

Synthesis and Coordination Chemistry of Multidentate Ligands
Based on Nitrogen-Containing Heterocyclic Phenanthridine
Moieties

by

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Department of Chemistry

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1^+ (S_0)	136
1^+ (T_1)	138
2^+ (S_0)	140
2^+ (T_1)	142
3^+ (S_0)	144
3^+ (T_1)	146

Chapter 2:

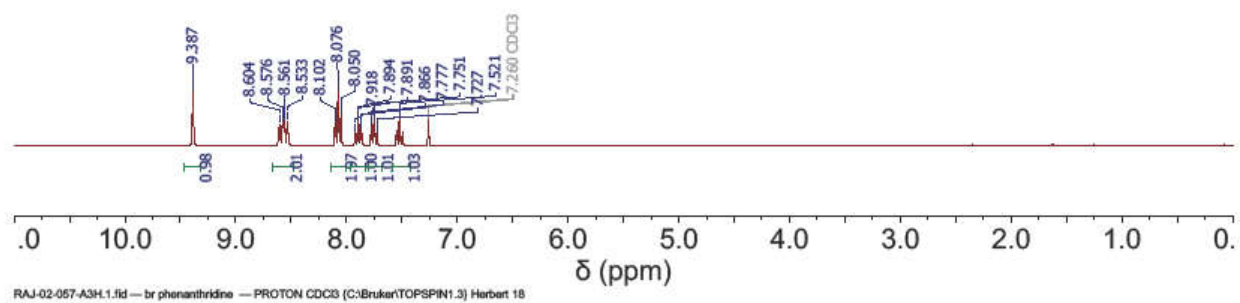


Figure S2.1. ^1H NMR (300 MHz, 22°C) spectrum of **1-Br** in CDCl_3 .

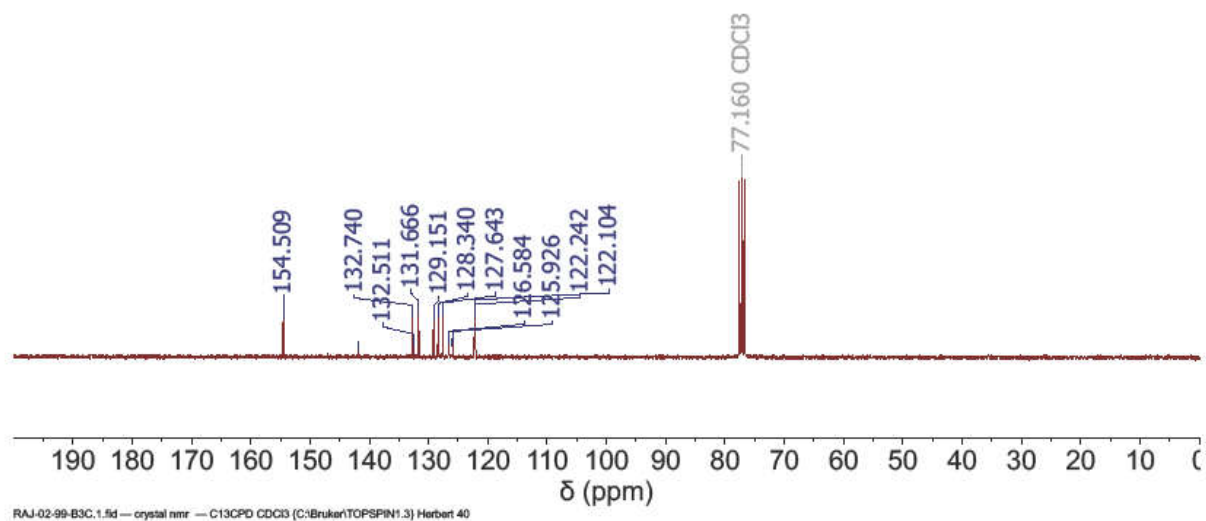


Figure S2.2. ¹³C NMR (75 MHz, 22°C) spectrum of **1-Br** in CDCl₃.

RAJ-0-4-048-DSH.2.fid
Acyl,MeBrPhenanthridine
PROTON CD2Cl2 C:\ Herbert 1

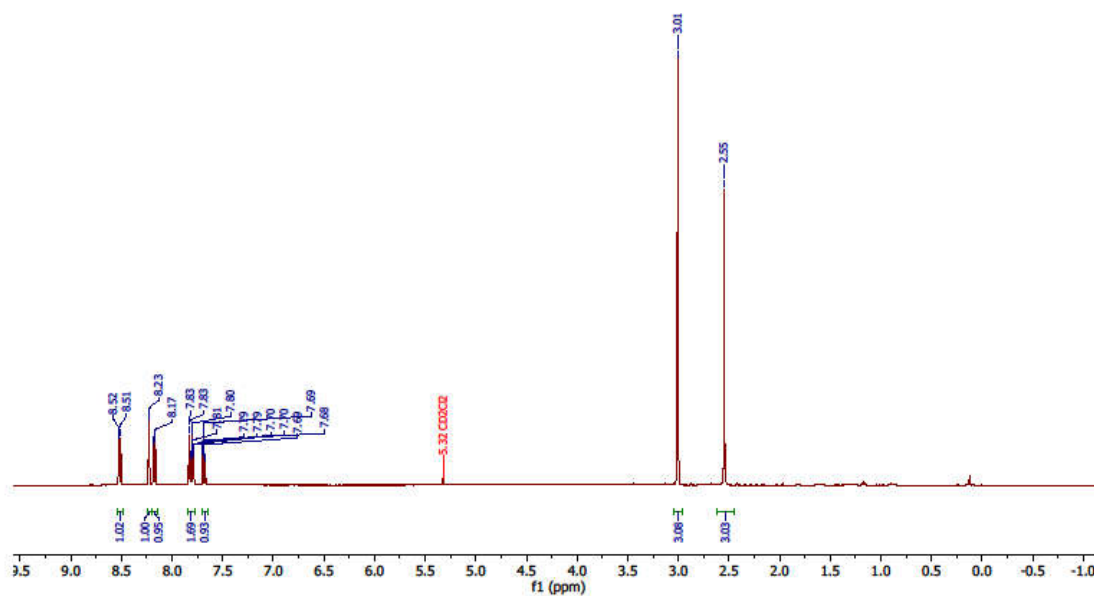


Figure S2.3. ^1H NMR (300 MHz, 22°C) spectrum of **3-Br** in CD_2Cl_2 .

RAJ-0-4-048-D5C.2.fid
Acyl_MeBrPhenanthridine
C13CPD CD2Cl2 C:\ Herbert 1

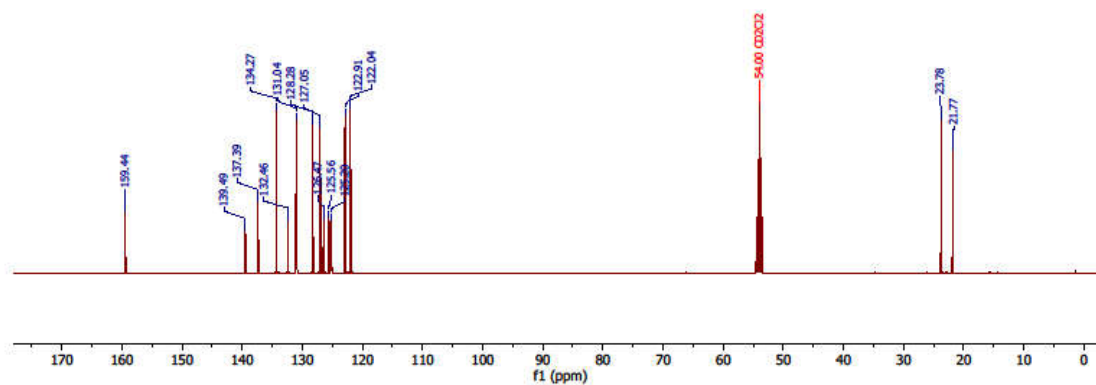


Figure S2.4. ^{13}C NMR (75 MHz, 22°C) spectrum of **3-Br** in CDCl_3 .

RAJ-03-121-A3H.1.fid
tBu, methylBromoPhen
PROTON CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 58

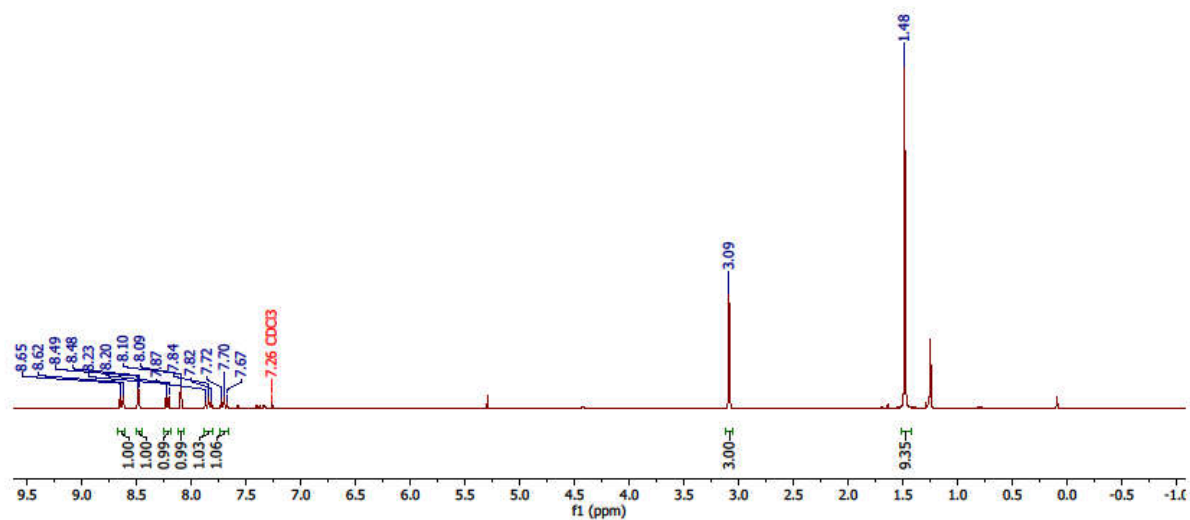


Figure S2.5. ^1H NMR (300 MHz, 22°C) spectrum of **4-Br** in CDCl_3 .

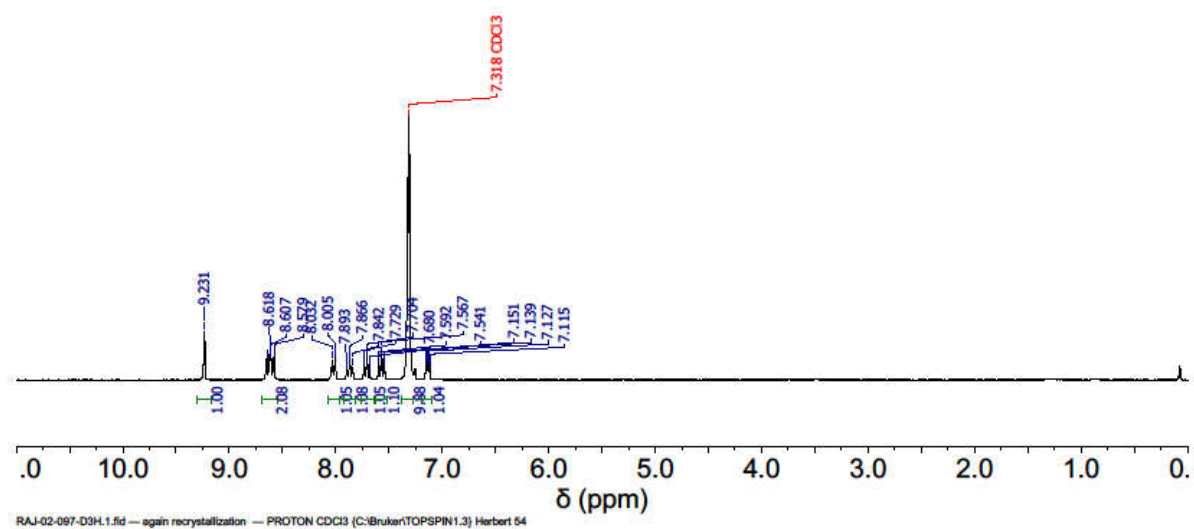


Figure S2.6. ^1H NMR (300 MHz, 22°C) spectrum of **L1** in CDCl_3 .

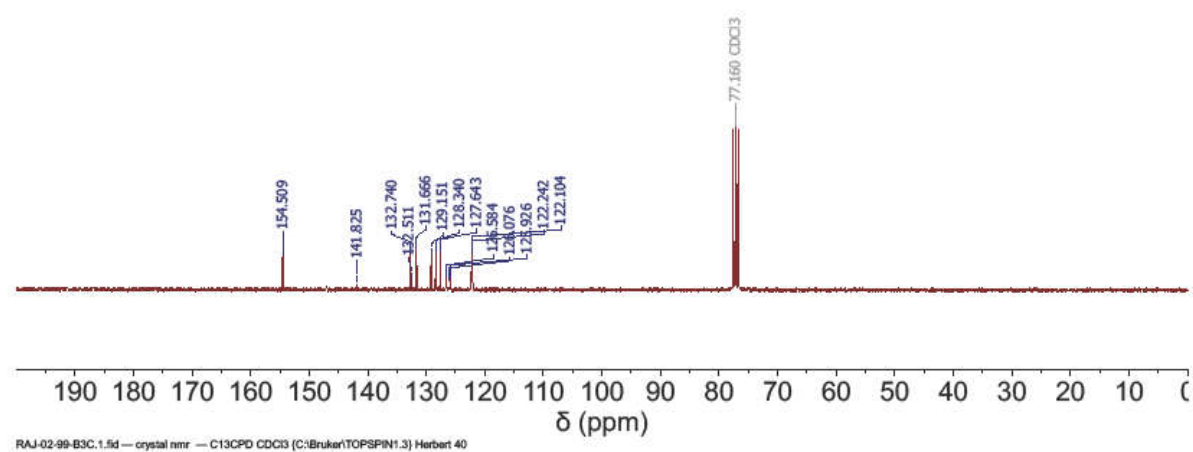


Figure S2.7. ¹³C NMR (75 MHz, 22°C) spectrum of **L1** in CDCl₃.

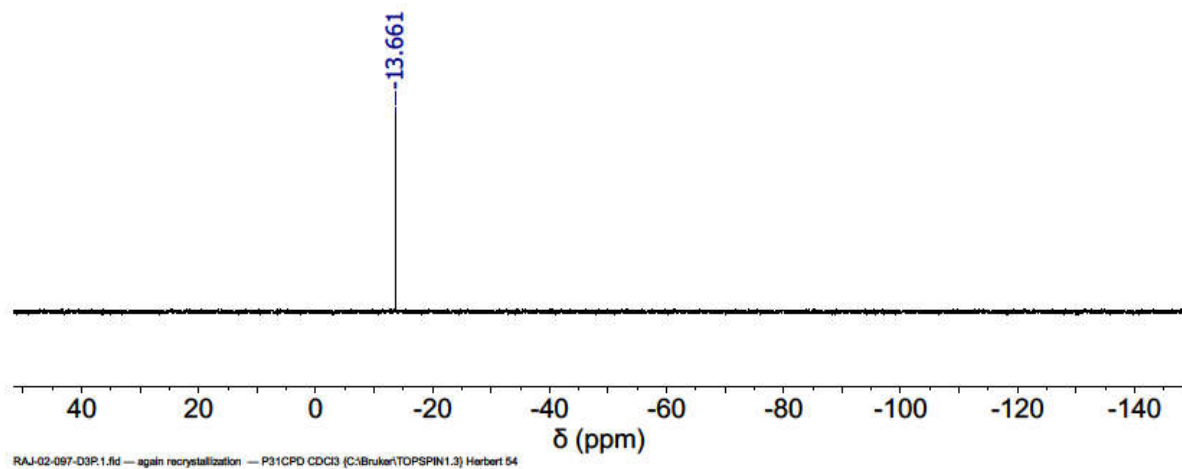


Figure S2.8. ^{31}P NMR (121 MHz, 22°C) spectrum of **L1** in CDCl_3 .

RAJ-03-141-B3H.1.fid
MePN
PROTON1.28 CDCl3 (C:\Bruker\TOPSPIN1.3) Herbert 41

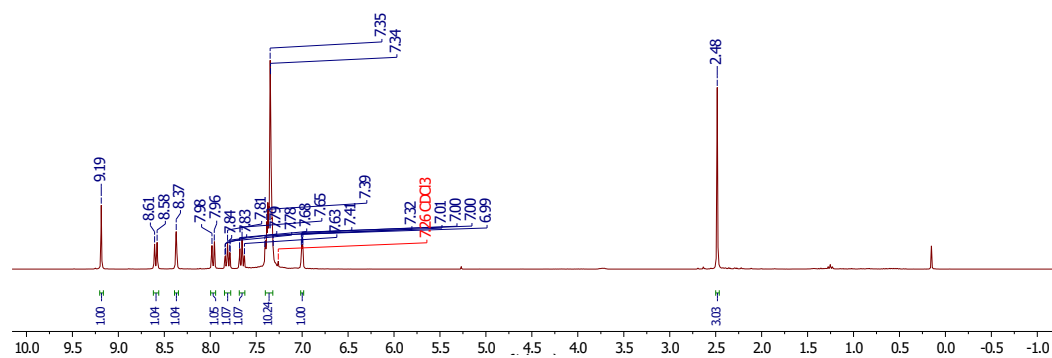


Figure S2.9. ^1H NMR (300 MHz, 22°C) spectrum of **L2** in CDCl_3 .

