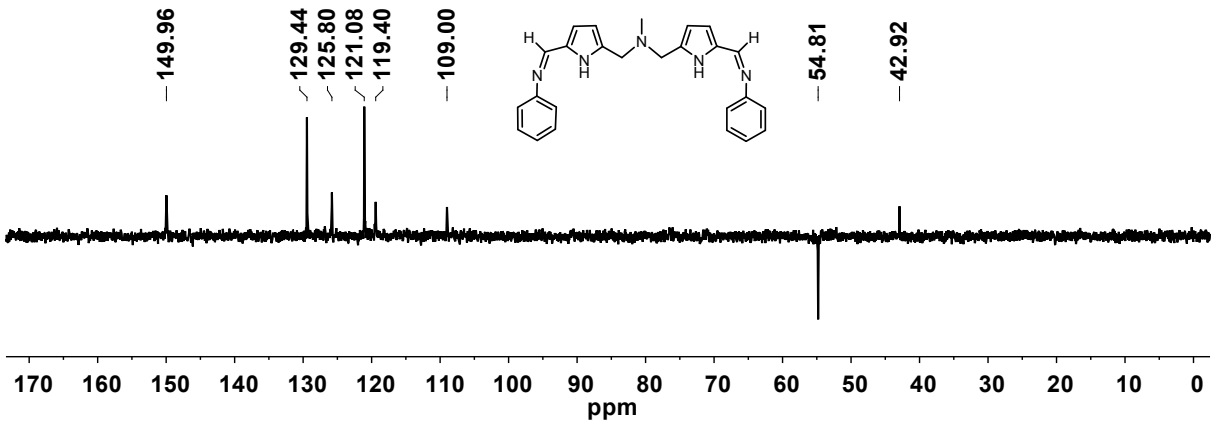

Figure S3: DEPT–135{^{1}H} NMR spectrum of **H_2L2** in $CDCl_3$.

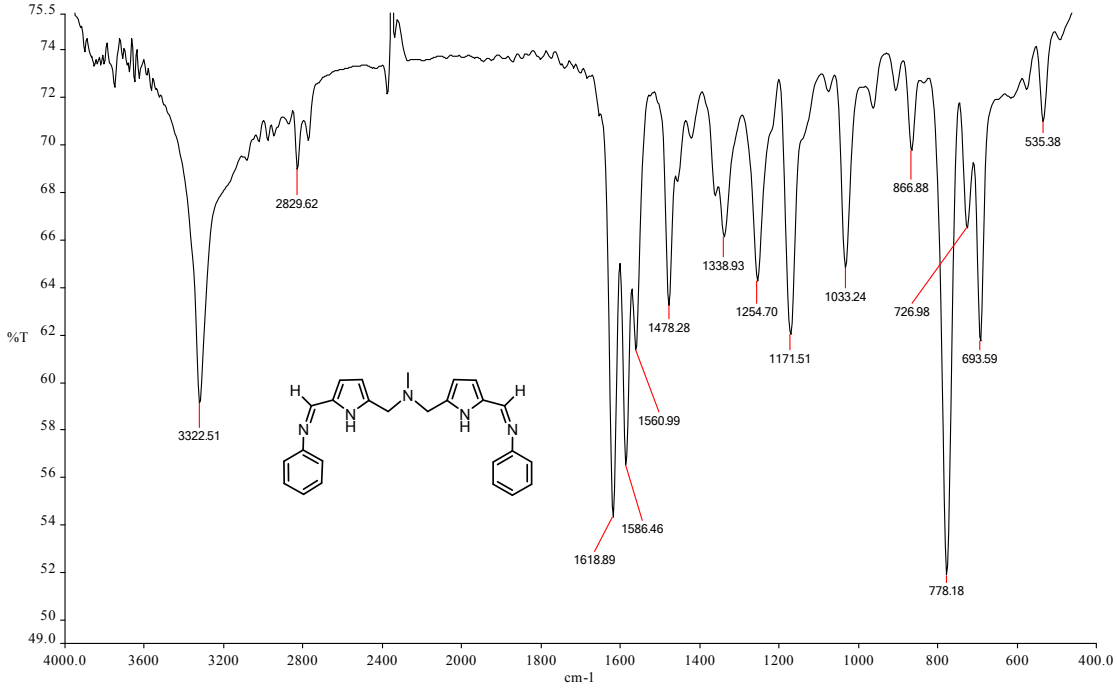

Figure S4: FTIR spectrum of **H_2L2** recorded as a KBr disc.

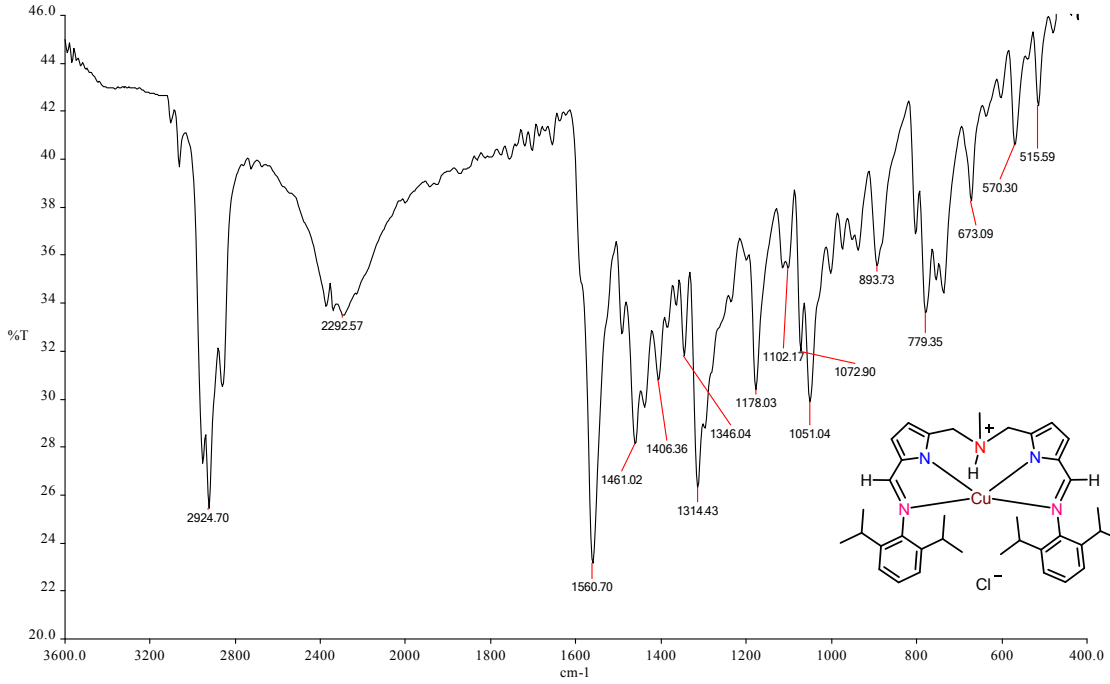

Figure S5: FTIR spectrum of the complex **1** recorded as a KBr disc.

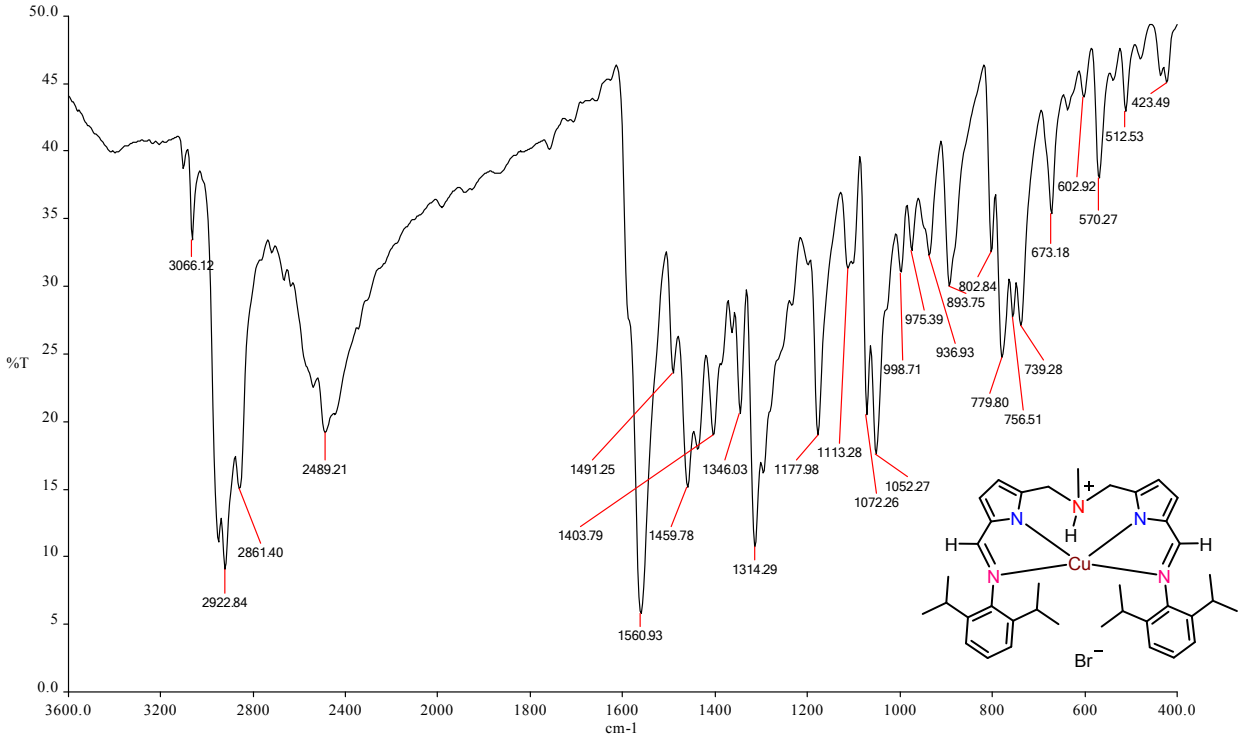

Figure S6: FTIR spectrum of complex **2** recorded as a KBr disc.