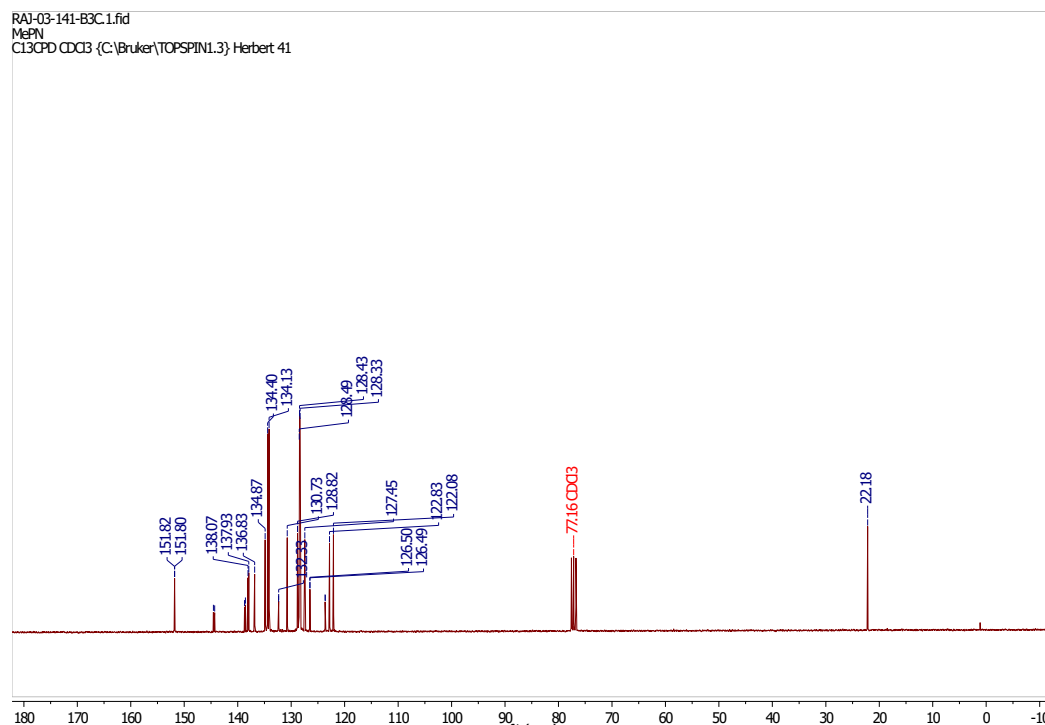


Figure S2.10. $^{13}\text{C}\{^1\text{H}\}$ (75 MHz, 22°C) NMR spectrum of **L2** in CDCl_3 .

RAJ-03-142-F3P1.fid
MePN ligand
P31CPD CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 41

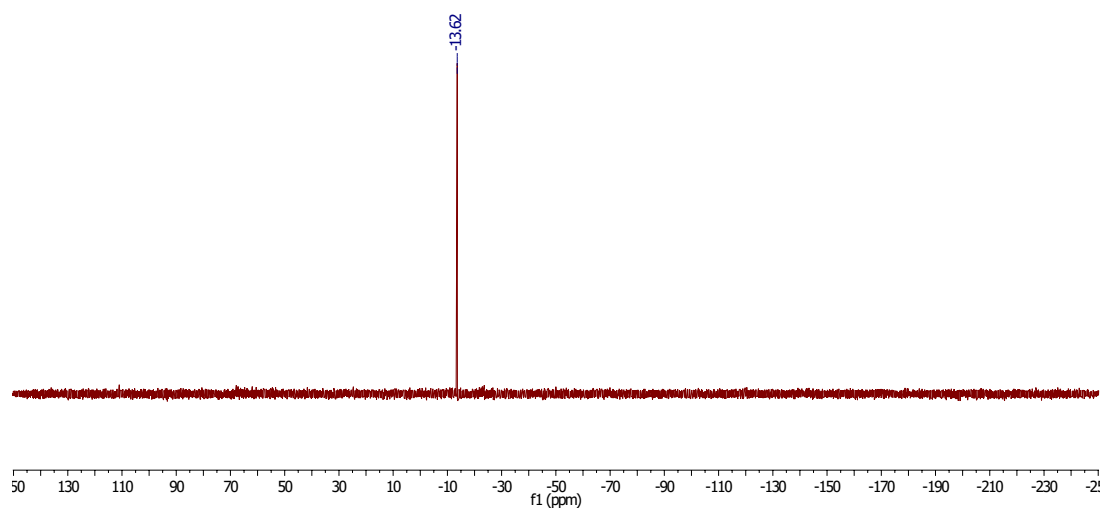


Figure S2.11. $^{31}\text{P}\{^1\text{H}\}$ NMR (121 MHz, 22°C) spectrum of **L2** in CDCl_3 .

RAJ-03-062-B3H.1.fid
quinolinephosphine after etoh wash
PROTON CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 27

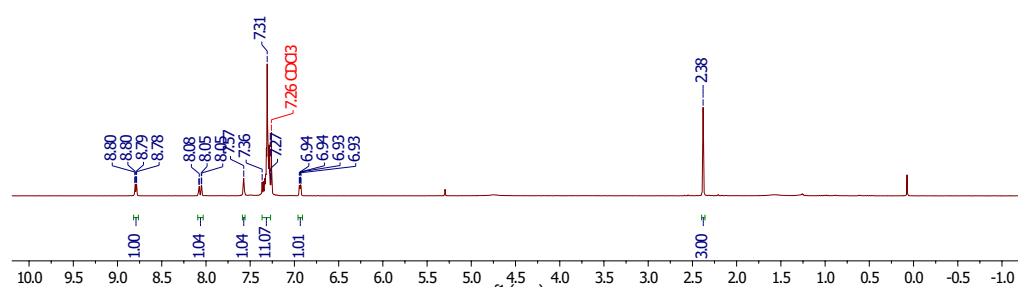


Figure S2.12. ^1H NMR (300 MHz, 22°C) spectrum of **L3** in CDCl_3 .

RAJ-03-141-D3C.1.fid
MeQuin
C13CPD CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 15

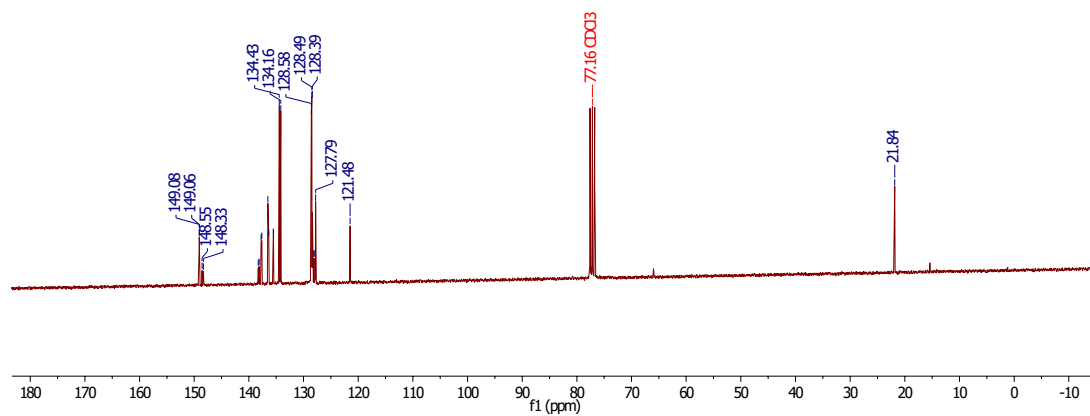


Figure S2.13. $^{13}\text{C}\{^1\text{H}\}$ (75 MHz, 22°C) NMR spectrum of **L3** in CDCl_3 .

RAJ-03-075-A3P1.fid
PN ligand check
P31CPD CDCl3 {C:\Bruker\TOPSPINL3} Herbert 21

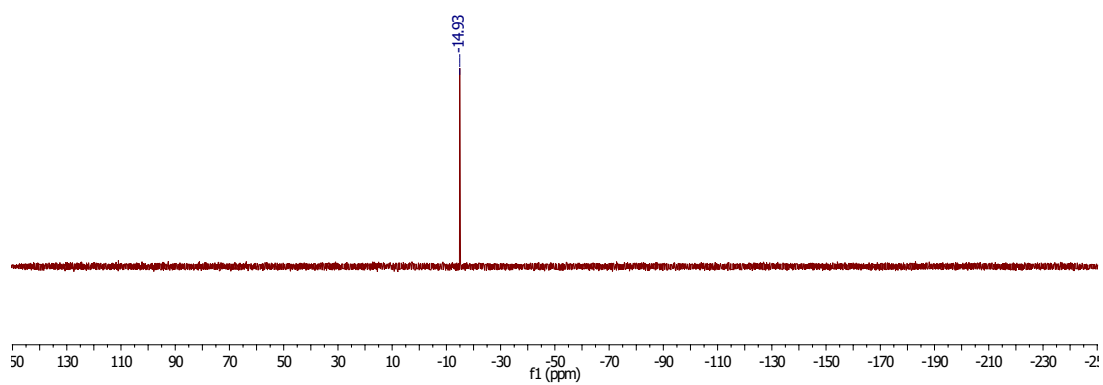


Figure S2.14. $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, 22°C) NMR spectrum of **L3** in CDCl_3 .

22

RAJ-04-059-DSC.2.fid
MePNIsoligand
C13CPD CDCl3 C:\\ Herbert 1

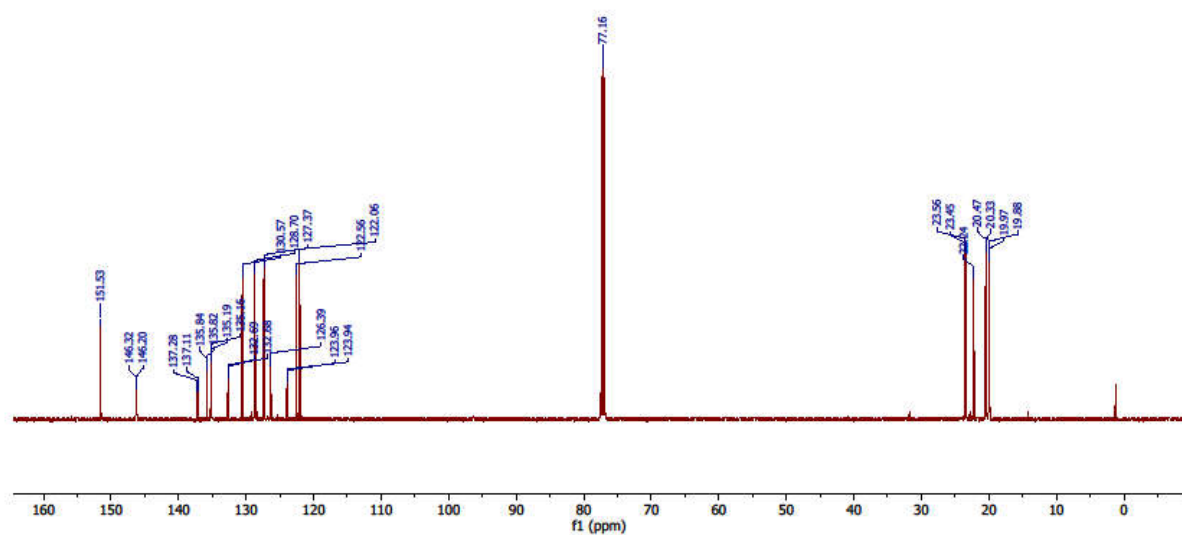


Figure S2.16. ^{13}C NMR (75 MHz, 22°C) spectrum of L4 in CDCl_3 .

RAJ-04-059-DSP.1.fid
MePNIsoligand
P31CPD CDCl3 C:\ Herbert 1

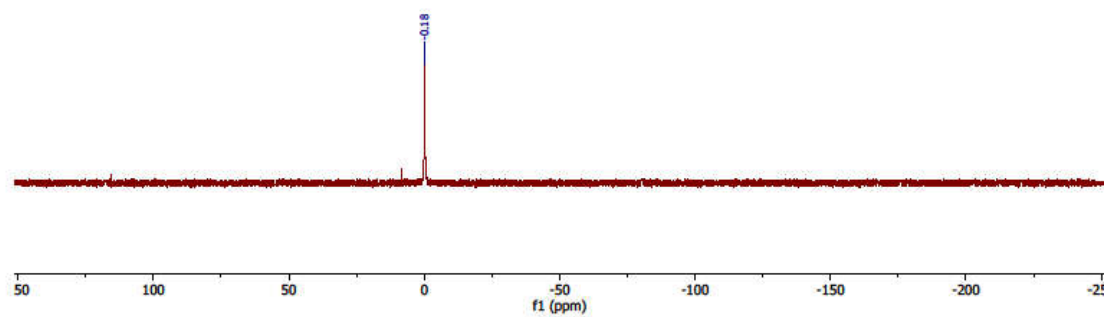


Figure S2.17. ^{31}P NMR (121 MHz, 22°C) spectrum of **L4** in CDCl_3 .

RAJ-04-048-G5H2.fid
Acyl/MePN ligand
PROTON CD2Cl2 C:\\ Herbert 1

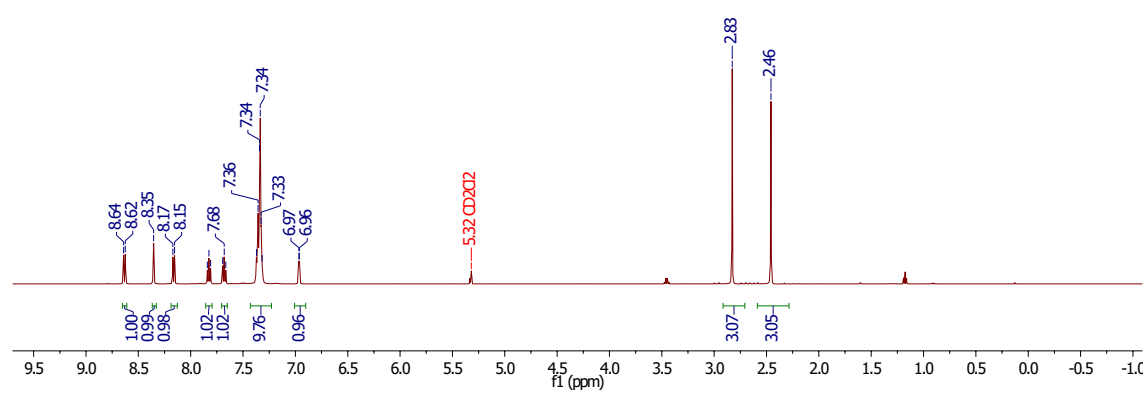


Figure S2.18. ¹H NMR (500 MHz, 22°C, CD₂Cl₂) spectrum of **L5**.

RAJ-04-048-G5C.1.fid
Acyl/MePN ligand
C13CPD CD202 C:\\ Herbert 1

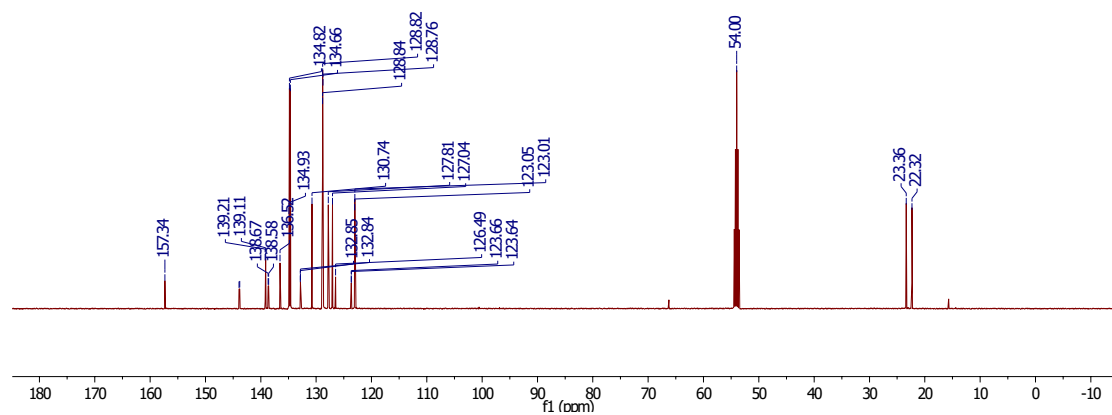


Figure S2.19. $^{13}\text{C}\{^1\text{H}\}$ (126 MHz, 22°C, CD_2Cl_2) NMR spectrum of **L5**.

RAJ-04-048-GSP.1.fid
Acyl/MePN ligand
P31CPD CD2Cl2 C:\\ Herbert 1

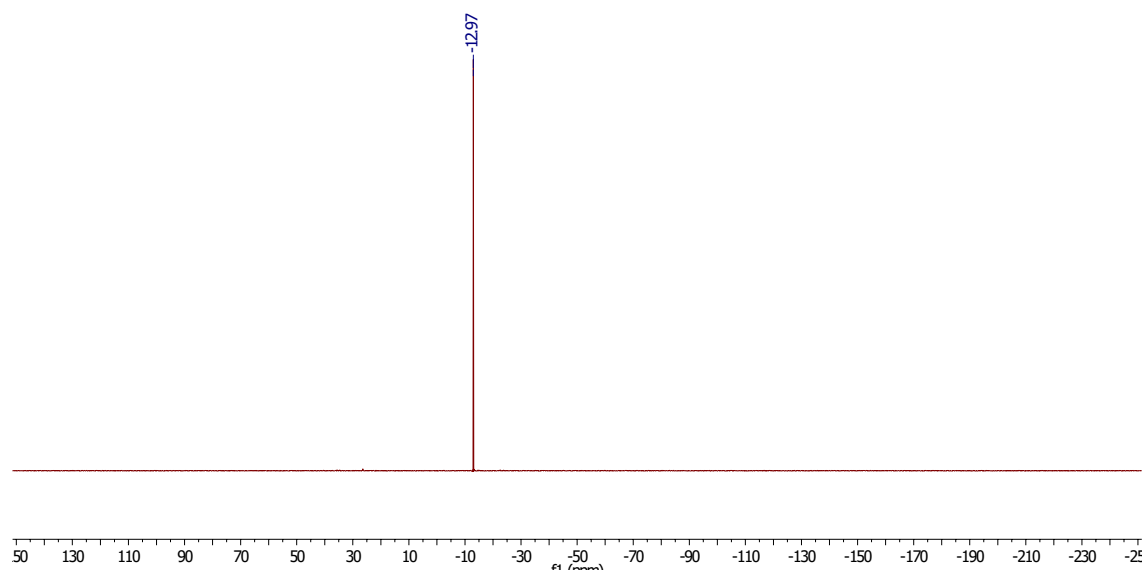


Figure S2.20. $^{31}\text{P}\{^1\text{H}\}$ (202 MHz, 22°C, CD_2Cl_2) NMR spectrum of **L5** in CD_2Cl_2 .