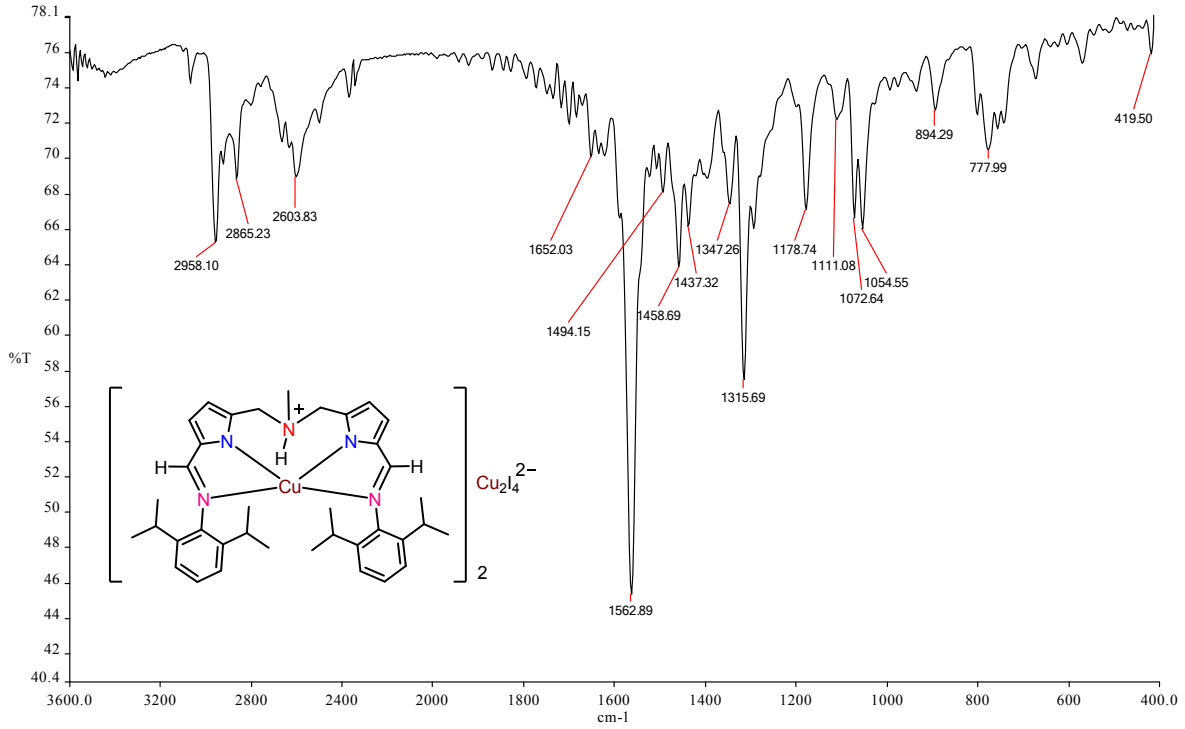

Figure S7: FTIR spectrum of the cationic complex **3** recorded as a KBr disc.

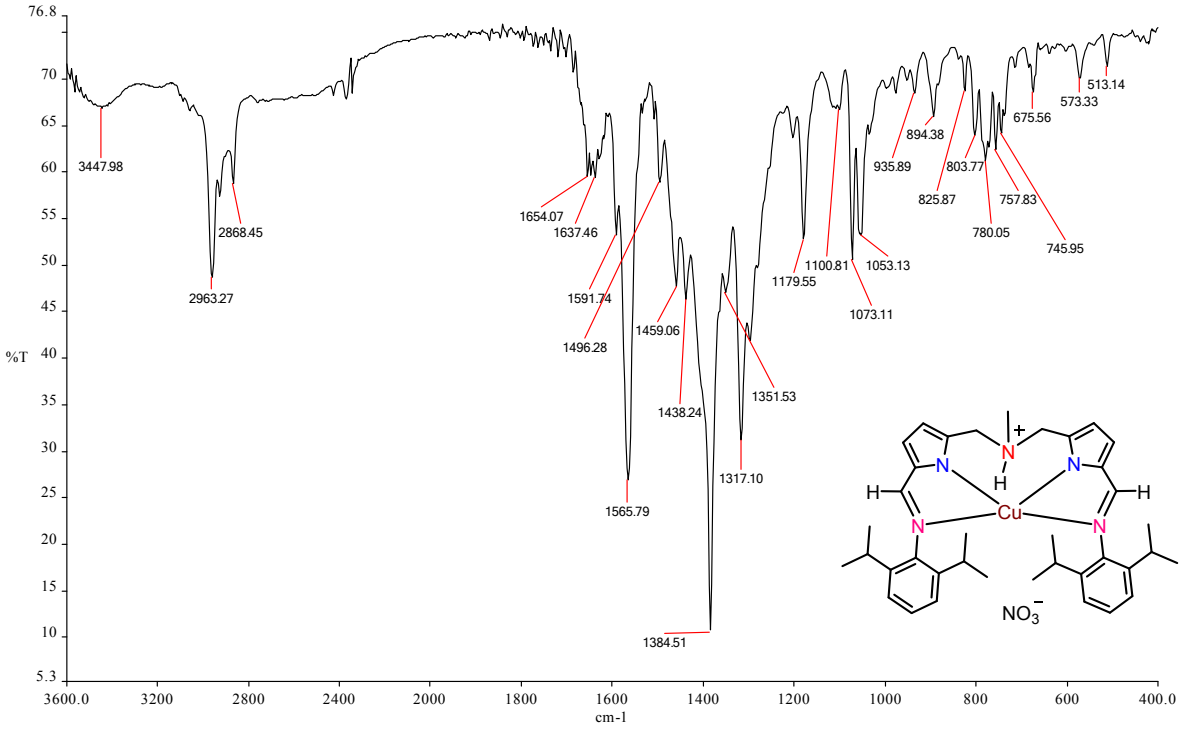

Figure S8: FTIR spectrum of the complex **4** recorded as a KBr disc.

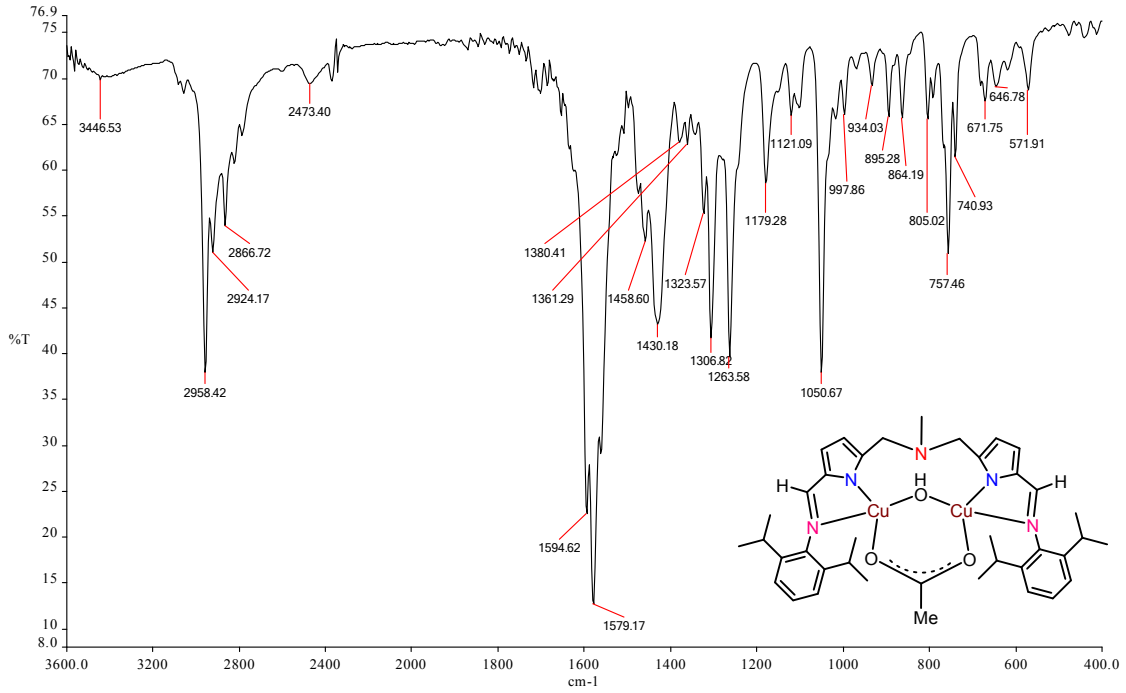

Figure S9: FTIR spectrum of the complex **5** recorded as a KBr disc.

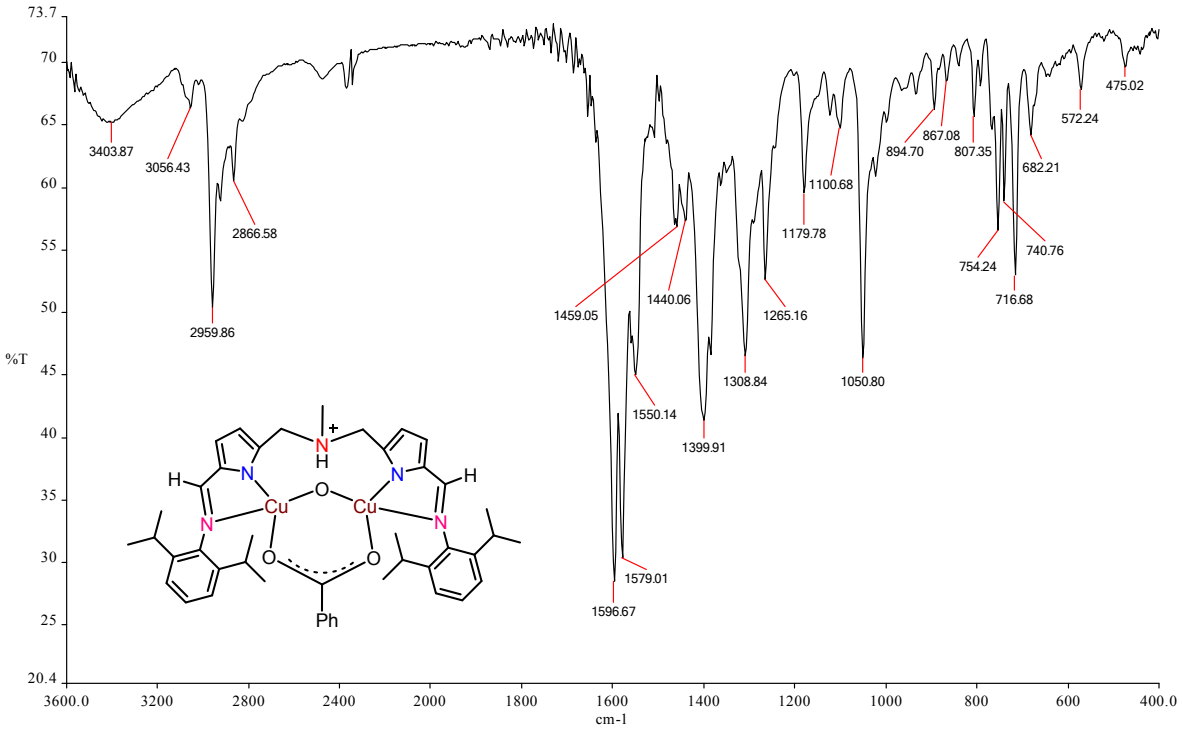

Figure S10: FTIR spectrum of the complex **6** recorded as a KBr disc.

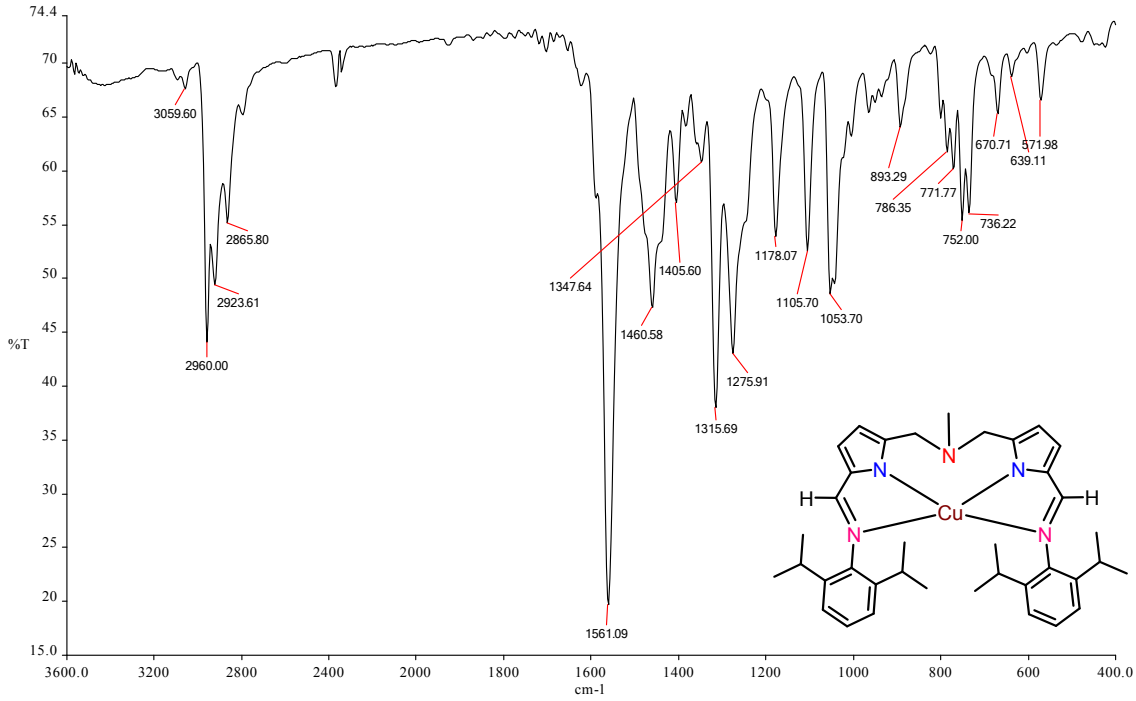

Figure S11: FTIR spectrum of the complex **7** recorded as a KBr disc.

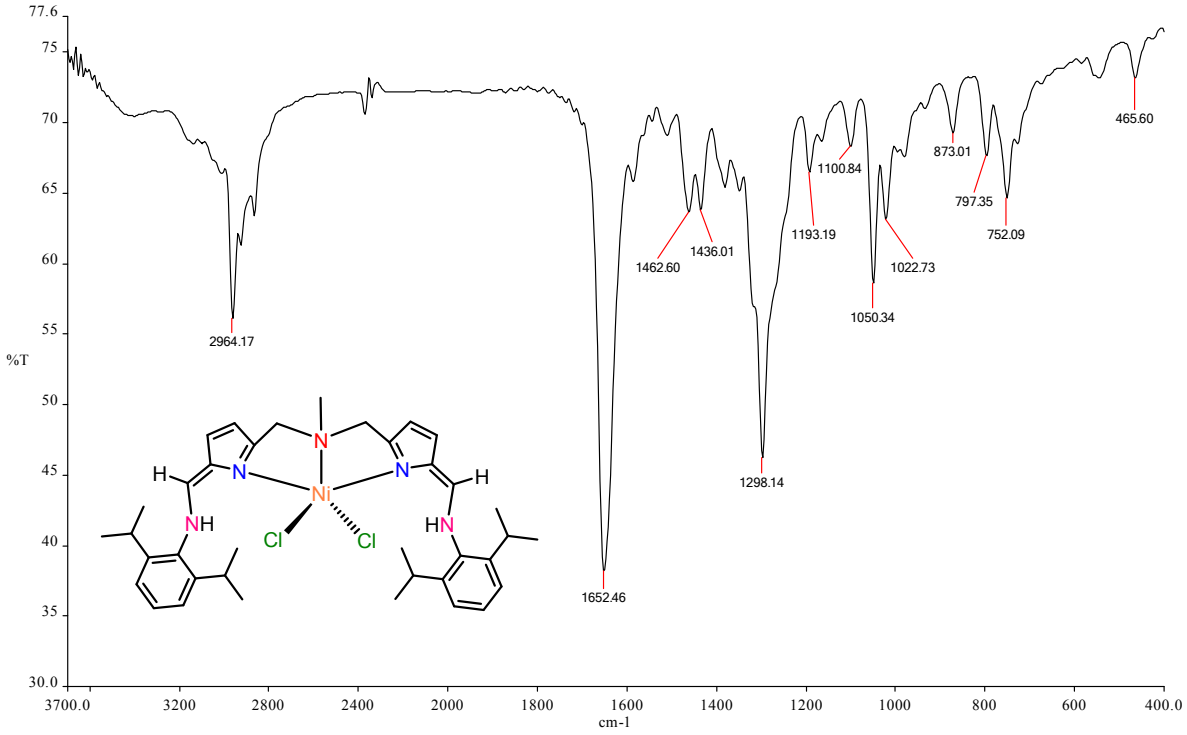

Figure S12: FTIR spectrum of the complex **8** recorded as a KBr disc.