RAJ-03-122-C3H.1.fid
tBuPNAC
PROTON CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 14

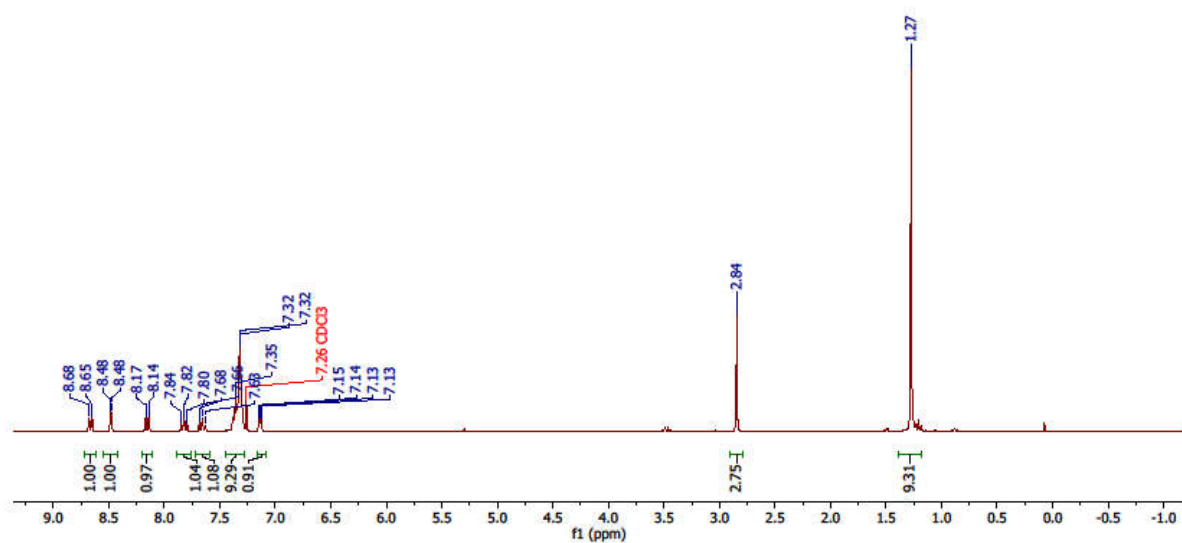


Figure S2.21. ^1H NMR (300 MHz, 22°C) spectrum of **L6** in CDCl_3 .

RAJ-03-122-C3P.1.fid
tBuPNAC
P31CPD CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 14

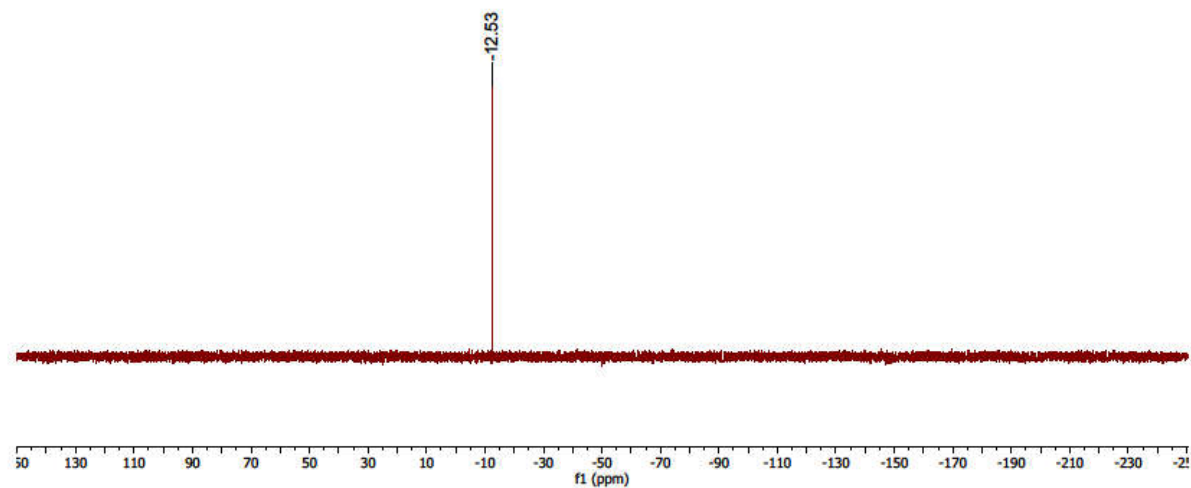


Figure S2.22. ^{31}P NMR (121 MHz, 22°C) spectrum of **L6** in CDCl_3 .

RAJ-04-016-A3H.2.fid
2nd time made starting material 6 bromo phen
PROTON CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 35

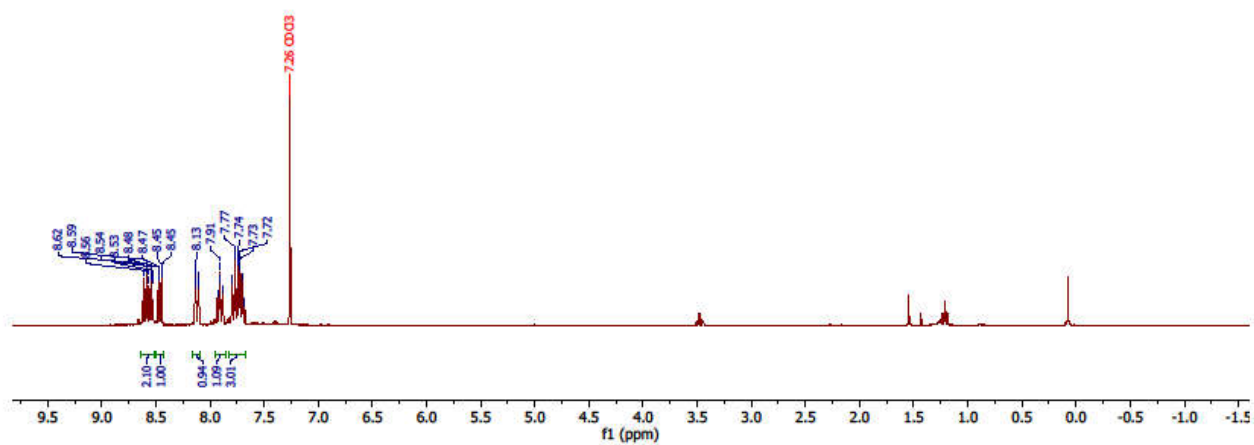


Figure S2.23. ^1H NMR (300 MHz, 22°C) spectrum of **6-Br** in CDCl_3 .

RAJ-04-063-A3H1.fid
6chlorophenanthridine
PROTON CDCl3 (C:\Bruker\TOPSPIN1.3) Herbert 40

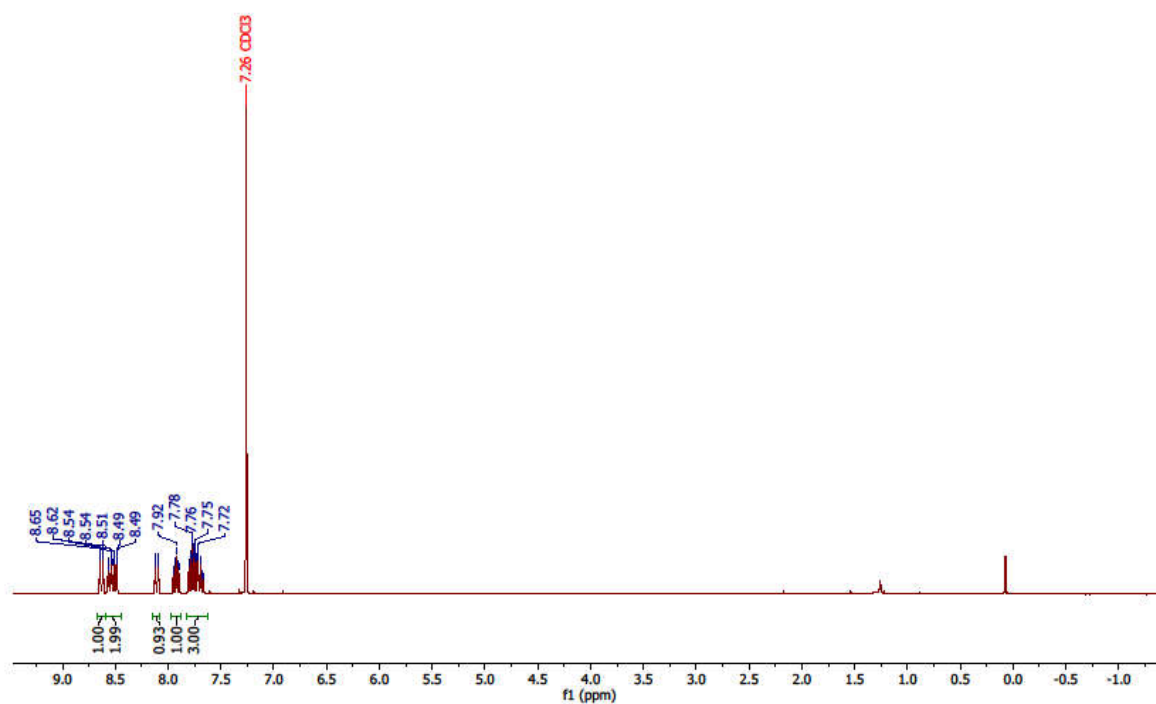


Figure S2.24. ^1H NMR (300 MHz, 22°C) spectrum of **6-Cl** in CDCl_3 .

RAJ-04-017-D3Hwide.1.fid
CN ligand in CD3CN starting mat
PROTON CD3CN (C:\Bruker\TOPSPIN1.3) Herbert 37

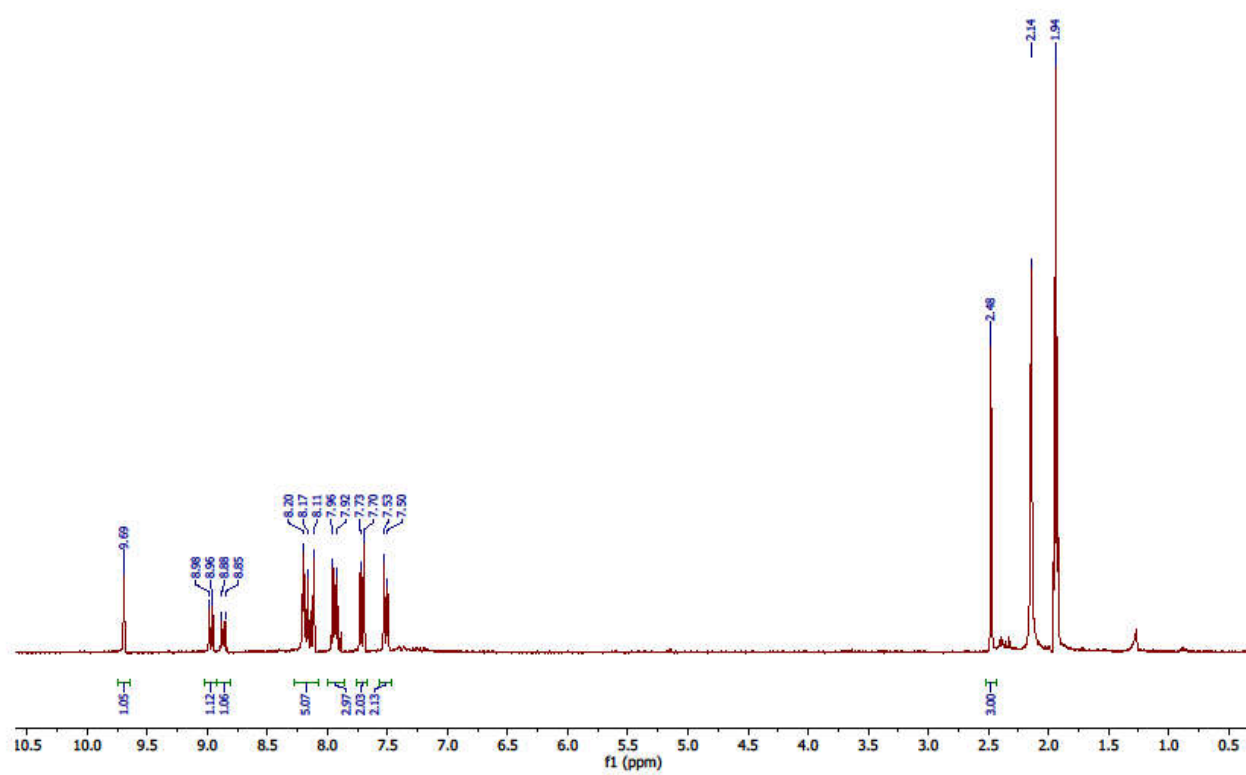


Figure S2.25. ^1H NMR (300 MHz, 22°C) spectrum of **L8.HBr** in CDCl_3 .

RAJ-03-189-D3H.1.fid
after work whole reaction wash with et2o
PROTON CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 11

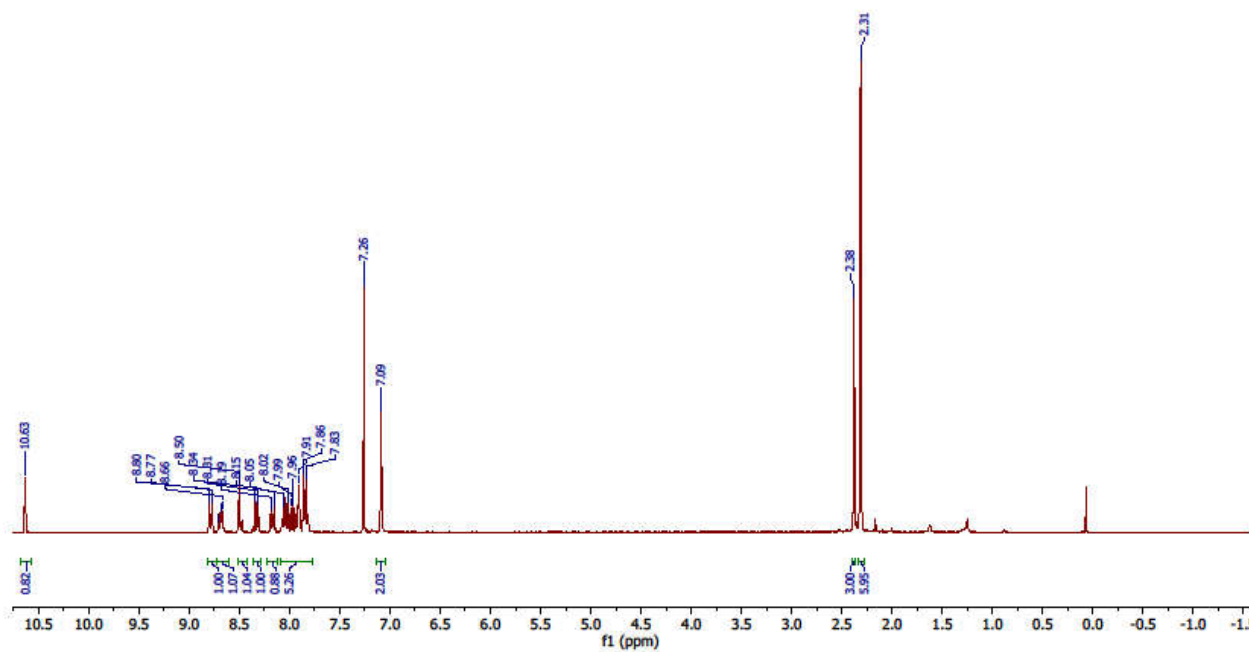


Figure S2.26. ^1H NMR (300 MHz, 22°C) spectrum of **L7.HBr** in CDCl_3 .

RAJ-04-079-N3H.1.fid
Mesityl CN chloride ligand
PROTON DMSO {C:\Bruker\TOPSPIN1.3} Herbert 18

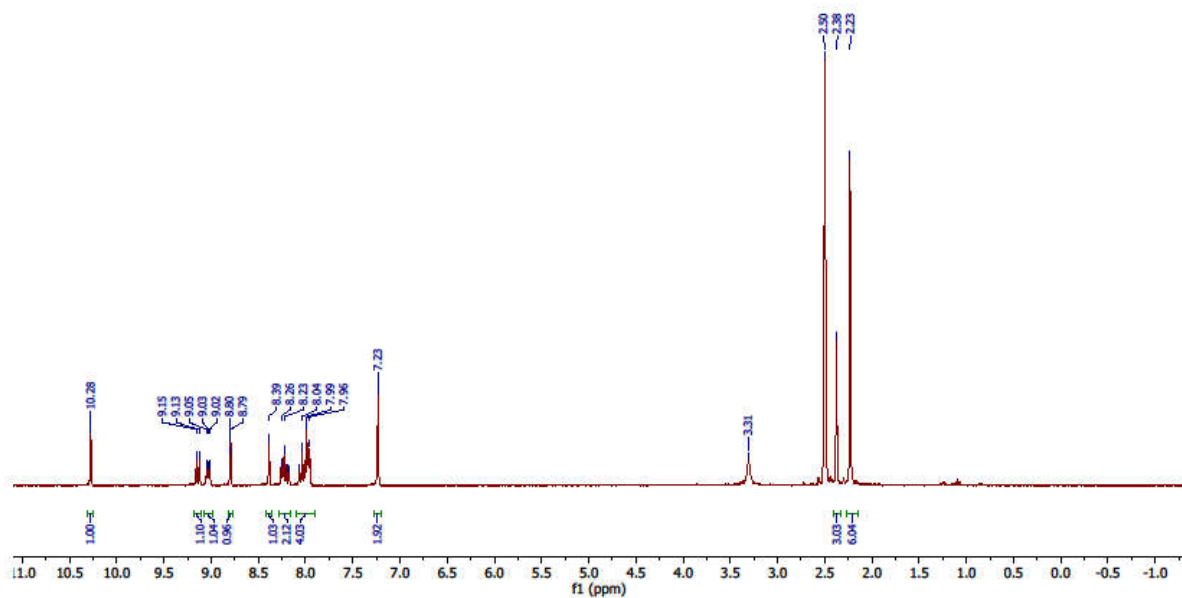


Figure S2.28. ^1H NMR (300 MHz, 22°C) spectrum of **L7.HCl** in CDCl_3 .