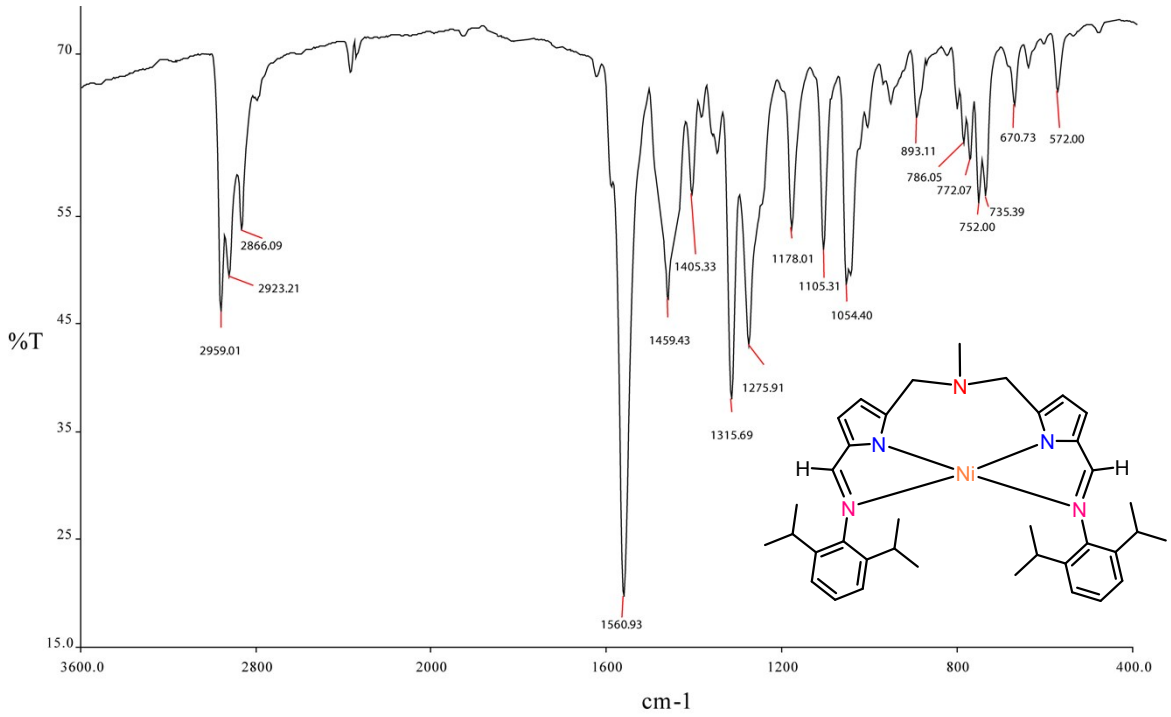

Figure S13: FTIR spectrum of the complex **9** recorded as a KBr disc.

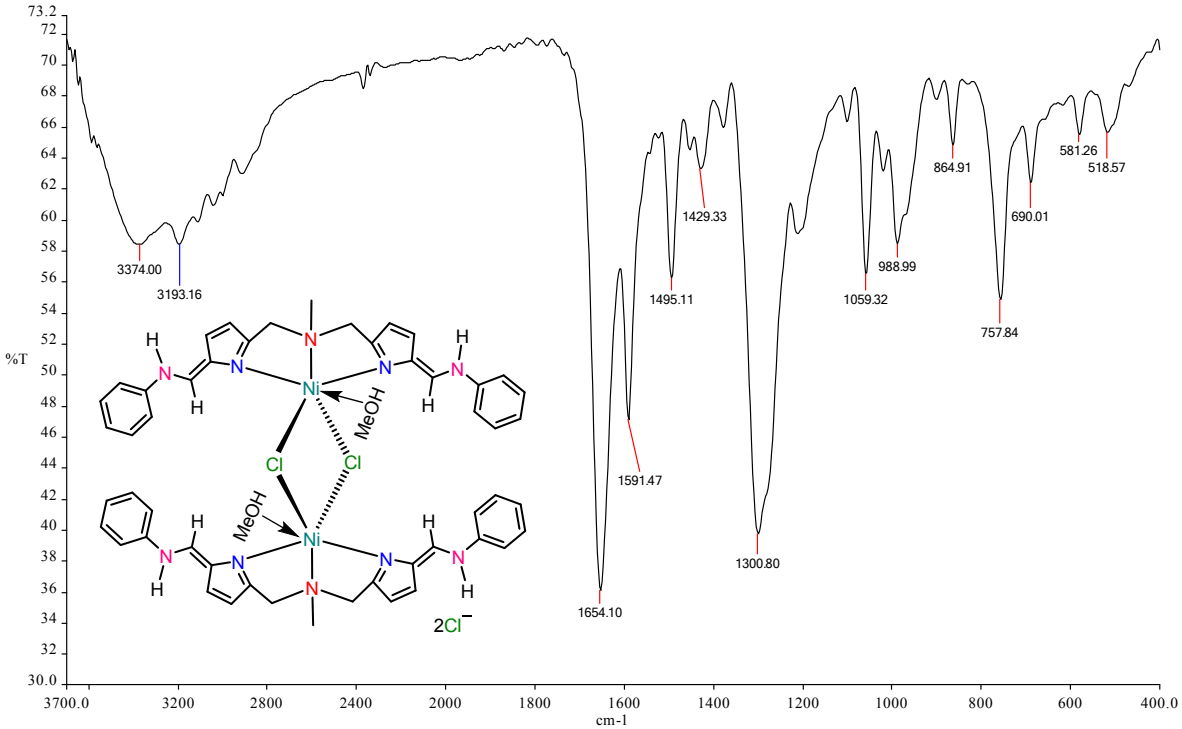

Figure S14: FTIR spectrum of the complex **10** recorded as a KBr disc.

2. X-ray Crystallography

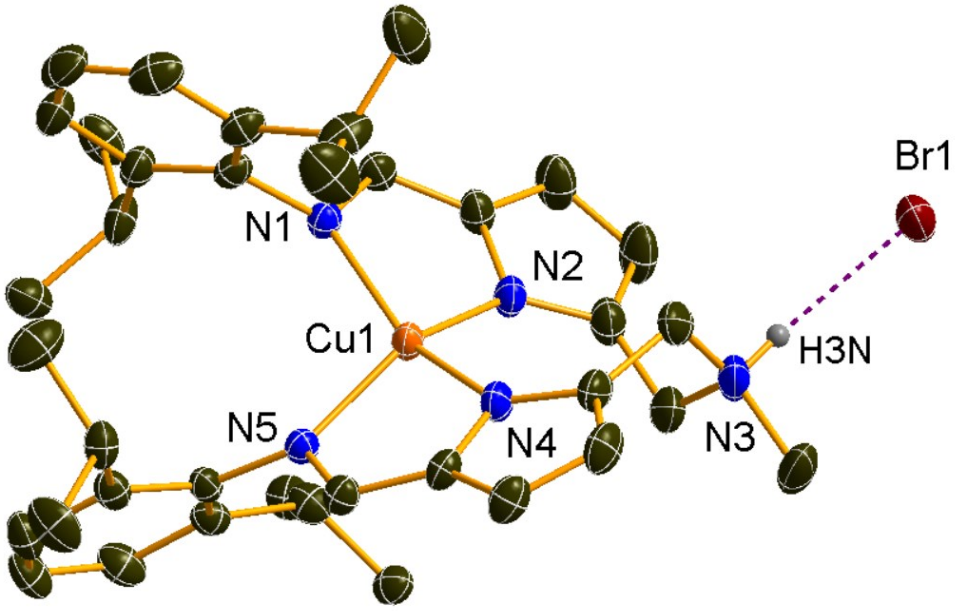

Figure S15: The molecular structure (30% probability ellipsoids) of the cationic copper(II) complex, **2**. Hydrogen atoms except the ammonium hydrogen are omitted for clarity. Selected bond lengths [Å] and angles [º]: N1–Cu1 2.022(3), N2–Cu1 1.927(3), N4–Cu1 1.935(3), N5–Cu1 2.034(3), N3···Br1 3.131(3), N1–Cu1–N2 82.77(12), N1–Cu1–N4 151.09(12), N2–Cu1–N5 152.44(12), N2–Cu1–N4 101.29(12), N4–Cu1–N5 82.71(11), N1–Cu1–N5, 106.95(11), N3–H3N···Br1 160.00(4). Symmetry transformations used to generate equivalent atoms: (i) x+1, y, z, (ii) x+1, y+1, z, (iii) x, y+1, z, (iv) –x+1, –y+1, –z.

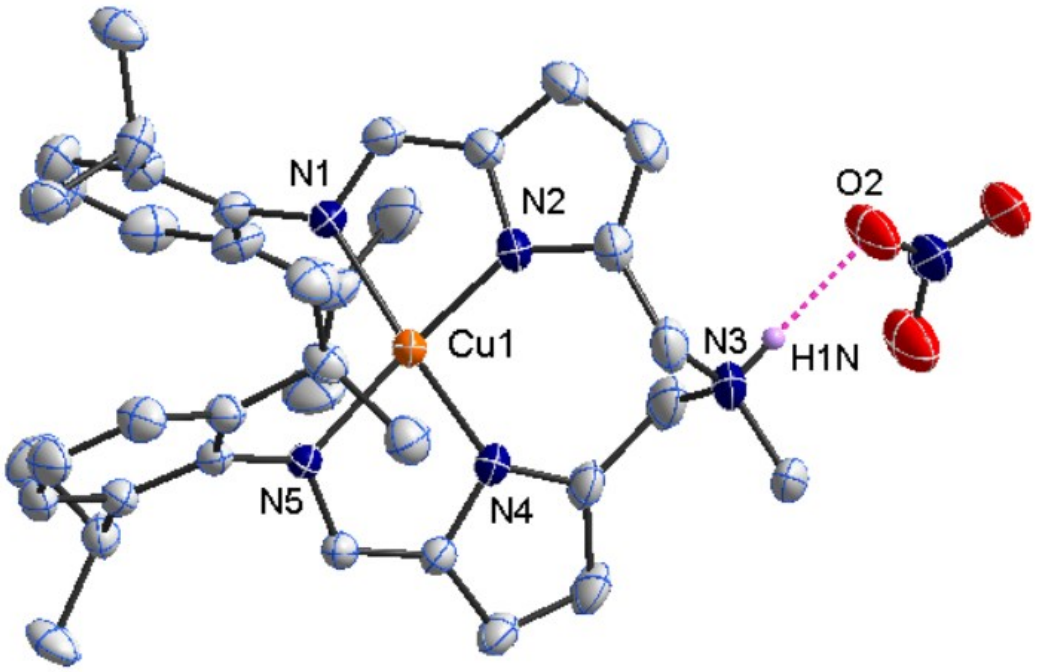

Figure S16: The molecular structure (30% probability ellipsoids) of the cationic copper(II) complex, **4**. Hydrogen atoms except the ammonium hydrogen are omitted for clarity. Selected bond lengths [Å] and angles [º]: N1–Cu1 2.017(3), N2–Cu1 1.920(3), N4–Cu1 1.933(3), N5–Cu1 2.029(3), N1–Cu1–N2 82.83(12), N1–Cu1–N4 150.85(12), N2–Cu1–N5 153.43(11), N2–Cu1–N4 101.27(12), N4–Cu1–N5 82.64(11), N1–Cu1–N5 106.62(10). Symmetry transformations used to generate equivalent atoms: (i) –x+1, –y+1, –z+1.

Table S1. Crystallographic data for the complexes **1-10**.

	1	**2**	**3**·$(MeCN)_{0.5}$
Empirical formula	$C_{37}H_{48}N_5CuCl$	$C_{37}H_{48}N_5CuBr$	$C_{77}H_{100.5}N_{11.5}Cu_4\ I_4$
CCDC number	2017163	2017164	2017165
Formula weight	661.79	706.25	1928.42
Wavelength (Å)	0.71073	0.71073	0.71073
Temperature (K)	293(2)	293(2)	293(2)
Crystal system	Triclinic	Triclinic	Triclinic
Color and shape	Dark Green, prism	Dark Green, prism	Dark Green, prism
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a/Å	8.9926(17)	9.013(2)	10.7497(11)
b/Å	10.728(2)	10.769(3)	17.8050(19)
c/Å	19.132(4)	19.466(5)	23.571(3)
α/degree	75.068(5)	75.451(5)	67.868(3)
β/degree	82.409(5)	82.408(6)	85.450(5)
γ/degree	86.015(6)	86.125(6)	87.076(4)
Volume ($Å^3$)	1766.5(6)	1811.6(7)	4164.8(8)
Z	2	2	2
D_{calcd}, g cm^{-3}	1.244	1.295	1.538
μ/mm^{-1}	0.726	1.737	2.535
F(000)	702	738	1920
Crystal size/mm	0.45×0.25×0.16	0.33×0.25×0.16	0.19×0.15×0.12
θ range (degree)	1.109 to 24.211	1.955 to 24.999	0.935 to 25.610
Limiting indices	−10<=h<=10, −12<=k<=12, −20<=l<=22	−10<=h<=10, −12<=k<=12, −20<=l<=23	−13<=h<=13, −21<=k<=21, −28<=l<=28
Total/ unique no. of reflns.	19707 / 5665	20485 / 6327	51199 / 15356
R_{int}	0.0330	0.0503	0.0621
Data / restr./ params.	5665 / 0 / 401	6327 / 0 / 400	15356 / 102 / 930
GOF (F^2)	1.026	1.037	1.018
R1, *wR2*	0.0382, 0.0939	0.0417, 0.0963	0.0529, 0.1359
R indices (all data) *R1*, *wR2*	0.0500, 0.1012	0.0748, 0.1119	0.1205, 0.1720
Largest different peak and hole (e $Å^{-3}$)	0.395 and −0.342	0.772 and −0.633	0.540 and −1.093

	4	**5**·$CHCl_3$	**6**·CH_3OH
Empirical formula	$C_{37}H_{48}N_6O_3Cu$	$C_{40}H_{52}N_5Cu_2O_3Cl_3$	$C_{45}H_{57}N_5Cu_2O_4$
CCDC number	2017166	2017167	2017168
Formula weight	688.35	884.29	859.03
Wavelength (Å)	0.71073	0.71073	0.71073
Temperature (K)	293(2)	293(2)	293(2)
Crystal system	Triclinic	Hexagonal	Hexagonal
Color and shape	Dark Green, prism	Dark Green, needle	Dark Green, prism
Space group	$P\bar{1}$	*P6(3)/m*	*P6(3)/m*
a/Å	8.955(3)	17.4202(9)	17.5728(4)
b/Å	10.717(4)	17.4202(9)	17.5728(4)
c/Å	20.003(7)	25.141(3)	25.5032(13)
α/degree	76.137(10)	90.00	90.00
β/degree	82.087(11)	90.00	90.00
γ/degree	85.491(10)	120.00	120.00
Volume ($Å^3$)	1843.9(11)	6607.1(9)	6820.4(5)
Z	2	6	6
D_{calcd}, g cm^{-3}	1.240	1.333	1.255
μ/mm^{-1}	0.635	1.188	0.980
F(000)	730	2760	2712
Crystal size/mm	0.43×0.34×0.14	0.18×0.14×0.09	0.23×0.21×0.15
θ range (degree)	1.056 to 24.948	2.109 to 24.998	2.084 to 26.044
Limiting indices	–10<=h<=10, –12<=k<=12, –23<=l<=23	–20<=h<=20, –20<=k<=20, –29<=l<=29	–21<=h<=21, –21<=k<=21, –31<=l<=31
Total/ unique no. of reflns.	21655 / 6401	79907 / 3983	110153 / 4619
R_{int}	0.0383	0.1325	0.0523
Data / restr./ params.	6401 / 0 / 428	3983 / 7 / 264	4619 / 39 / 291
GOF (F^2)	1.022	1.015	1.062
R1, *wR2*	0.0501, 0.1250	0.0583, 0.1494	0.0671, 0.2084
R indices (all data) *R1*, *wR2*	0.0742, 0.1395	0.1058, 0.1809	0.0843, 0.2362
Largest different peak and hole (e $Å^{-3}$)	0.592 and –0.313	0.687 and –0.957	2.241 and –0.676

	7·CH_3OH	**8**	**9**
Empirical formula	$C_{38}H_{51}N_5OCu$	$C_{37}H_{49}N_5Cl_2Ni$	$C_{37}H_{47}N_5Ni$
CCDC number	2017169	2017170	2017171
Formula weight	657.37	693.42	620.50
Wavelength (Å)	0.71073	0.71073	0.71073
Temperature (K)	293(2)	293(2)	293(2)
Crystal system	Triclinic	Triclinic	Triclinic
Color and shape	Dark Green, prism	Yellow, needle	Yellow, needle
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a/Å	10.1009(10)	10.9516(5)	12.096(2)
b/Å	10.6823(11)	11.4362(5)	13.620(2)
c/Å	19.141(2)	16.4132(7)	21.043(3)
α/degree	82.590(3)	75.1680(10)	87.403(5)
β/degree	85.574(3)	80.0740(10)	81.329(5)
γ/degree	63.203(3)	68.8550(10)	87.201(6)
Volume (Å^3)	1827.7(3)	1846.06(14)	4496.4(5)
Z	2	2	4
D_{calcd} , g cm^{-3}	1.195	1.247	1.205
μ/mm^{-1}	0.632	0.702	0.599
F(000)	702	736	1328
Crystal size/mm	0.52×0.33×0.13	0.13×0.06×0.04	0.26×0.21×0.18
θ range (degree)	1.073 to 24.995	1.953 to 24.735	0.980 to 25.000
Limiting indices	−11<=h<=11, −11<=k<=12, −22<=l<=22	−12<=h<=12, −13<=k<=12, −19<=l<=19	−14<=h<=14, −16<=k<=16, −23<=l<=25
Total/ unique no. of reflns.	21694 / 6358	20395 / 6144	11909 / 11909
R_{int}	0.0606	0.0583	*hklf5*
Data / restr./ params.	6358 / 0 / 411	6144 / 0 / 414	11909 / 134 / 794
GOF (F^2)	1.072	1.010	1.053
R1, *wR2*	0.0596, 0.1446	0.0385, 0.0881	0.0686, 0.1454
R indices (all data) *R1*, *wR2*	0.0970, 0.1641	0.0630, 0.0996	0.1323, 0.1826
Largest different peak and hole (e Å^{-3})	0.853 and −0.317	0.429 and −0.540	0.720 and −0.966

	10
Empirical formula	$C_{52}H_{58}N_{10}O_2Cl_4Ni_2$
CCDC number	2017172
Formula weight	1114.30
Wavelength (Å)	0.71073
Temperature (K)	293(2)
Crystal system	Monoclinic
Color and shape	Brown, prism
Space group	*P2(1)/c*
a/Å	11.73(2)
b/Å	23.36(5)
c/Å	11.47(2)
α/degree	90.00
β/degree	93.73(3)
γ/degree	90.00
Volume (Å^3)	3136(11)
Z	2
D_{calcd} , g cm^{-3}	1.180
μ/mm^{-1}	0.813
F(000)	1160
Crystal size/mm	0.21×0.15×0.10
θ range (degree)	1.740 to 24.921
Limiting indices	−13<=h<=13, −27<=k<=26, −12<=l<=13
Total/ unique no. of reflns.	20017 / 5302
R_{int}	0.0939
Data / restr./ params.	5302 / 0 / 320
GOF (F^2)	0.979
R1, *wR2*	0.0634, 0.1649
R indices (all data) *R1*, *wR2*	0.1171, 0.1997
Largest different peak and hole (e Å^{-3})	0.806 and −0.549

3. Mass Spectra

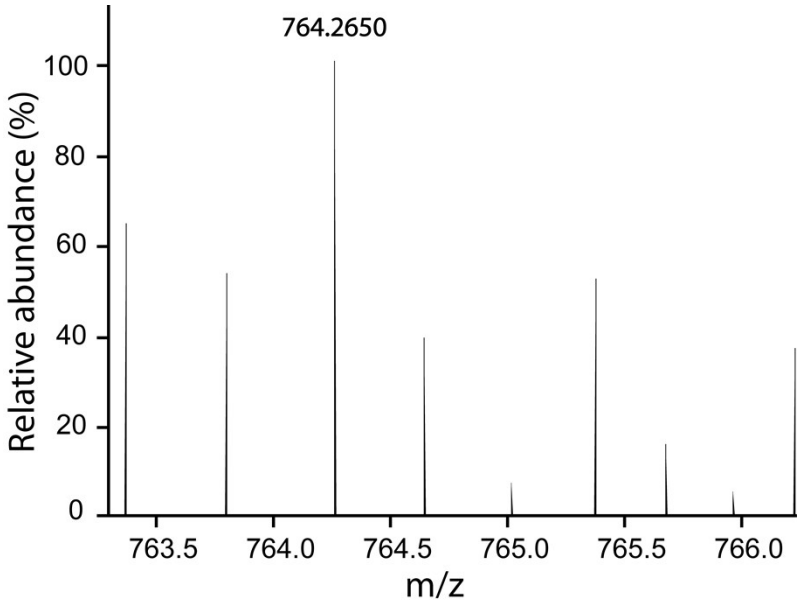

Figure S17: Portion of ESI(+)-MS spectrum of **5**, showing [**5** + H]$^+$ peak.