RAJ-04-079-DSH.2.fid
chloro methyl imidazolium lidand nmr check
PROTON CDCl3 C:\ Herbert 1

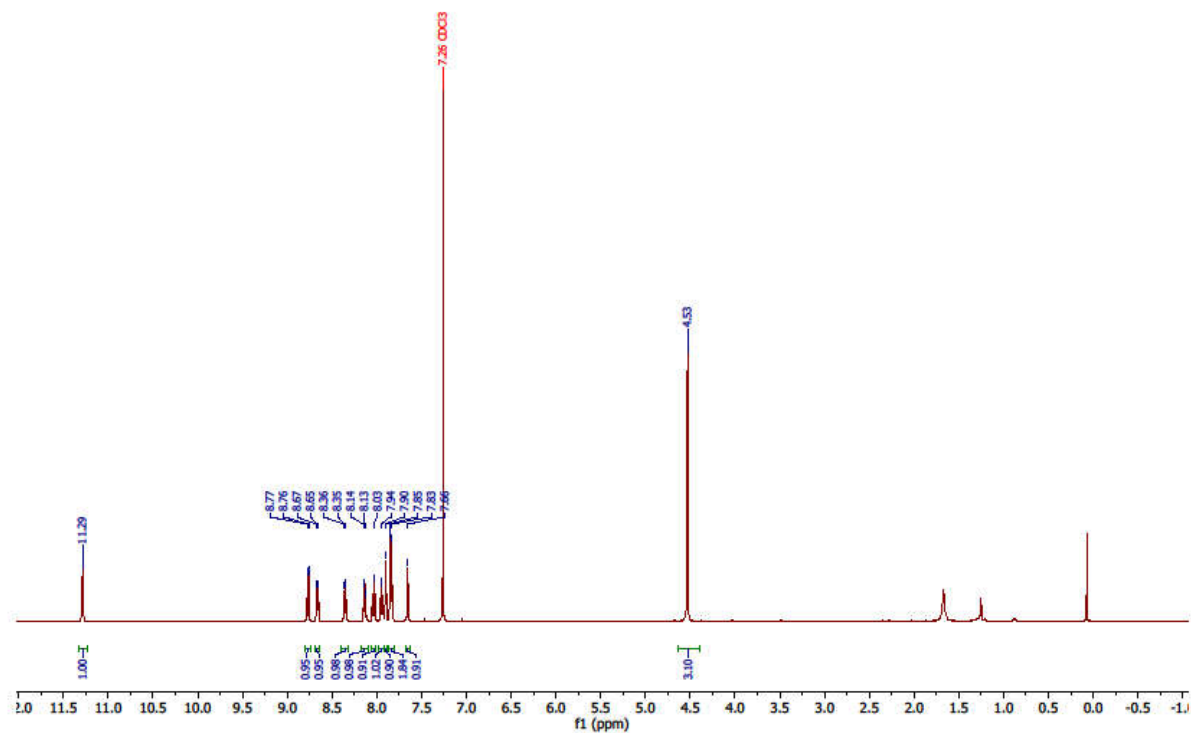


Figure S2.29. ^1H NMR (300 MHz, 22°C) spectrum of **L9.HCl** in CDCl_3 .

RJO-01-034-A3H.1.fid
Methyl-Phenanthridine-Imidazolium
PROTON CD2Cl2 {C:\Bruker\TOPSPIN1.3} Herbert 5

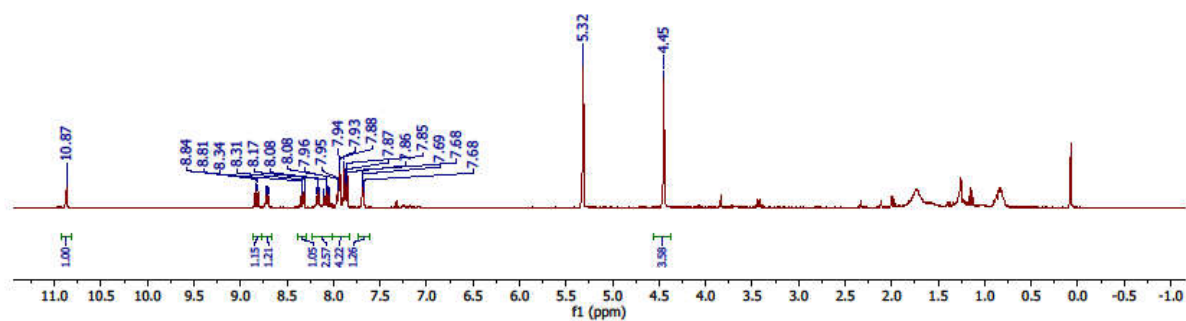


Figure S2.30. ^1H NMR (300 MHz, 22°C) spectrum of **L9.HBr** in CD_2Cl_2 .

RAJ-04-027-B3H.2.fid
imidazole of 6bromophen
PROTON CDCl3 (C:\Bruker\TOPSPIN1.3) Herbert 28

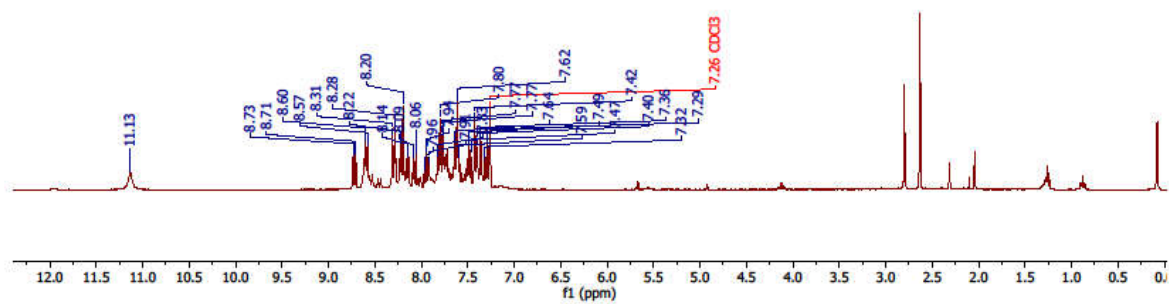


Figure S2.31. ^1H NMR (300 MHz, 22°C) spectrum of 6-imidazolephenanthridine in CDCl_3 .

RAJ-04-30-A3H.1.fid
 NCN ligand,insoluble solid,insoluble in dcm ch3cn,nmr in dmsd
 PROTON DMSO {C:\Bruker\TOPSPIN1.3} Herbert 37

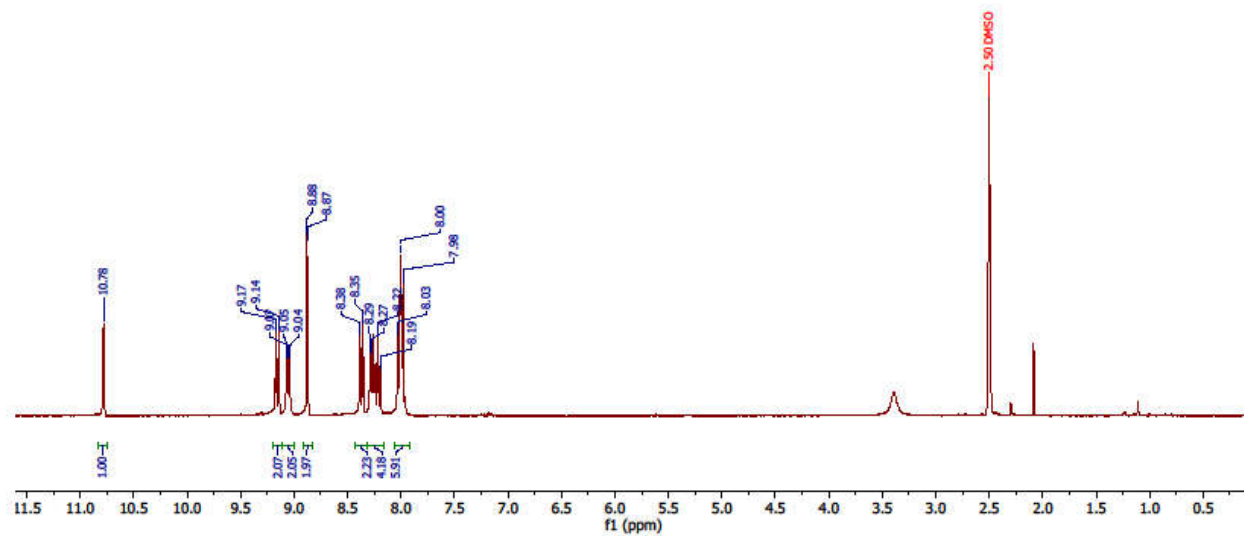


Figure S2.32. ^1H NMR (300 MHz, 22°C) spectrum of **L10.HBr** in CDCl_3 .

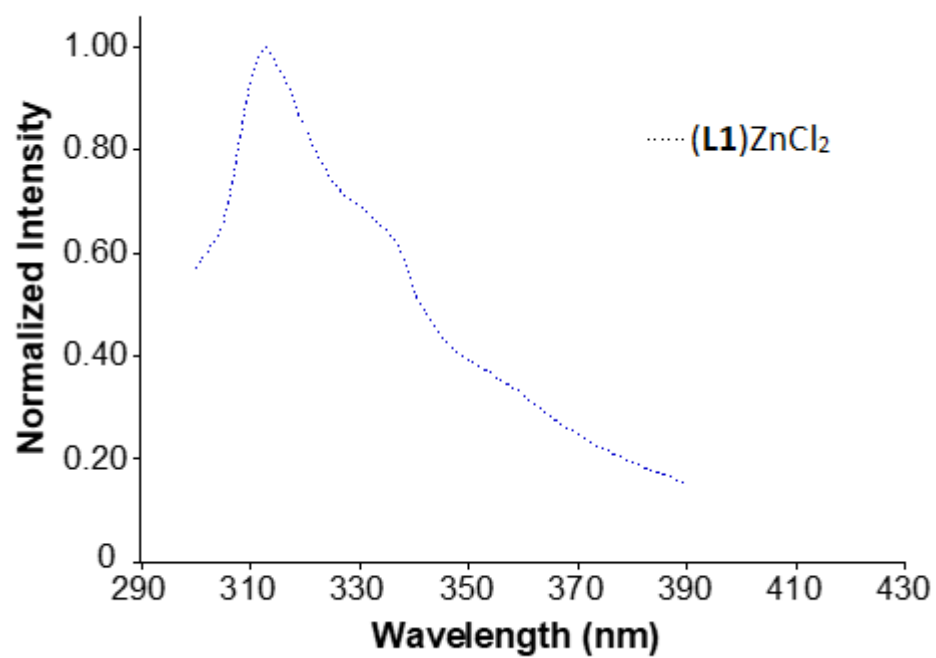


Figure S1.33. Excitation spectra in CH₂Cl₂ for **(L1)ZnCl₂** ([**(L1)ZnCl₂**] = 1 x 10⁻⁴ M, λ = 400 nm, 2 nm slit width).

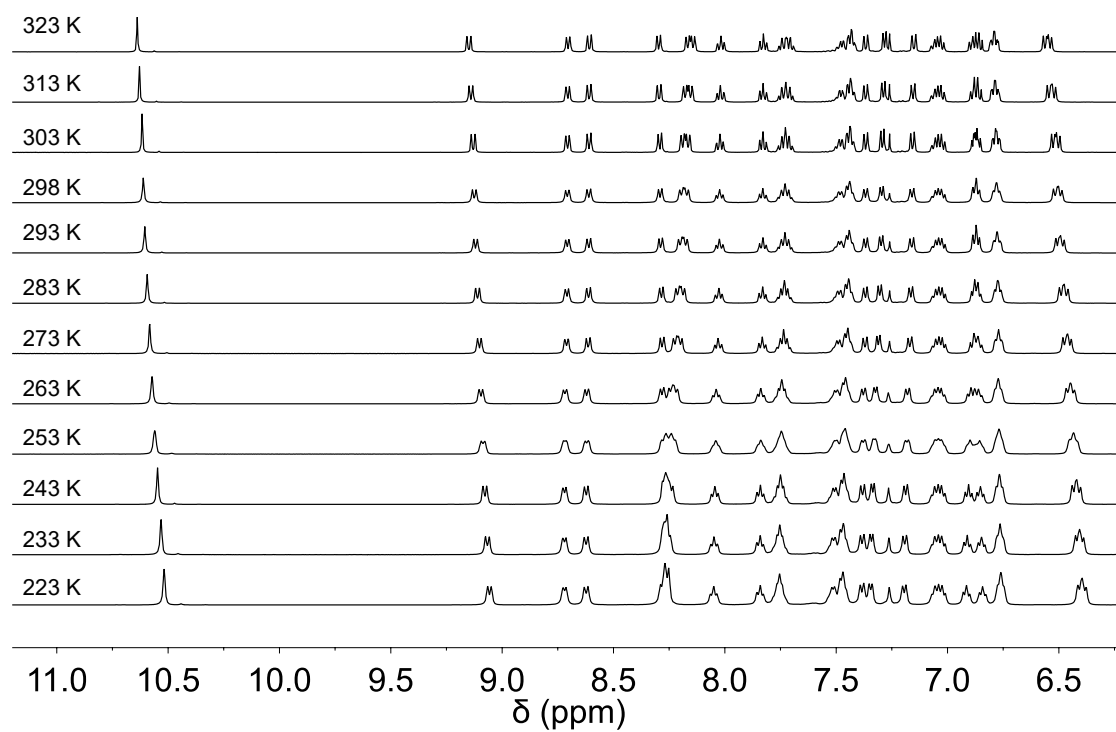


Figure S1.34. Variable temperature (223-323 K) ¹H NMR spectra (aromatic region) of (L1)Ni(Cl)(1-naphthyl) in CDCl₃.

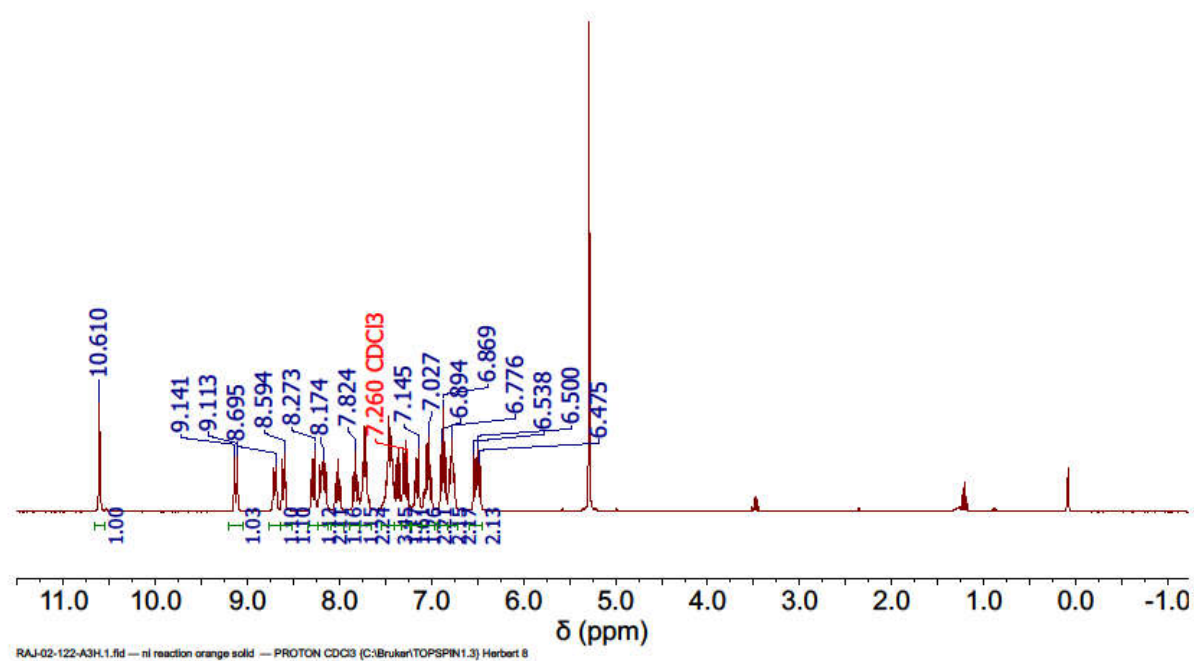


Figure S1.35. ¹H NMR (300 MHz, 22°C) spectrum of (L1)Ni(Cl)(1-naphthyl) in CDCl₃.

RAJ-02-116-A3H.1.fid
zn complex nmr
PROTON CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 18

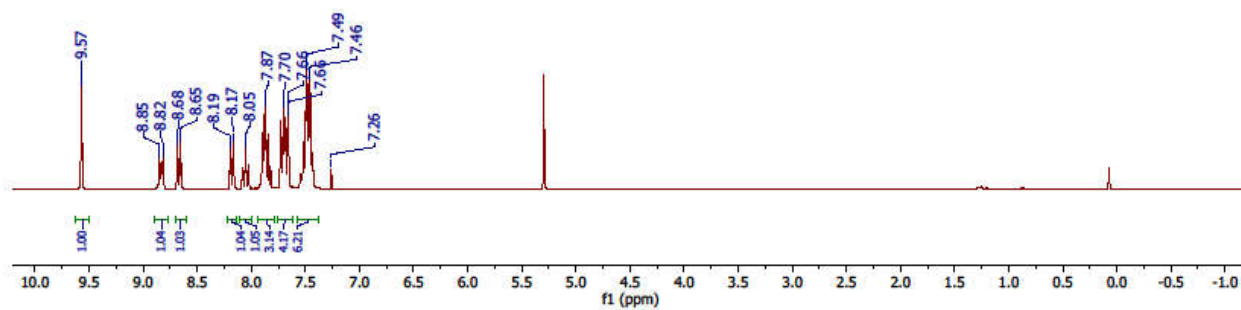


Figure S1.36. ^1H NMR (300 MHz, 22°C) spectrum of $(\text{L1})\text{ZnCl}_2$ in CDCl_3 .