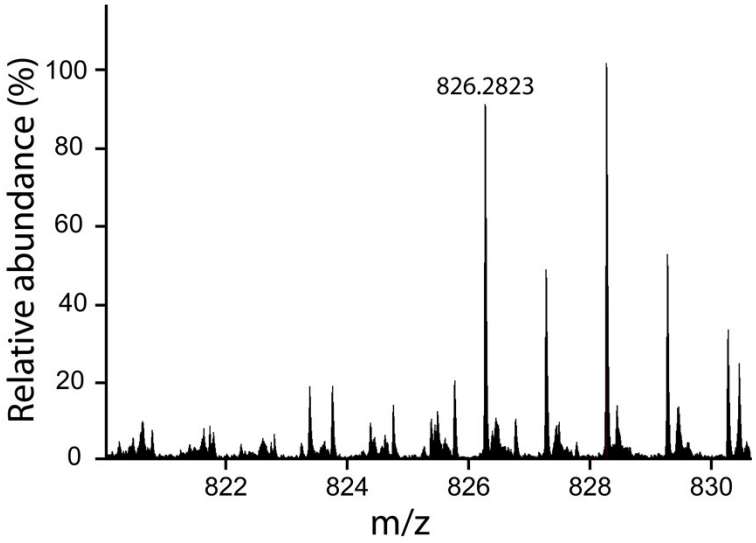

Figure S18: Portion of ESI(+)-MS spectrum of **6**, showing [**6** + H]$^+$ peak.

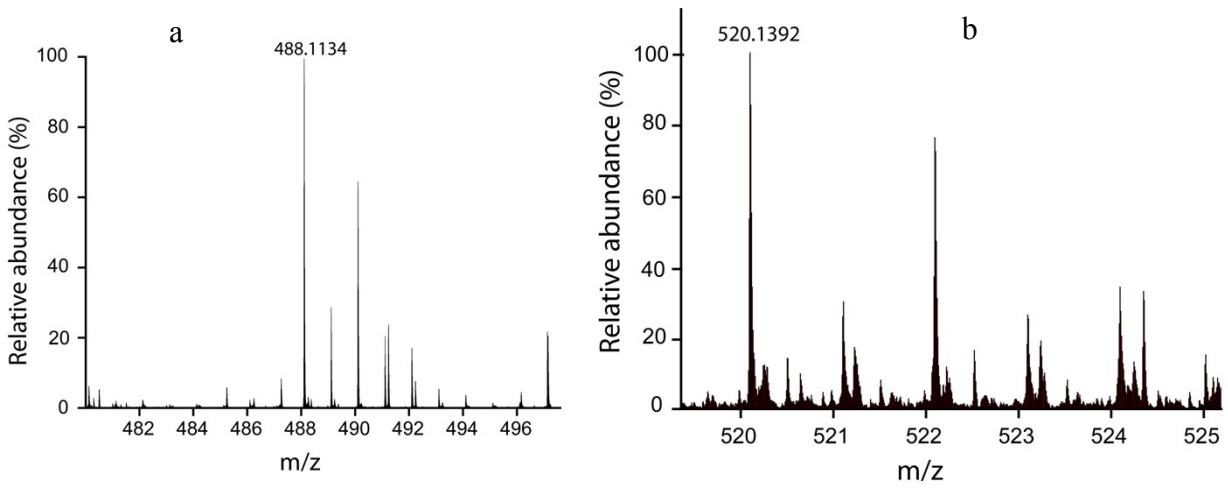

Figure S19: Portions of ESI(+)-MS spectrum of **10**, showing (a) [**10** – 2Cl – 2MeOH]$^{2+}$ and (b) [**10** – 2Cl]$^{2+}$ peaks.

4. DFT Calculation

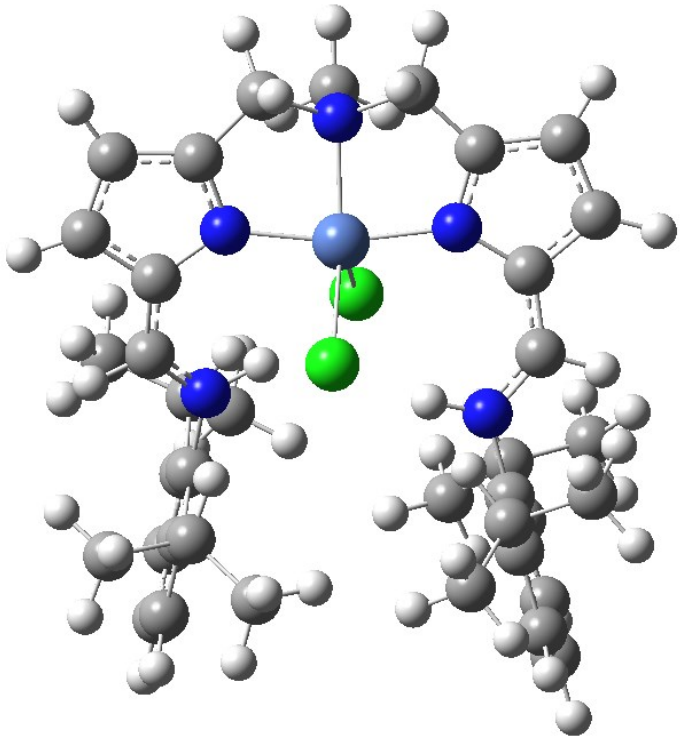

Figure S20. Optimized geometry of complex **8**.

E = -1912.307156 hartree

The atomic coordinates of complex **8**.

Ni -2.33584600 -0.62408400 -0.26994500
Cl -0.66302500 -0.63838000 -1.93710100
Cl -0.97043100 0.24253900 1.87016900
N 1.03133000 -2.22630000 0.14488000
N -2.11569400 -2.45115800 0.31613700
N -4.29437300 -0.89133800 0.25521800
N -2.96502600 1.10648900 -0.81098800
N -0.18565700 2.40959300 -0.22970600
C 2.93561000 0.05635000 3.06320600
H 2.32530000 0.41211800 3.90274700
H 3.98131300 0.01592400 3.39744800
H 2.86105200 0.79426300 2.25566400
C 2.41821500 -1.32901300 2.60093300
H 1.35888800 -1.19388500 2.35989600
C 2.52361300 -2.36085800 3.75626800
H 2.11729100 -3.33895500 3.46522400
H 3.56780600 -2.51177900 4.06310000
H 1.95948700 -2.00746800 4.62889700
C 3.15856300 -1.82279800 1.35347500
C 4.57054200 -1.87971000 1.34783100
H 5.11820500 -1.57727200 2.23657000
C 5.27535600 -2.30166400 0.21163600
H 6.36248800 -2.33280000 0.22809100
C 4.58246000 -2.67746300 -0.95206200
H 5.14138400 -2.99376400 -1.82789100
C 3.17416300 -2.65228800 -0.99671000
C 3.10460400 -2.73541200 -3.56777600
H 2.45377600 -2.99442200 -4.41265300
H 3.30166800 -1.65773300 -3.60926500
H 4.05583300 -3.26513900 -3.71183200
C 2.41437400 -3.12951300 -2.24077200
H 1.42358900 -2.66035400 -2.24436000
C 2.20212800 -4.66852700 -2.17926400
H 1.63104100 -5.00916100 -3.05283600
H 3.16604500 -5.19533800 -2.17133600

H 1.64795000 -4.96343400 -1.27927100
C 2.48480500 -2.23180100 0.17407200
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H 0.86243700 -3.94078700 1.24734800
C -1.09967800 -3.30420900 0.78812100
C -1.71146300 -4.47284500 1.35787800
H -1.17431800 -5.30366000 1.79822700
C -3.09645800 -4.33079800 1.22539200
H -3.86628100 -5.01981800 1.54423500
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H -5.40464600 -2.65656200 0.82661600
C -4.48741800 -0.37122800 1.65135800
H -3.81067900 -0.89698800 2.32735300
H -4.22334800 0.68699600 1.68060700
H -5.53361400 -0.51164200 1.96803700
C -5.09051600 -0.09641400 -0.74756700
H -6.09048200 0.14956300 -0.35883500
H -5.22285600 -0.71634000 -1.64396500
C -4.30126400 1.13667900 -1.07561200
C -4.68440100 2.36720800 -1.67729300
H -5.68198000 2.65185000 -1.98210800
C -3.50829900 3.12079900 -1.78966800
H -3.40708400 4.12431900 -2.18383000
C -2.44239900 2.34301200 -1.22349400
C -1.15682900 2.87485300 -1.00717700
H -0.94797800 3.81777100 -1.50946600
C 1.09431200 3.08249800 -0.09541100
C 2.00287800 3.08547400 -1.18586300
C 3.22049200 3.78284700 -1.01833900
H 3.93618100 3.80677500 -1.83612700
C 3.52864300 4.42617600 0.18803800
H 4.47459500 4.95179300 0.29714700
C 2.62063900 4.38796100 1.26027400
H 2.87411800 4.88451300 2.19206200
C 1.38516300 3.72106800 1.14301700
C 1.00144900 3.72500600 3.68871300
H 0.21628000 3.61933700 4.44806100
H 1.68869700 2.87744800 3.79429700

H 1.55286100 4.64853800 3.91229600
C 0.35906500 3.75212800 2.28255800
H -0.27091900 2.85832800 2.20870600
C -0.56169200 4.99618200 2.13323300
H -1.31979100 5.00454200 2.92744900
H 0.02061900 5.92521200 2.20416000
H -1.08538800 4.99730800 1.16877100
C 1.53069200 3.36502600 -3.67284300
H 1.30013700 2.82778400 -4.60192200
H 0.70701900 4.06338700 -3.47237500
H 2.43764200 3.96130100 -3.84139500
C 1.72604800 2.35878100 -2.50709800
H 0.80810400 1.77152700 -2.40766600
C 2.85246300 1.34908100 -2.84522800
H 2.58843300 0.79255600 -3.75372700
H 3.81293200 1.85086400 -3.02361400
H 2.99080700 0.62688200 -2.03183200
H 0.55020900 -1.50793900 -0.42676000
H -0.37284000 1.58097400 0.38378300

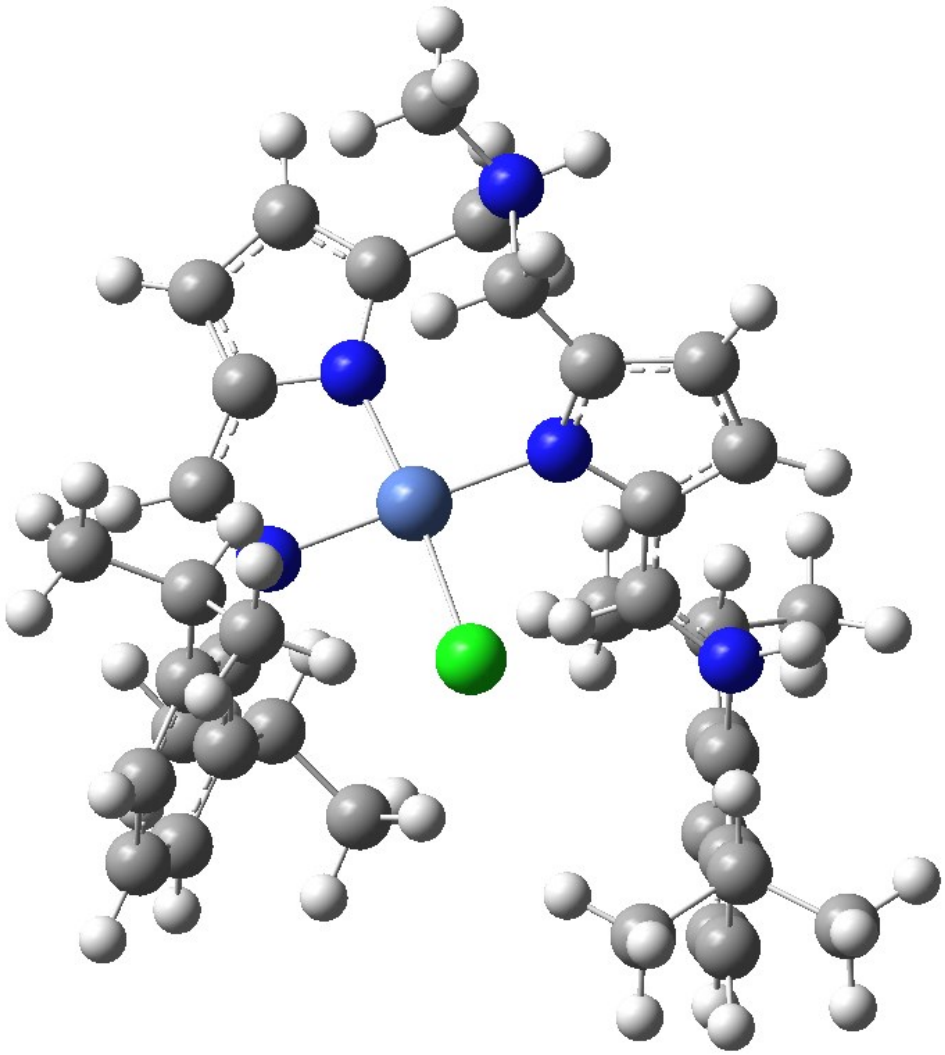

Figure S21. Optimized geometry of model complex **I**.

E = -1897.096184 hartree

The atomic coordinates of model complex **I**.

C 1.53627100 2.66109200 1.92508100

H 1.76992700 2.34695500 0.90052700
H 2.12984200 2.05502900 2.62329300
H 1.85900400 3.70344000 2.03875800
C 0.02293800 2.49812200 2.22104500
H -0.20556000 1.42707400 2.15141000
C -0.30937100 2.95249100 3.66722800
H -1.36780500 2.78760100 3.90858900

H -0.10243300 4.02180500 3.80183900
H 0.29703700 2.39787100 4.39552700
C -0.83277400 3.24004300 1.18904200
C -0.63112100 4.61817900 0.97021000
H 0.12213000 5.14757600 1.54809500
C -1.38495300 5.31754600 0.01517900
H -1.21814600 6.38093600 -0.13638700
C -2.34795400 4.64234100 -0.75063000
H -2.91590900 5.19003100 -1.49809900
C -2.58740900 3.26517500 -0.56885600
C -1.83317900 2.58901800 0.42340800
C -3.35641700 2.73704100 -2.94140300
H -4.08066900 2.16201600 -3.53451200
H -2.34679100 2.39357300 -3.19372900
H -3.44580300 3.78827300 -3.24277800
C -3.63576200 2.55111400 -1.42785800
H -3.57245100 1.47534300 -1.22077700
C -5.07186800 3.01550200 -1.06511800
H -5.81494300 2.48002900 -1.67106700
H -5.19789200 4.08946600 -1.25255700
H -5.29938400 2.83556100 -0.00574600
C -2.99593400 0.89080100 1.62553000
H -3.49391100 1.67107800 2.19784100
C -3.26531800 -0.49341900 1.84711200
C -4.11503200 -1.20414100 2.72139400
H -4.76598700 -0.78336900 3.47509700
C -3.93129400 -2.57092000 2.41155400
H -4.40642100 -3.41628000 2.89278900
C -2.97320900 -2.64138800 1.36476700
C -2.48092100 -3.88785400 0.72543500
H -2.75672500 -4.76335200 1.32052200
H -1.40224600 -3.88683700 0.55753700
C -4.61698500 -4.31486500 -0.63209300
H -5.00134900 -4.47105600 -1.64347100
H -5.05318500 -3.41521700 -0.19571800
H -4.85656700 -5.17731800 -0.00458900
C -2.71035600 -3.03213900 -1.70738000
H -3.11510400 -3.34797600 -2.67397700
H -3.20882700 -2.11934300 -1.37811100
C -1.22698400 -2.88824500 -1.74095300

C -0.30464400 -3.72561800 -2.43815000
H -0.55358500 -4.52773500 -3.12129300
C 0.97783100 -3.28182800 -2.09316100
H 1.91408600 -3.70363400 -2.43581300
C 0.80556800 -2.18573000 -1.19249300
C 1.78671600 -1.36115000 -0.59171500
H 1.48697200 -0.64077700 0.16022000
C 4.10204400 -0.58718200 -0.21502800
C 3.65623500 2.28778600 -2.45091000
H 3.33606300 2.50599200 -3.47722900
H 4.40625000 3.03678600 -2.16711800
H 2.78520200 2.40356500 -1.79581800
C 4.23197500 0.84896300 -2.37085100
H 3.42296900 0.17421900 -2.67824900
C 5.40675700 0.66347800 -3.36885800
H 5.06926600 0.87026900 -4.39209500
H 5.80959100 -0.35786100 -3.34050500
H 6.23145300 1.35143500 -3.14452800
C 4.66158300 0.49566100 -0.94249000
C 5.65091100 1.26505400 -0.29665200
H 6.10089100 2.10390000 -0.81993400
C 6.05425500 0.97125600 1.01515900
H 6.81441100 1.58066200 1.49677600
C 5.48368700 -0.10773900 1.70720400
H 5.81345700 -0.32683900 2.71898500
C 4.49991900 -0.92160700 1.10645200
C 5.04676800 -3.10169500 2.31020800
H 5.61735200 -3.45751600 1.44328000
H 4.60984100 -3.97311300 2.81454000
H 5.75397800 -2.63594700 3.00713300
C 3.92918300 -2.11227600 1.88671400
H 3.24256400 -2.66937200 1.23699100
C 3.11758300 -1.63861000 3.12261800
H 2.29637600 -0.96808800 2.83574900
H 3.75609500 -1.09572400 3.83037100
H 2.68934000 -2.49982700 3.65137000
N -2.12187400 1.18497600 0.68777200
N -2.55951800 -1.36629800 1.02118600
N -3.11318200 -4.14042200 -0.69246300
H -2.69191600 -5.01518200 -1.03605200