Chapter 3:

RAJ-03-142-D5H1.1.fid
PNCuCl Parent
PROTON CDCl3 C:\ Herbert 1

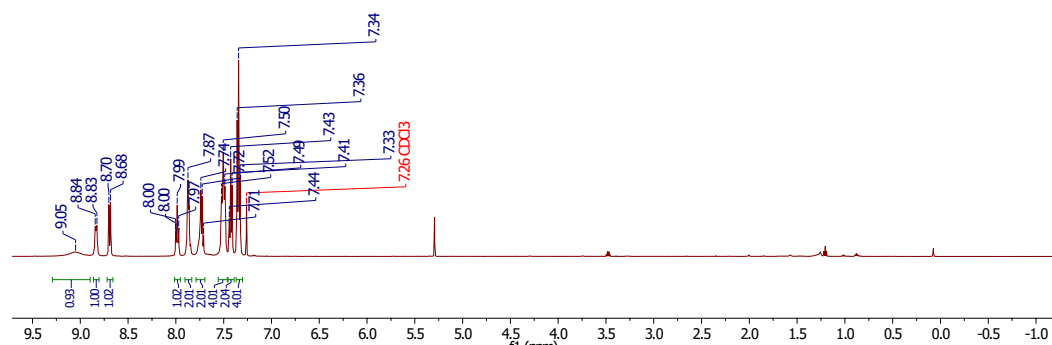


Figure S3.1. ^1H NMR (500 MHz, 22 °C) spectrum of $(\text{L1})_2\text{Cu}_2\text{Cl}_2$ in CDCl_3 .

RAJ-03-142-D5C.1.fid
PNCuCl Parent
C13CPD CDCl3 C:\\ Herbert 1

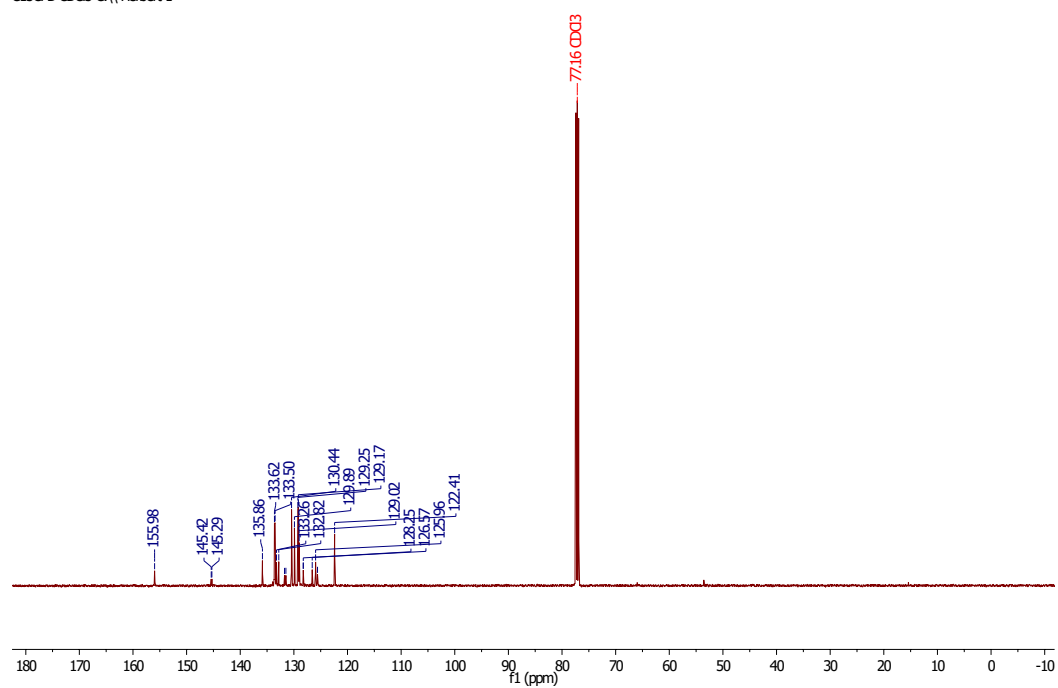


Figure S3.2. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, 22°C) spectrum of $(\text{L1})_2\text{Cu}_2\text{Cl}_2$ in CDCl_3 .

RAJ-03-142-D5P1.fid
PNCuCl Parent
P31CPD CDCl3 C:\\ Herbert 1

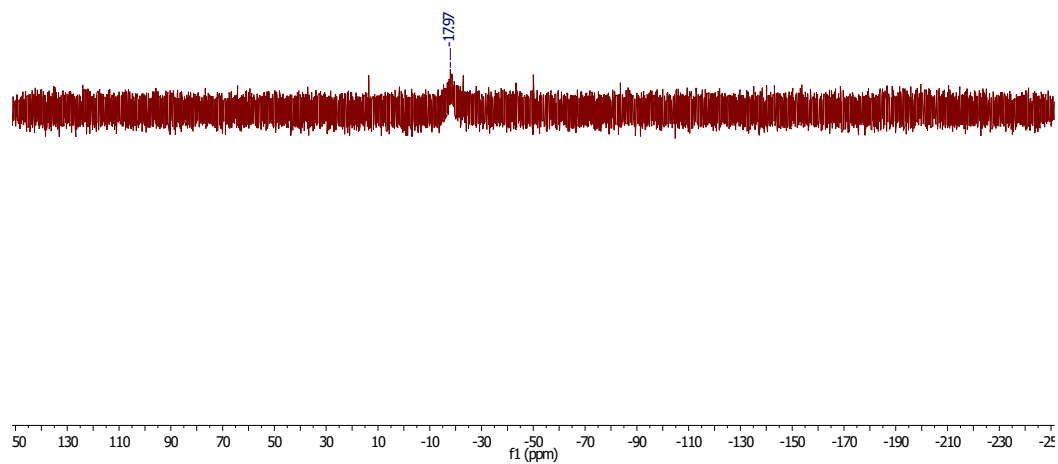


Figure S3.3. $^{31}\text{P}\{^1\text{H}\}$ NMR (202 MHz, 22°C) spectrum of $(\text{L1})_2\text{Cu}_2\text{Cl}_2$ in CDCl_3 .

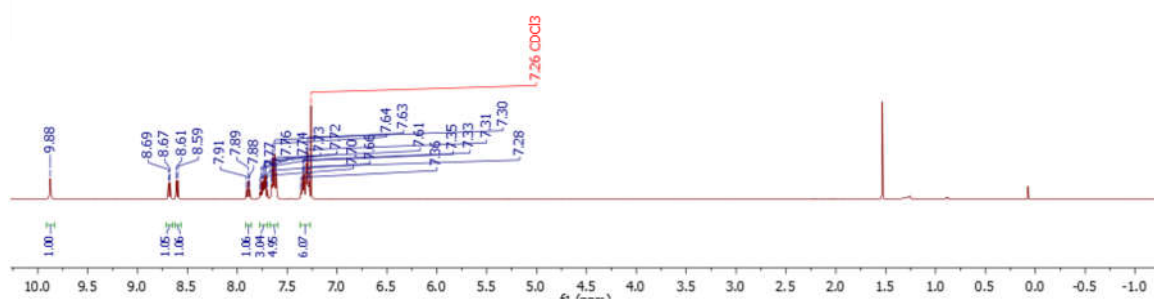


Figure S3.4. ^1H NMR (500 MHz, 22°C) spectrum of $(\text{L1})_2\text{Cu}_2\text{I}_2$ in CDCl_3 .

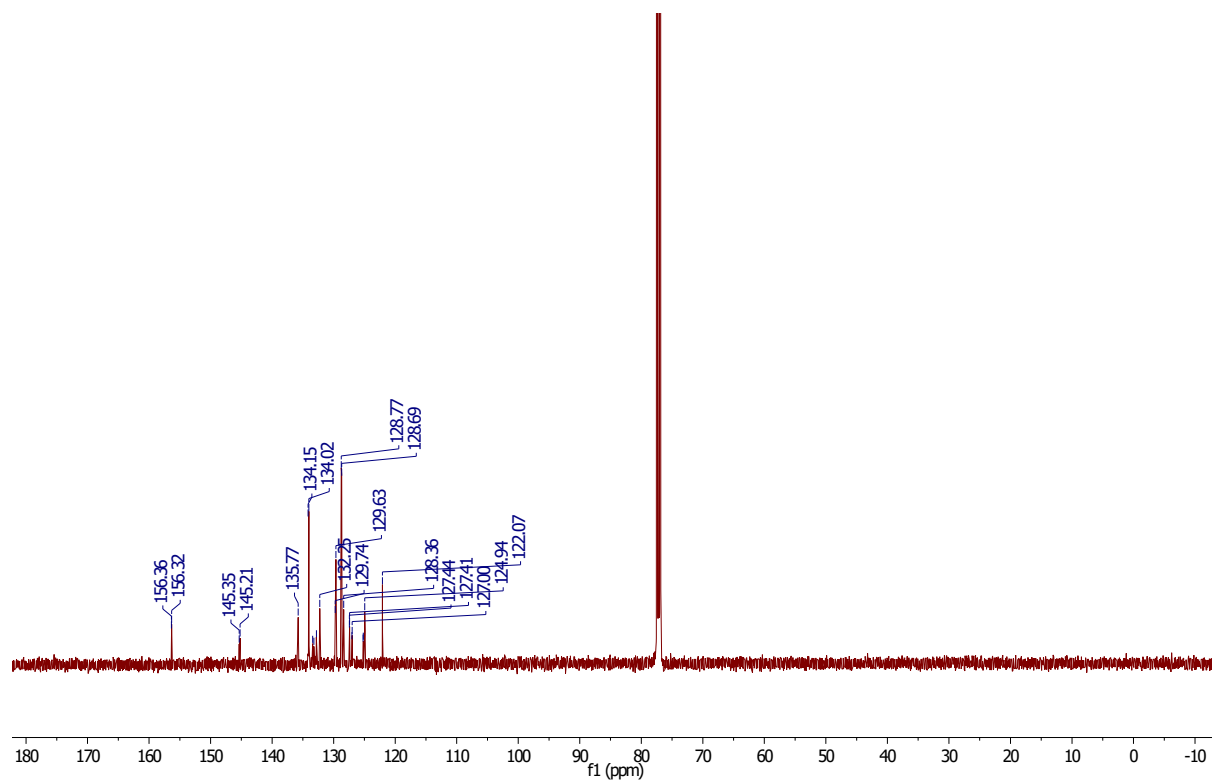


Figure S3.5. $^{13}\text{C}\{^1\text{H}\}$ (126 MHz, 22°C) NMR spectrum of $(\text{L1})_2\text{Cu}_2\text{I}_2$ in CDCl_3 .

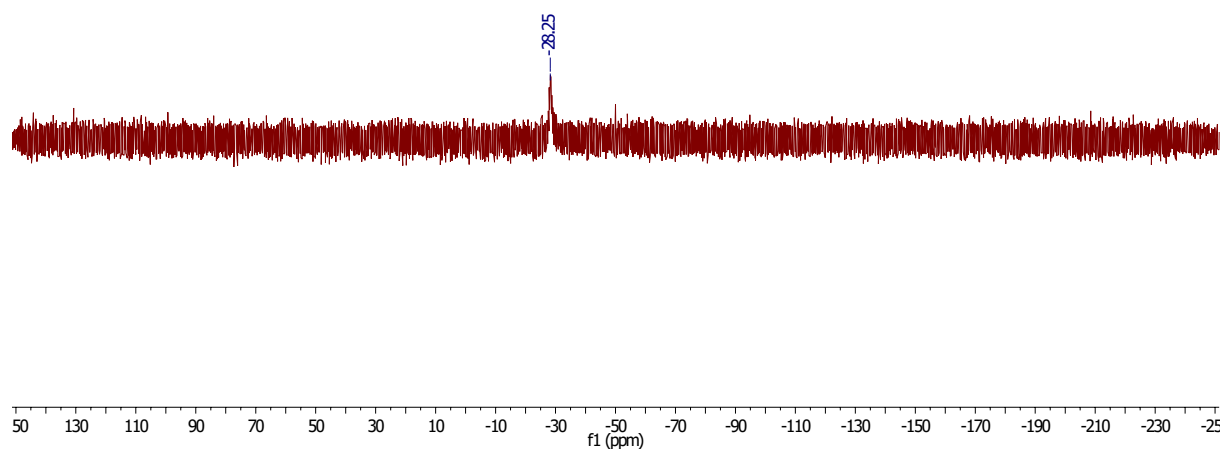


Figure S3.6. $^{31}\text{P}\{^1\text{H}\}$ (202 MHz, 22°C) NMR spectrum of **(L1)₂Cu₂I₂** in CDCl_3 .

RAJ-03-051-C3H.1.fid
MePNCuCl
PROTON1128 CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 51

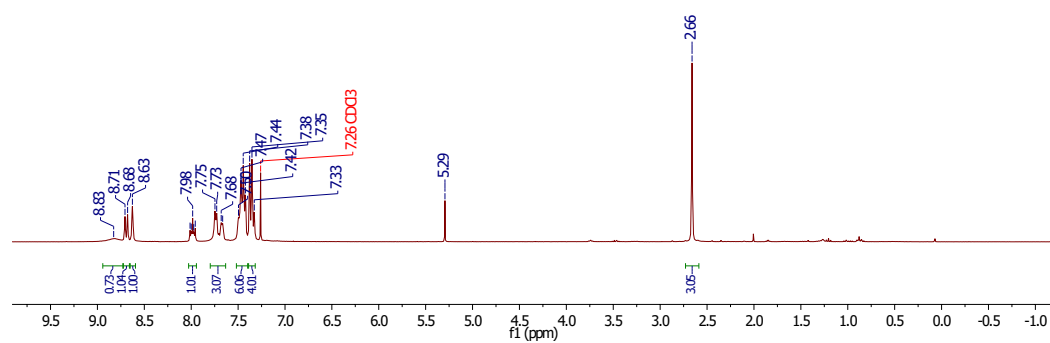


Figure S3.7. ^1H NMR (300 MHz, 22°C) spectrum of $(\text{L2})_2\text{Cu}_2\text{Cl}_2$ in CDCl_3 .

RAJ-03-142-B5C.1.fid
MePNCuCl
C13CPD CDCl3 C:\\ Herbert 1

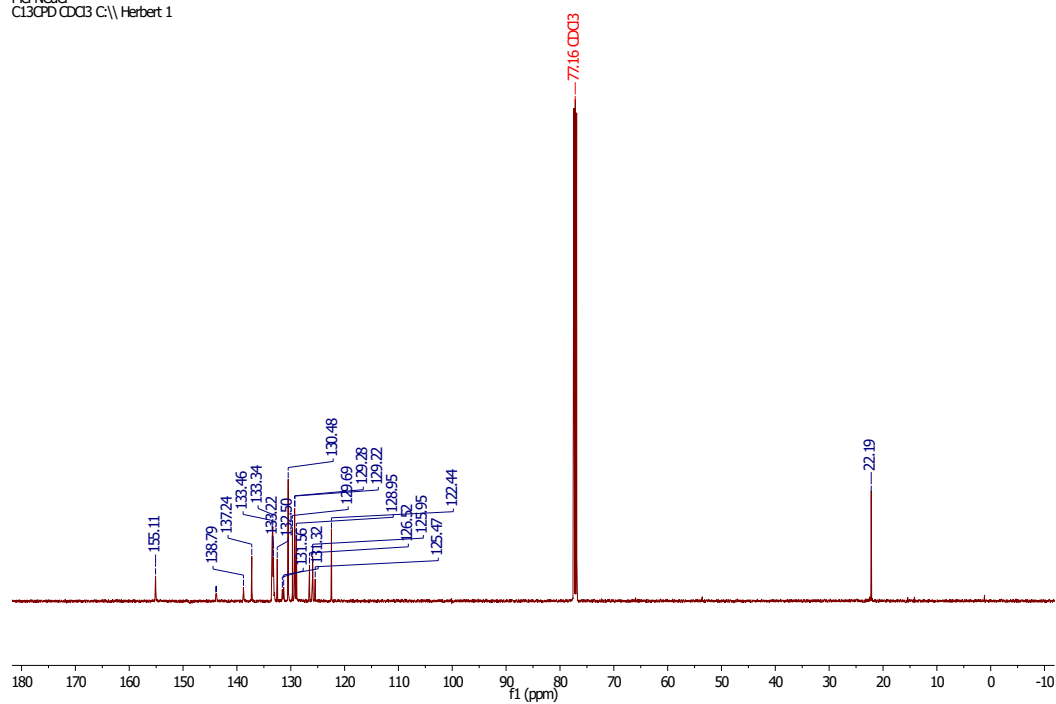


Figure S3.8. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, 22°C) spectrum of $(\text{L}2)_2\text{Cu}_2\text{Cl}_2$ in CDCl_3 .

RAJ-03-142-B3P1.fid
MePNCuCl
P31CPD CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 29

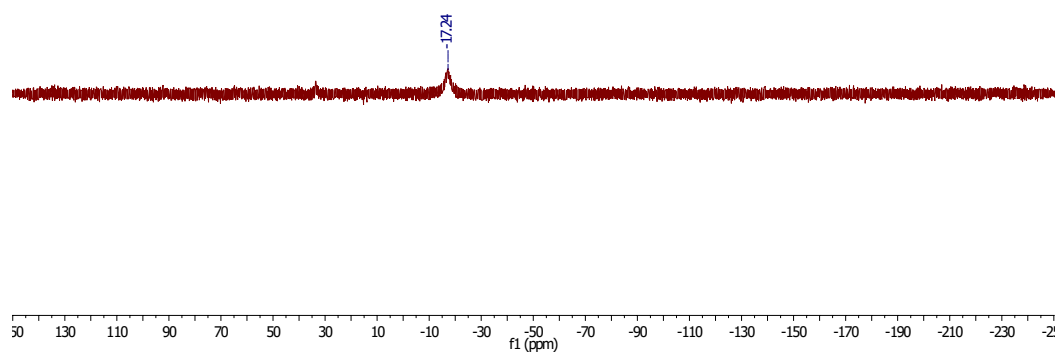


Figure S3.9. $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, 22°C) NMR spectrum of $(\text{L}2)_2\text{Cu}_2\text{Cl}_2$ in CDCl_3 .

RAJ-03-142-ESH.1.fid
MePNCuBr
PROTON CDCl3 C:\ Herbert 1

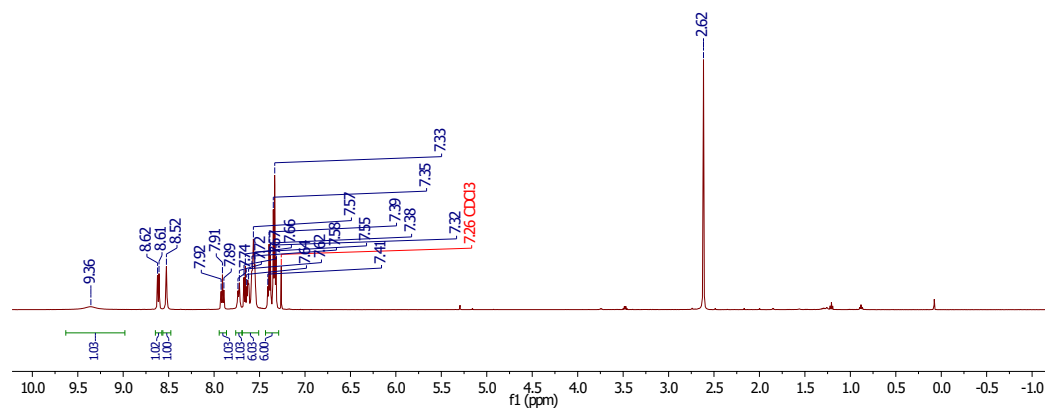


Figure S3.10. ^1H NMR(500 MHz, 22°C) spectrum of $(\text{L2})_2\text{Cu}_2\text{Br}_2$ in CDCl_3 .

RAJ-03-142-ESC.1.fid
MePNCuBr
C13CPD CDCl3 C:\\ Herbert 2

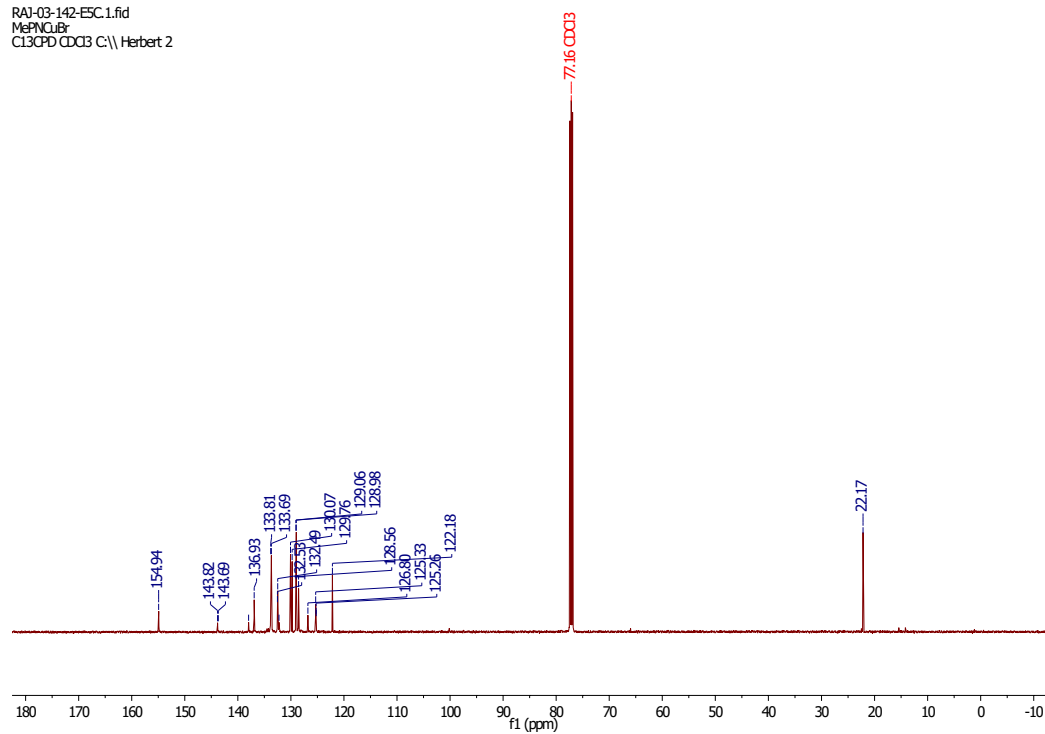


Figure S3.11. $^{13}\text{C}\{^1\text{H}\}$ (126 MHz, 22°C) NMR spectrum of $(\text{L2})_2\text{Cu}_2\text{Br}_2$ in CDCl_3 .

RAJ-03-051-B3P1.fid
MePNCuBr
P31CPD CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert.55

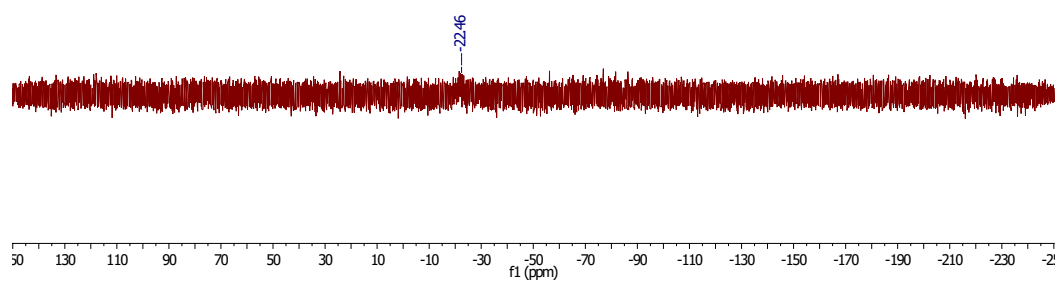


Figure S3.12. $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, 22°C) NMR spectrum of **(L2)₂Cu₂Br₂** in CDCl_3 .

[illegible]

55

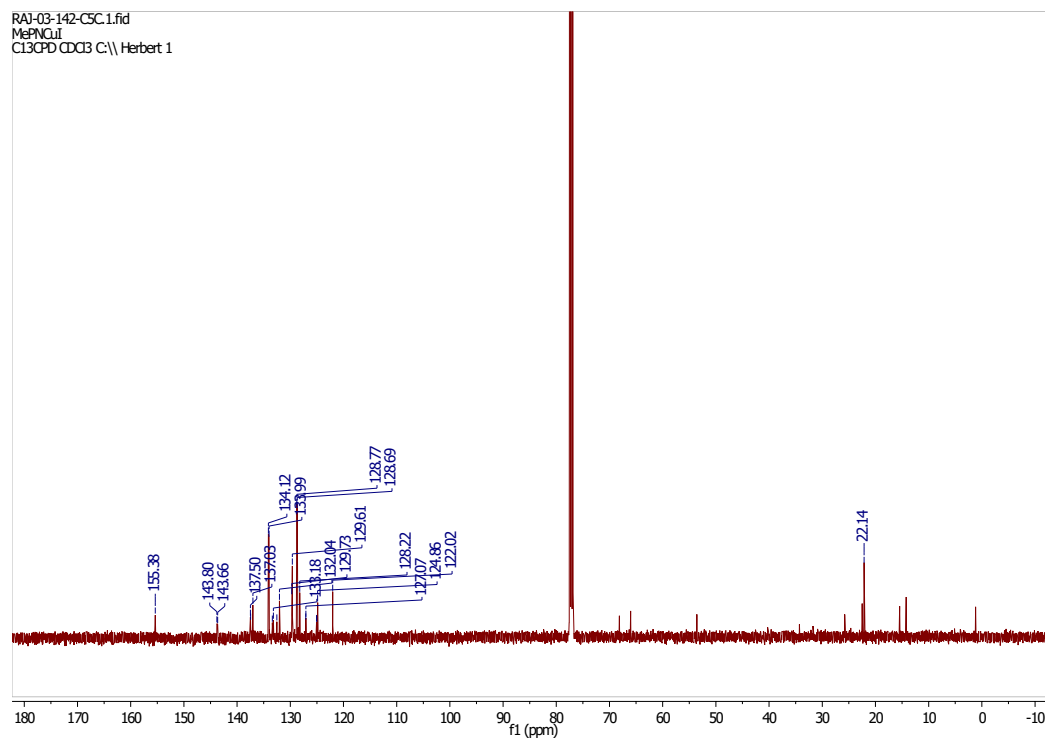


Figure S3.14. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, 22°C) spectrum of $(\text{L2})_2\text{Cu}_2\text{I}_2$ in CDCl_3 .

RAJ-03-142-GSP2.fid
MePNCuI
P31CPD CDCl3 C:\\ Herbert 1

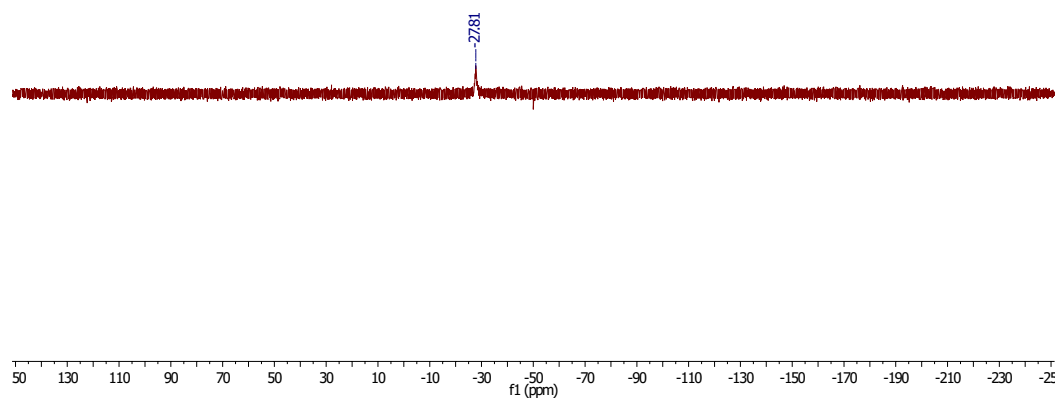


Figure S3.15. $^{31}\text{P}\{^1\text{H}\}$ (202 MHz, 22°C) NMR spectrum of **(L2)₂Cu₂I₂** in CDCl_3 .

RAI-03-062-C3H.1.fid
P1NguihCuCl
PROTON128 CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 49

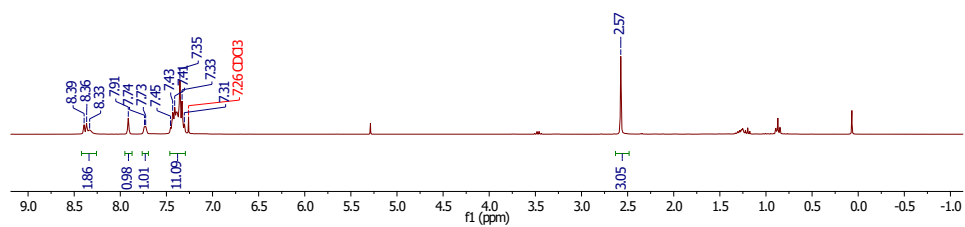


Figure S3.16. ^1H NMR (300 MHz, 22°C) spectrum of $(\text{L3})_2\text{Cu}_2\text{Cl}_2$ in CDCl_3 .

RAJ-03-062-C3C.1.fid
PNquinCuD
C13CPD CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 49

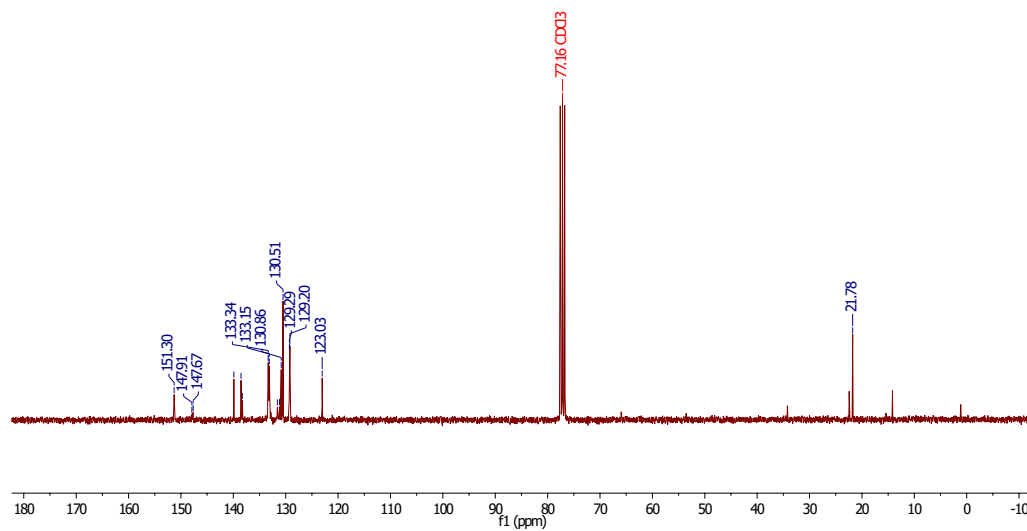


Figure S3.17. $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, 22°C) spectrum of $(\text{L3})_2\text{Cu}_2\text{Cl}_2$ in CDCl_3 .

RAJ-03-062-CSP1.fid
P1NquinCuCl
P31CPD CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 49

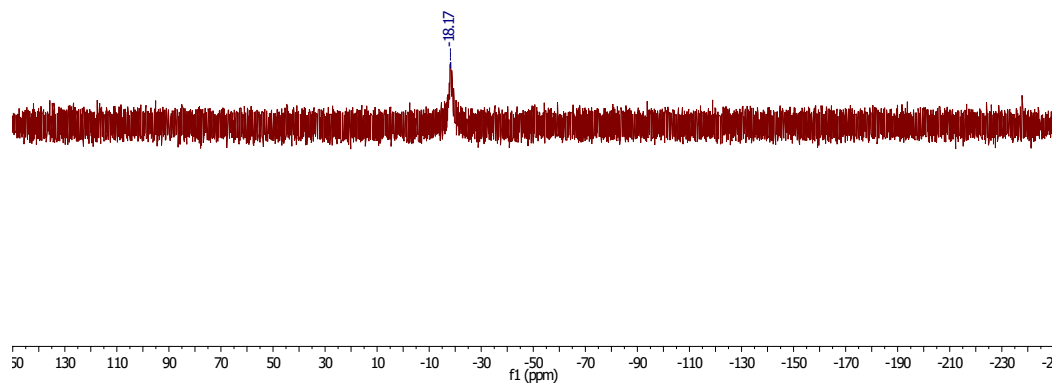


Figure S3.18. $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, 22°C) NMR spectrum of **(L3) $_2$ Cu $_2$ Cl $_2$** in CDCl_3 .

RAJ-03-141-C3H.1.fid
QuindineCubr
PROTON128 CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 52

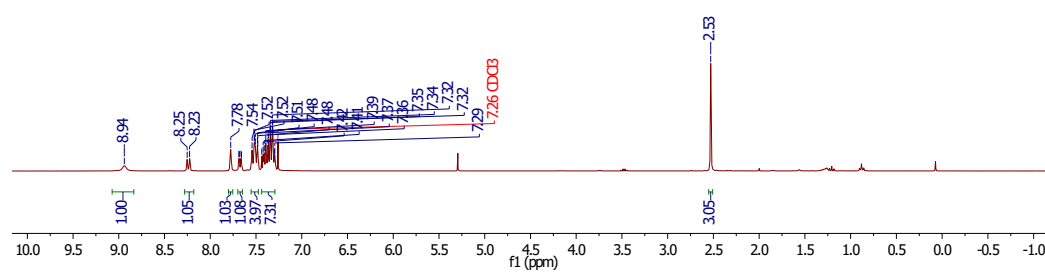


Figure S3.19. ^1H NMR (300 MHz, 22°C) spectrum of $(\text{L3})_2\text{Cu}_2\text{Br}_2$ in CDCl_3 .

RAJ-03-141-C3C.1.fid
QuindineCubr
C13CPD CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert.52

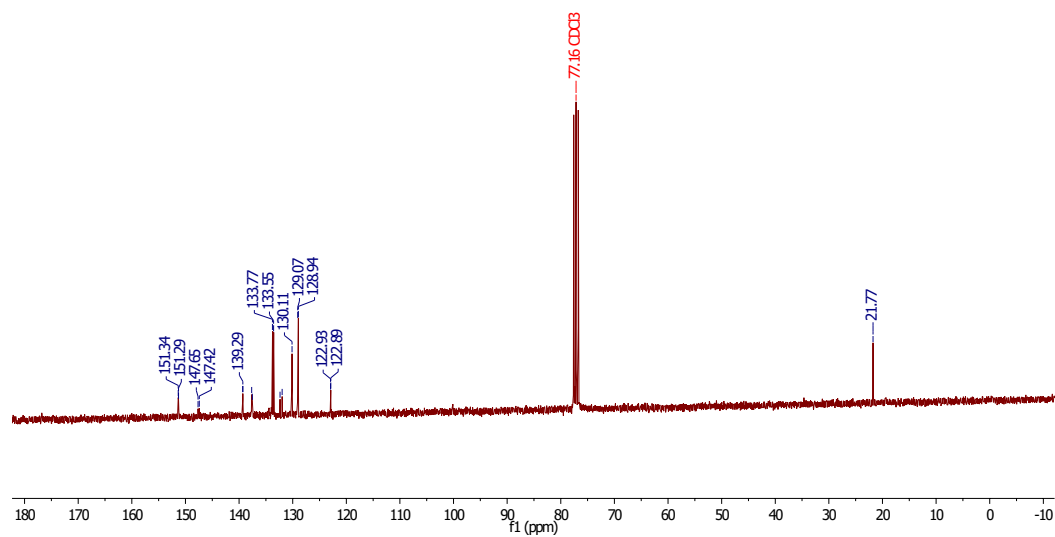


Figure S3.20. $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, 22°C) spectrum of $(\text{L3})_2\text{Cu}_2\text{Br}_2$ in CDCl_3 .