N -0.56505500 -1.96235200 -0.98591000
N 3.08564600 -1.40047400 -0.87840400
H 3.39957400 -1.99932700 -1.64008700
Cl -0.07178000 0.88537700 -1.50660900
Ni -1.35265500 -0.39692000 -0.16158500

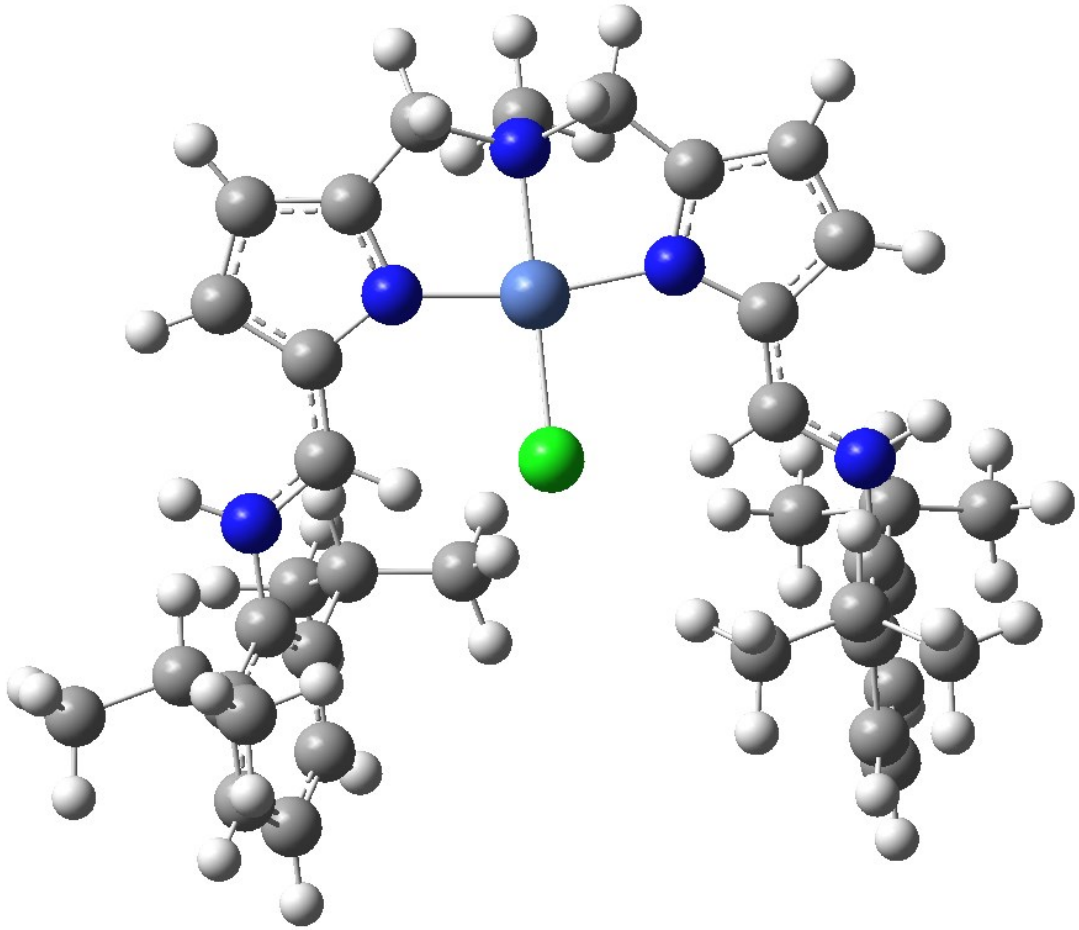

Figure S22. Optimized geometry of model complex **II**.

E = -1897.123576 hartree

The atomic coordinates of model complex **II**.

Cl	0.06408100	0.40832600	-1.02386300
N	-4.15691000	-0.30948200	-0.28262600

N	-1.93299500	2.68497400	-0.30785200
N	-0.07581800	4.43369900	0.30557200
N	1.89429800	2.72455800	-0.01434100
N	4.15132200	-0.22667200	0.30870500
C	-4.86864200	-2.31954100	-3.76662700
H	-4.78454900	-1.78505000	-4.72128600
H	-4.77519400	-3.39199500	-3.97799300
H	-5.87446300	-2.14466900	-3.36352300
C	-3.76758600	-1.83484200	-2.78648800
H	-3.89318900	-0.75139900	-2.66954800
C	-2.35293800	-2.06961700	-3.38141900
H	-1.56957600	-1.67213200	-2.72507800
H	-2.16057100	-3.13924800	-3.53455100
H	-2.26566200	-1.57022800	-4.35477300
C	-3.90960700	-2.50088500	-1.41334000
C	-3.85416200	-3.90728600	-1.31107800
H	-3.70498300	-4.50202400	-2.20794100
C	-3.99354000	-4.55013300	-0.07177000
H	-3.95018800	-5.63487100	-0.01737400
C	-4.19435300	-3.79951700	1.09715100
H	-4.30649500	-4.31153000	2.04902400
C	-4.25380900	-2.39108900	1.05369900
C	-5.80650800	-1.98701900	3.03629700
H	-5.96695900	-1.36921800	3.92908400
H	-6.66213700	-1.84578400	2.36379500
H	-5.80327500	-3.03672000	3.35483200
C	-4.47155200	-1.59896100	2.34761300
H	-4.53118000	-0.53131700	2.10101900
C	-3.27595200	-1.77734400	3.32164600
H	-3.42709000	-1.17240000	4.22494400
H	-3.17172100	-2.82430500	3.63302100
H	-2.32999700	-1.47138400	2.85554200
C	-4.09984900	-1.76856900	-0.21249400
C	-3.07620300	0.48010600	-0.25270300
H	-2.11486900	-0.01841100	-0.17855700
C	-3.10060700	1.88205000	-0.33550800
C	-4.24095000	2.75127000	-0.42166700
H	-5.28070300	2.45045600	-0.45651000
C	-3.76967700	4.06732300	-0.43553400
H	-4.35601500	4.97377700	-0.48985300

C	-2.35169800	3.97922000	-0.36350900
C	-1.29180300	5.03742200	-0.35975900
H	-1.01842300	5.31590800	-1.38519100
H	-1.61492900	5.94891300	0.16079400
C	-0.20195500	4.50408000	1.80746900
H	-1.11484700	3.99214900	2.11931000
H	0.65892500	4.01330700	2.26670400
H	-0.24147300	5.55278500	2.13435000
C	1.22061300	5.06498200	-0.14847400
H	1.43469300	5.97963600	0.42039600
H	1.11454700	5.34378700	-1.20434300
C	2.28779500	4.02794600	0.01938300
C	3.69432100	4.14523500	0.19469400
H	4.26065900	5.06392700	0.25534300
C	4.18561500	2.83858200	0.27305500
H	5.22181100	2.55915800	0.41830100
C	3.06777500	1.94587300	0.14627700
C	3.06239600	0.54170700	0.17902500
H	2.11448100	0.02611900	0.06479100
C	4.12947600	-1.68311700	0.35843300
C	3.52107400	-2.33566200	1.46430600
C	3.52034700	-3.74694000	1.46070500
H	3.05932100	-4.28168000	2.28648200
C	4.11917000	-4.47273600	0.42042700
H	4.11208400	-5.55927400	0.44447800
C	4.73062000	-3.80028800	-0.64888100
H	5.19061800	-4.37377500	-1.44885200
C	4.74336900	-2.39219600	-0.70807600
C	6.89531700	-2.02489500	-2.02851500
H	7.34206600	-1.47397900	-2.86577100
H	7.44207100	-1.76122300	-1.11369600
H	7.05364100	-3.09464700	-2.21269900
C	5.38478700	-1.69024000	-1.91077800
H	5.29669500	-0.60371600	-1.77961800
C	4.63480300	-2.03847300	-3.22492200
H	5.07807800	-1.49576100	-4.06937300
H	4.69730700	-3.11124800	-3.44605300
H	3.57336900	-1.76825000	-3.16214500
C	1.34669500	-1.79007600	2.67203200
H	0.90601900	-1.22871400	3.50658000

H	0.87755400	-1.44992100	1.73970700
H	1.09038400	-2.84842600	2.80726500
C	2.88688400	-1.59056000	2.64566200
H	3.07766300	-0.51637300	2.53483600
C	3.52030100	-2.01742500	3.99574200
H	3.09687000	-1.42309900	4.81566000
H	3.32591700	-3.07369600	4.21837100
H	4.60745400	-1.87026100	3.99259800
H	-5.07813600	0.11309500	-0.37888400
H	5.06496000	0.21849900	0.35831800
Ni	-0.01317900	2.51406500	-0.22231800

Energy of Chloride anion = -15.11520744

The difference in energy between complex 8 and model complex I = E(8) - [E(I)+E(Cl)]
E(8) = energy of complex 8 = -1912.307156 hartree
E(I) = energy of model complex I = -1897.096184 hartree
E(Cl) = energy of chloride = -15.11520744
the difference in energy = 0.09576456 hartree = 60.09 kcal/mol.

The difference in energy between complex 8 and model complex II = = E(8) - [E(II)+E(Cl)]
E(8) = energy of complex 8 = -1912.307156 hartree
E(II) = energy of model complex I = -1897.123576 hartree
E(Cl) = energy of chloride = -15.11520744
the difference in energy = 0.06837256 hartree = 42.90 kcal/mol