RAJ-03-062-D3P1.fid
P1NquinCUBr
P31CPD CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 50

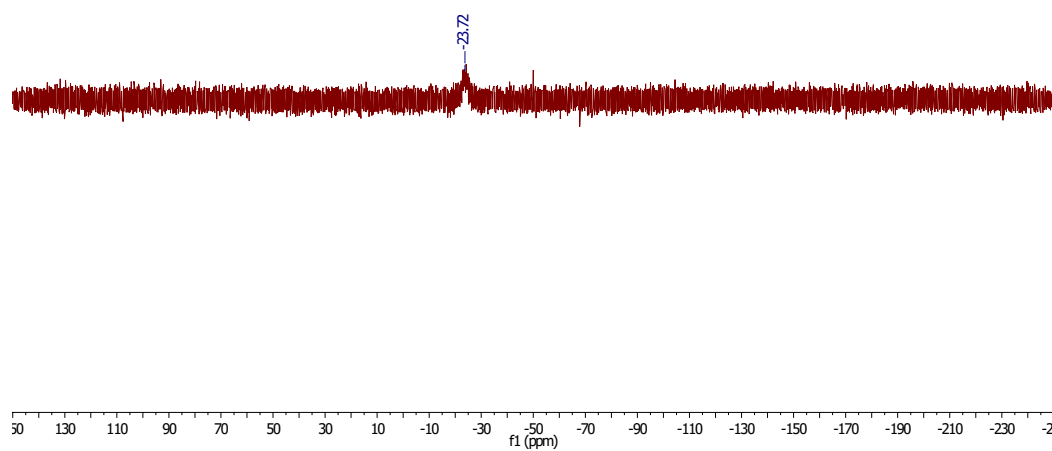


Figure S3.21. $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, 22°C) NMR spectrum of **(L3)₂Cu₂Br₂** in CDCl_3 .

RAJ-03-191-ASH2.fid
MeguinCui
PROTON CDCl3 C:\\ Herbert 1

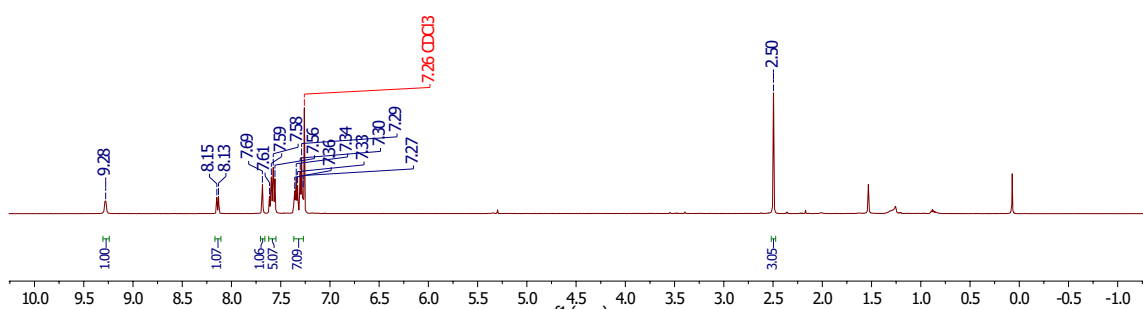


Figure S3.22 ^1H NMR (500 MHz, 22°C) spectrum of $(\text{L3})_2\text{Cu}_2\text{I}_2$ in CDCl_3 .

RAJ-03-191-ASC.1.fid
MequinCui
C13CPD CDCl3 C:\\ Herbert 1

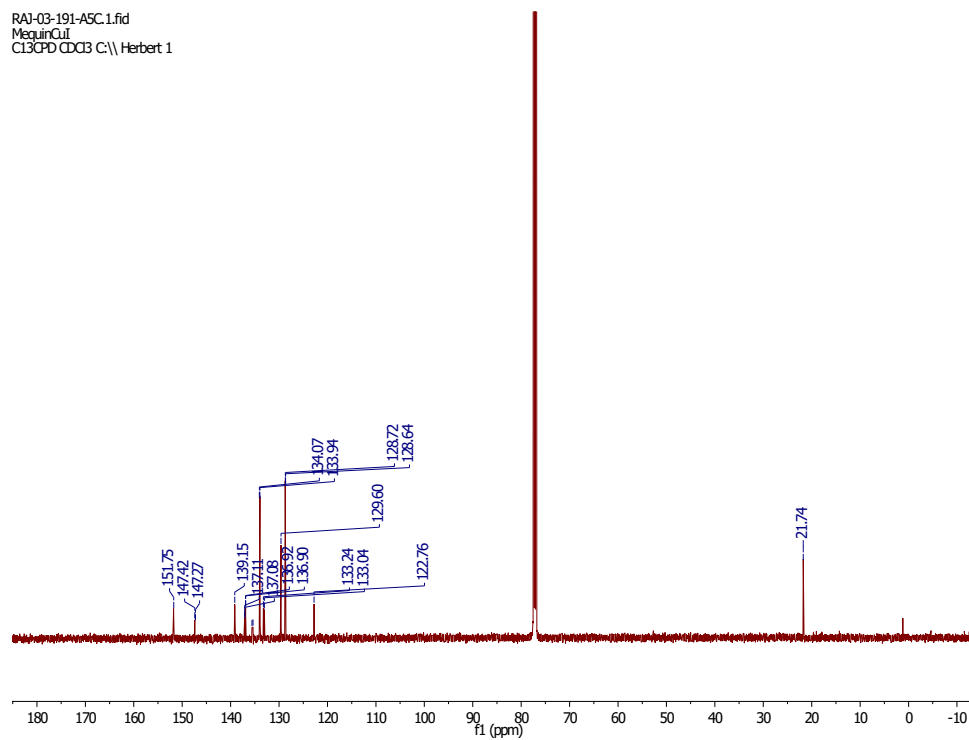


Figure S3.23. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, 22°C) spectrum of $(\text{L3})_2\text{Cu}_2\text{I}_2$ in CDCl_3 .

RAI-03-062-E3P1.fid
P31CPD CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 51

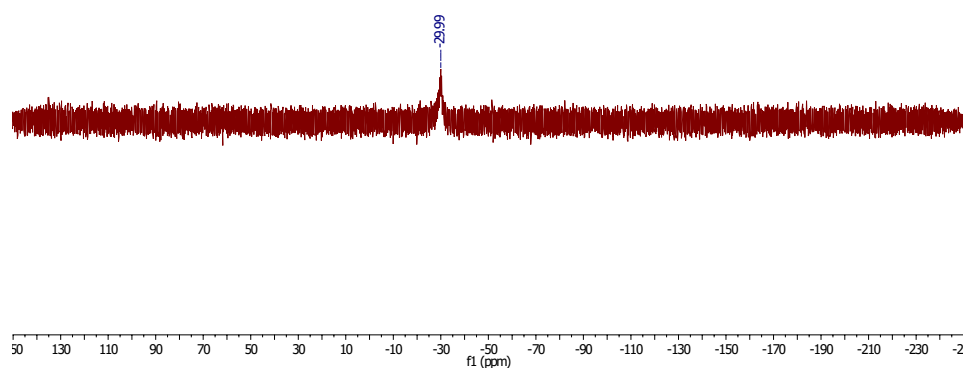


Figure S3.24. $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, 22°C) NMR spectrum of $(\text{L3})_2\text{Cu}_2\text{I}_2$ in CDCl_3 .

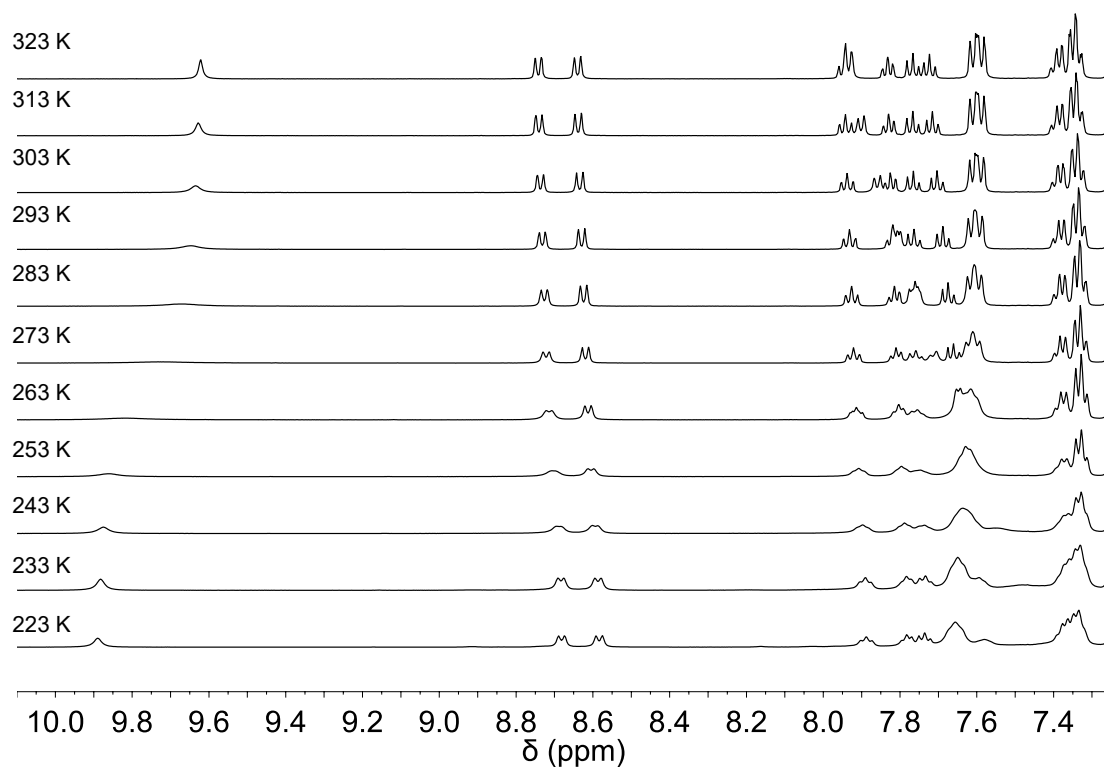


Figure S3.25. Variable temperature (223-323 K) ^1H NMR spectra (aromatic region) of $(\text{L1})_2\text{Cu}_2\text{Br}_2$ in CDCl_3 .

Computational Details:

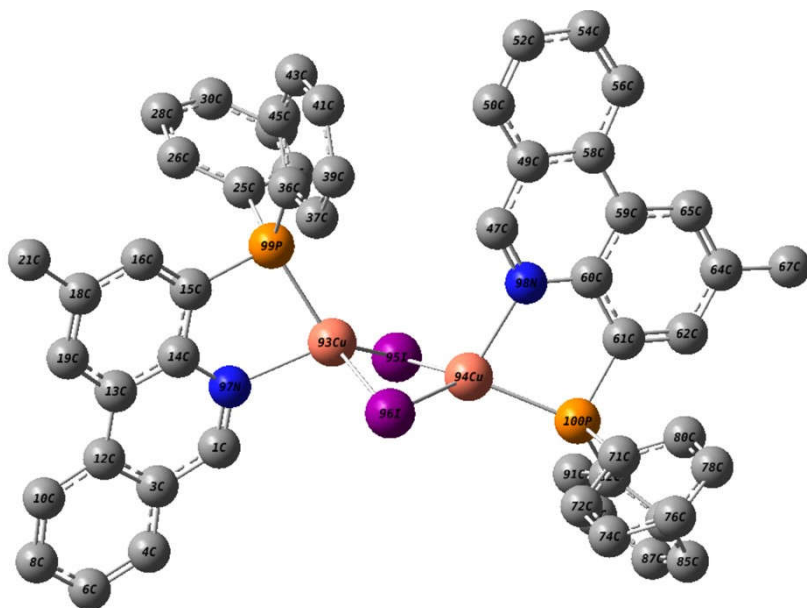


Figure S3.26. Optimized (S₀) structure of (L2)₂Cu₂I₂ and atom assignments.

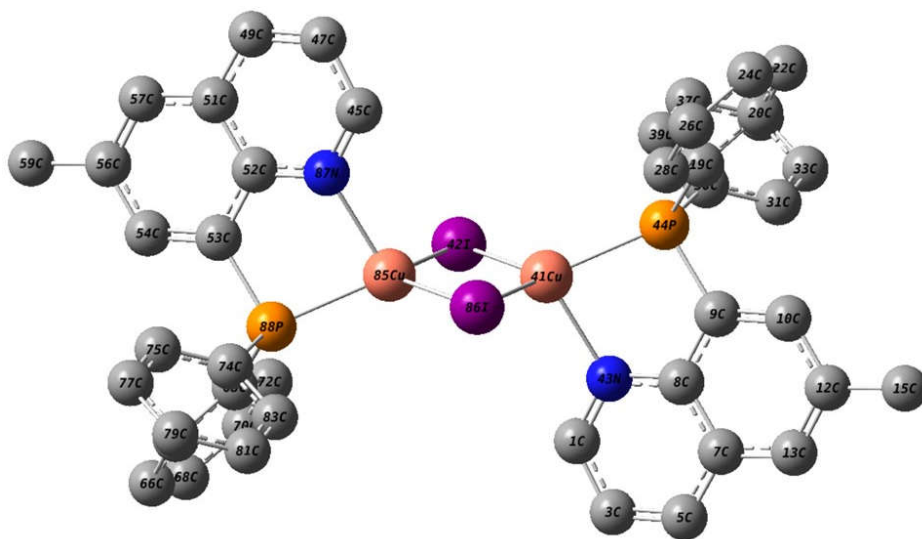


Figure S3.27. Optimized structure (S₀) of (L3)₂Cu₂I₂ and atom assignments.

Table S1. Selected bond distances and angles of optimized structures of (L3)₂Cu₂I₂.

Bond (Å)	Crystal	Calculated (DFT)
43N-41Cu	2.108	2.180
44P-41Cu	2.237	2.299
41Cu-42I	2.607	2.670
41Cu-86I	2.626	2.710
42I-86I	4.469	4.590
41Cu-85Cu	2.723	2.806
42I-85Cu	2.626	2.710
86I-85Cu	2.607	2.670
85Cu-88P	2.236	2.299
85Cu-87N	2.108	2.180
Angle (°)	Crystal	Calculated (DFT)
43N-41Cu-44P	86.0	83.2
42I-41Cu-86I	117.3	117.1
41Cu-42I-85Cu	62.7	62.9
41Cu-86I-85Cu	62.7	62.9
42I-85Cu-86I	117.3	117.1
87N-85Cu-88P	86.0	83.2
44P-41Cu-42I	123.6	121.1
44P-41Cu-86I	111.7	114.9
43N-41Cu-42I	101.5	108.2
43N-41Cu-86I	110.0	104.4
88P-85Cu-42I	111.7	114.9
88P-85Cu-86I	123.6	121.1
87N-85Cu-42I	110.0	104.4
87N-85Cu-86I	101.5	108.2

Table S2. Selected bond distances and angles of optimized structures of **(L2)₂Cu₂I₂**.

Bond (Å)	Crystal	Calculated (DFT)
97N-93Cu	2.100	2.171
99P-93Cu	2.229	2.292
93Cu-95I	2.571	2.665
93Cu-96I	2.685	2.717
95I-96I	4.358	4.524
93Cu-94Cu	2.708	2.735
95I-94Cu	2.654	2.731
96I-94Cu	2.594	2.674
94Cu-100P	2.237	2.297
94Cu-98N	2.101	2.182
Angle (°)	Crystal	Calculated (DFT)
97N-93Cu-99P	84.8	82.7
95I-93Cu-96I	112.0	114.4
93Cu-95I-94Cu	62.4	61.0
93Cu-96I-94Cu	61.7	61.0
95I-94Cu-96I	112.3	113.7
98N-94Cu-100P	85.2	82.5
99P-93Cu-95I	128.5	124.1
99P-93Cu-96I	114.6	115.3
97N-93Cu-95I	110.6	108.7
97N-93Cu-96I	96.4	103.6
100P-94Cu-95I	114.5	114.6
100P-94Cu-96I	122.3	121.6
98N-94Cu-95I	106.8	109.1
98N-94Cu-96I	111.5	110.2

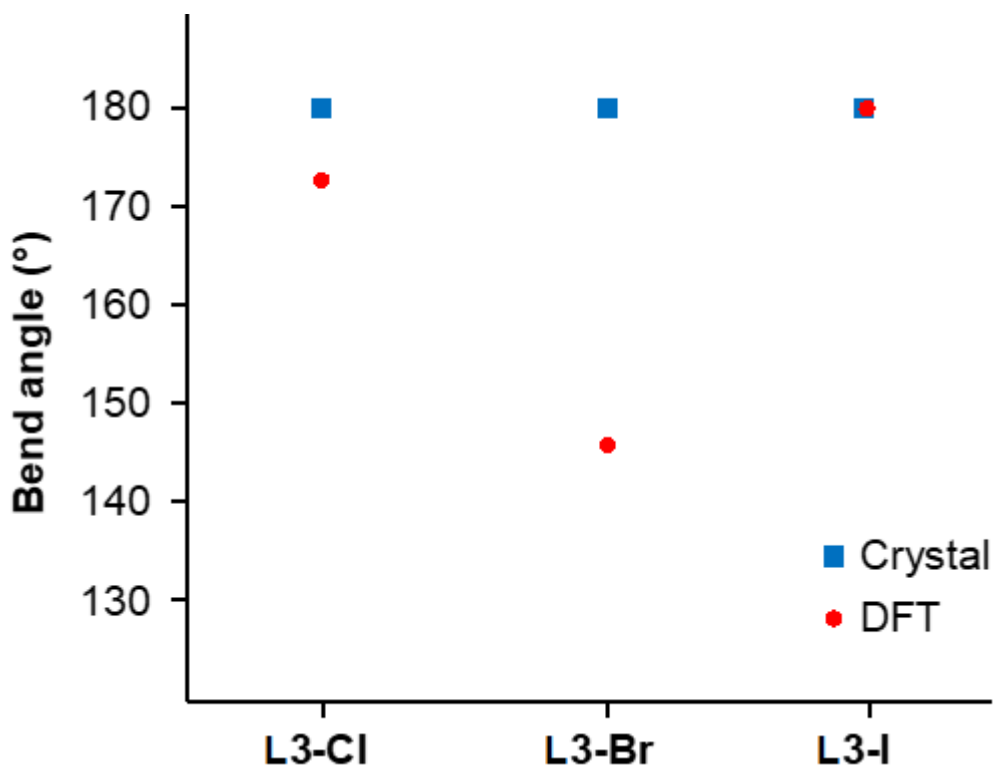


Figure S3.28. Calculated and experimental bend angles for $(\text{L3})_2\text{Cu}_2\text{X}_2$. Bend angles is defined as the dihedral angle between the two X-Cu-X triangles in $(\text{L3})_2\text{Cu}_2\text{X}_2$.

Table S3. Atomic contributions (Mulliken) to the HOMO of $(\text{L2})_2\text{Cu}_2\text{I}_2$ and $(\text{L3})_2\text{Cu}_2\text{I}_2$ (S_0).

	Cu1	Cu2	I1	I2	P1	P2	Ph1	Ph2	N-hc1 ^a	N-hc2 ^a
2-I	20.14	33.19	12.82	11.56	0.66	11.08	0.63	4.94	1.78	3.19
3-I	24.57	24.57	15.11	15.11	6.31	6.31	3.21	3.21	0.80	0.80

^a N-hc = N-heterocyclic ligand backbone (i.e. Me-phen for **2-I** or Me-quin for **3-I**).

Table S4. Atomic contributions (Mulliken) to the LUMO (TD-DFT) of **(L2)₂Cu₂I₂** (S₁ state) and **(L3)₂Cu₂I₂** (S₂ state) from the first allowed excited state.

	Cu1	Cu2	I1	I2	P1	P2	Ph1	Ph2	N-hc1^a	N-hc2^a
2-I (S ₁)	1.45	0.89	0.02	0.13	0.53	0.13	2.88	0.13	89.33	4.50
3-I (S ₂)	0.54	0.54	0.09	0.09	0.98	0.98	2.44	2.44	45.94	45.97

^a N-hc = N-heterocyclic ligand backbone (i.e. Me-phen for **2-I** or Me-quin for **3-I**).

Table S5. Atomic contributions (Mulliken) to the LUMO+1 (TD-DFT) of **(L2)₂Cu₂I₂** (S₁ state) and **(L3)₂Cu₂I₂** (S₂ state) from the first allowed excited state.

	Cu1	Cu2	I1	I2	P1	P2	Ph1	Ph2	N-hc1^a	N-hc2^a
2-I (S ₁)	4.87	3.94	0.19	0.01	0.27	0.62	2.88	0.13	0.13	83.09
3-I (S ₂)	2.52	2.52	0.12	0.12	0.76	0.76	2.26	2.26	44.35	44.32

^a N-hc = N-heterocyclic ligand backbone (i.e. Me-Phenan for **2-I** or Me-quin for **3-I**).

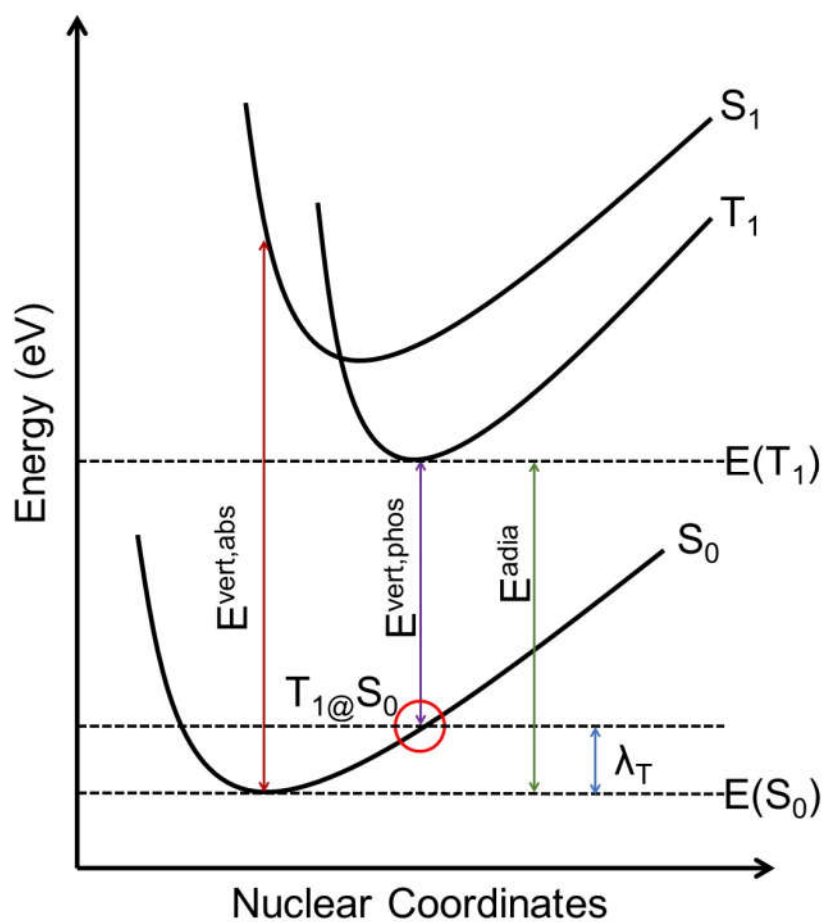


Figure S3.29. Diagram illustrating parameters calculated using protocol described in experimental section.

Table S6. Calculated photophysical parameters for (L2)₂Cu₂I₂ and (L3)₂Cu₂I₂

E (eV)	2-I	3-I
E _{adia}	1.909	1.801
E _{vert-abs}	3.166	3.218
E _{vert-phos}	1.519	1.410
λ _T	0.390	0.391

Table S7. TD-DFT calculated electronic transitions for **(L2)₂Cu₂I₂** along with their corresponding excitation energies and oscillator strengths (FWHM: 3000 cm⁻¹; σ : 0.2).

Transition	λ (nm)	Osc. Strength	Major contributions
S1	391.6	0.0040	H-3->L+1 (17%), HOMO->L+1 (69%)
S2	376.3	0.0007	H-2->LUMO (22%), H-1->LUMO (43%), HOMO->LUMO (12%)
S3	359.5	0.0147	H-3->LUMO (10%), HOMO->LUMO (69%)
S4	345.3	0.0048	H-3->L+1 (37%), H-1->L+1 (20%), HOMO->L+1 (17%)
S5	329.7	0.0075	H-2->LUMO (10%), H-2->L+1 (36%), H-1->L+1 (34%)
T1	816.2	0.0000	HOMO(A)->LUMO(A) (38%), HOMO(B)->LUMO(B) (38%)

Table S8. TD-DFT calculated electronic transitions for **(L3)₂Cu₂I₂** along with their corresponding excitation energies and oscillator strengths (FWHM: 3000 cm⁻¹; σ : 0.2).

Transition	λ (nm)	Osc. Strength	Major contributions
S1	385.3	0.0000	H-3->L+1 (29%), HOMO->LUMO (51%)
S2	384.8	0.0123	H-3->LUMO (31%), HOMO->L+1 (49%)
S3	362.0	0.0000	H-3->L+1 (11%), H-2->LUMO (14%), H-1->LUMO (24%), HOMO->LUMO (38%)
S4	361.4	0.0064	H-3->LUMO (11%), H-2->L+1 (13%), H-1->L+1 (23%), HOMO->L+1 (40%)
S5	327.1	0.0000	H-2->LUMO (50%), H-1->LUMO (38%)
T1	879.1	0.0000	HOMO(A)->LUMO(A) (38%), HOMO(B)->LUMO(B) (38%)

Table S9. Structural comparison between the S₀ and T₁ gas phase structures of (L2)₂Cu₂I₂.

(L2) ₂ Cu ₂ I ₂			
Structural Parameters	Gas phase		
Bond	S ₀	T ₁	ΔS ₀ -T ₁
97N-93Cu	2.1714	1.9877	0.1837
99P-93Cu	2.2921	2.2825	0.0096
93Cu-95I	2.6650	2.7372	-0.0722
93Cu-96I	2.7166	2.6253	0.0913
95I-96I	4.5243	4.2091	0.3152
93Cu-94Cu	2.7352	2.6918	0.0434
95I-94Cu	2.7305	2.6320	0.0985
96I-94Cu	2.6740	2.7989	-0.1249
94Cu-100P	2.2970	2.3293	-0.0323
94Cu-98N	2.1818	1.9877	0.1941
Angle	S ₀	T ₁	ΔS ₀ -T ₁
97N-93Cu-99P	82.692	85.708	-3.016
95I-93Cu-96I	114.426	103.407	11.018
93Cu-95I-94Cu	60.907	60.140	0.767
93Cu-96I-94Cu	60.977	59.404	1.573
95I-94Cu-96I	113.674	101.570	12.104
98N-94Cu-100P	82.518	83.988	-1.470
99P-93Cu-95I	124.056	115.532	8.524
99P-93Cu-96I	115.311	132.049	-16.739
97N-93Cu-95I	108.728	104.541	4.187
97N-93Cu-96I	103.603	111.252	-7.649
100P-94Cu-95I	114.590	102.517	12.073
100P-94Cu-96I	121.607	125.390	-3.783
98N-94Cu-95I	109.134	141.543	-32.409
98N-94Cu-96I	110.235	105.092	5.144

Table S10. Structural comparison between the S_0 and T_1 gas phase structures of $(L3)_2Cu_2I_2$.

$(L3)_2Cu_2I_2$			
Structural Parameters	Gas phase		
Bond	S_0	T_1	ΔS_0-T_1
43N-41Cu	2.1800	1.9883	0.1917
44P-41Cu	2.2992	2.3325	-0.0333
41Cu-42I	2.6696	2.7812	-0.1115
41Cu-86I	2.7103	2.6323	0.0781
42I-86I	4.5904	4.2082	0.3822
41Cu-85Cu	2.8061	2.7229	0.0832
42I-85Cu	2.7103	2.6369	0.0735
86I-85Cu	2.6696	2.7228	-0.0532
85Cu-88P	2.2992	2.2914	0.0078
85Cu-87N	2.1800	2.1230	0.0570
Angle	S_0	T_1	ΔS_0-T_1
43N-41Cu-44P	83.216	84.078	-0.862
42I-41Cu-86I	117.129	102.004	15.125
41Cu-42I-85Cu	62.871	60.269	2.603
41Cu-86I-85Cu	62.871	61.095	1.776
42I-85Cu-86I	117.129	103.460	13.668
87N-85Cu-88P	83.216	86.084	-2.868
44P-41Cu-42I	121.088	127.642	-6.554
44P-41Cu-86I	114.891	102.854	12.036
43N-41Cu-42I	108.211	104.845	3.366
43N-41Cu-86I	104.356	139.351	-34.995
88P-85Cu-42I	114.890	129.144	-14.254
88P-85Cu-86I	121.088	117.828	3.260
87N-85Cu-42I	104.356	111.393	-7.038
87N-85Cu-86I	108.211	105.232	2.979

Chapter 4:

RAJ-04-022-13H.2.fid
ParentPhenCuPF6
PROTON CDCl3 C:\\ Herbert.1

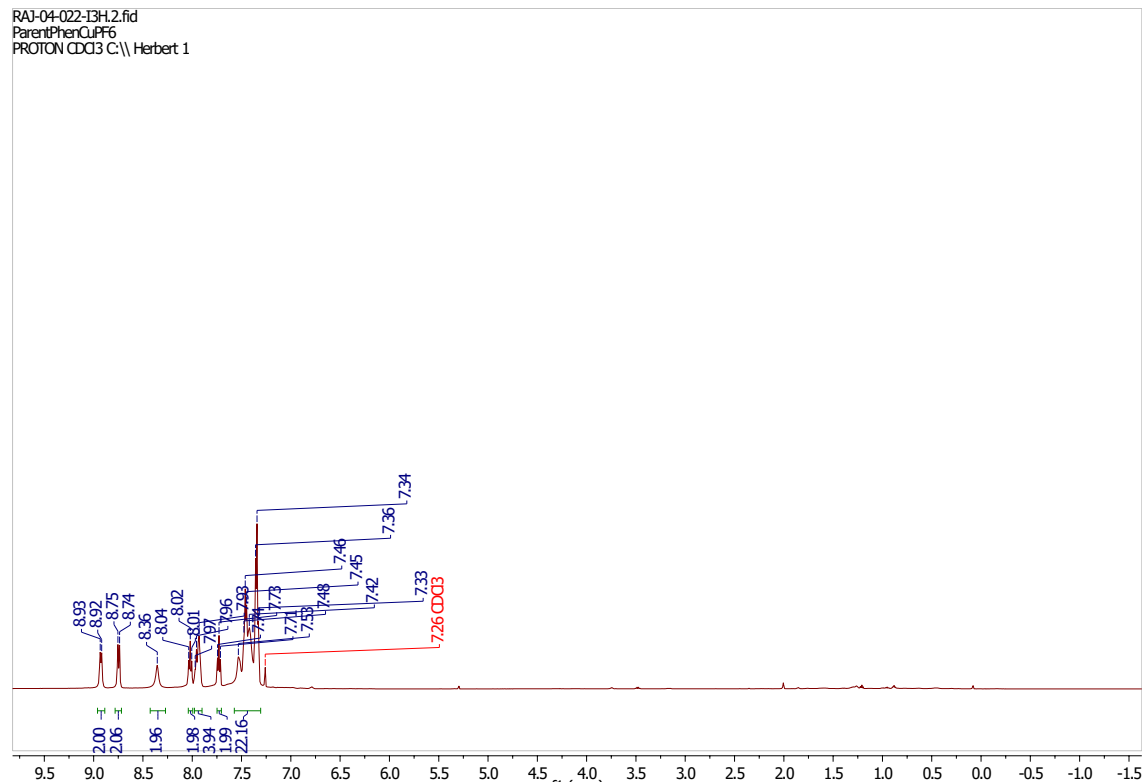


Figure S4.1. ^1H NMR (300 MHz, 22°C) spectrum of $(\text{L1})\text{CuPF}_6$ in CDCl_3 .

RAJ-04-022-13C1.fid
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C13CPD CDCl3 C\\ Herbert 1

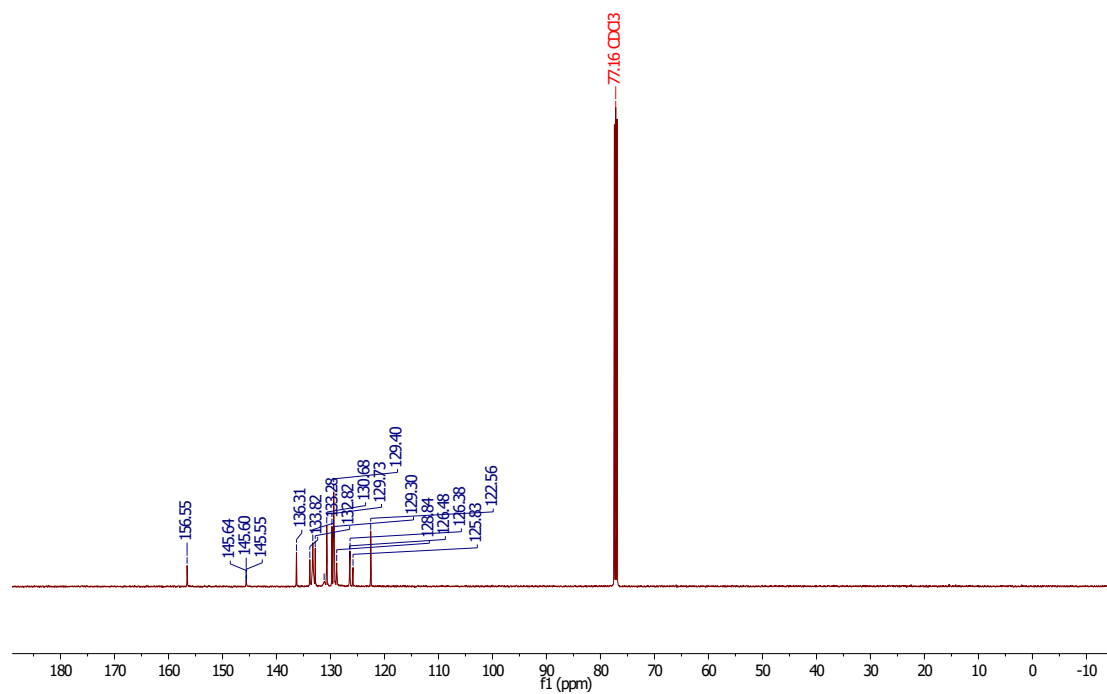


Figure S.4.2. $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, 22°C) spectrum of **(L1)CuPF₆** in CDCl_3 .

RAJ-04-022-I3P1.fid
ParentPhenCuPF6
P31CPD CDCl3 C:\\ Herbert 1

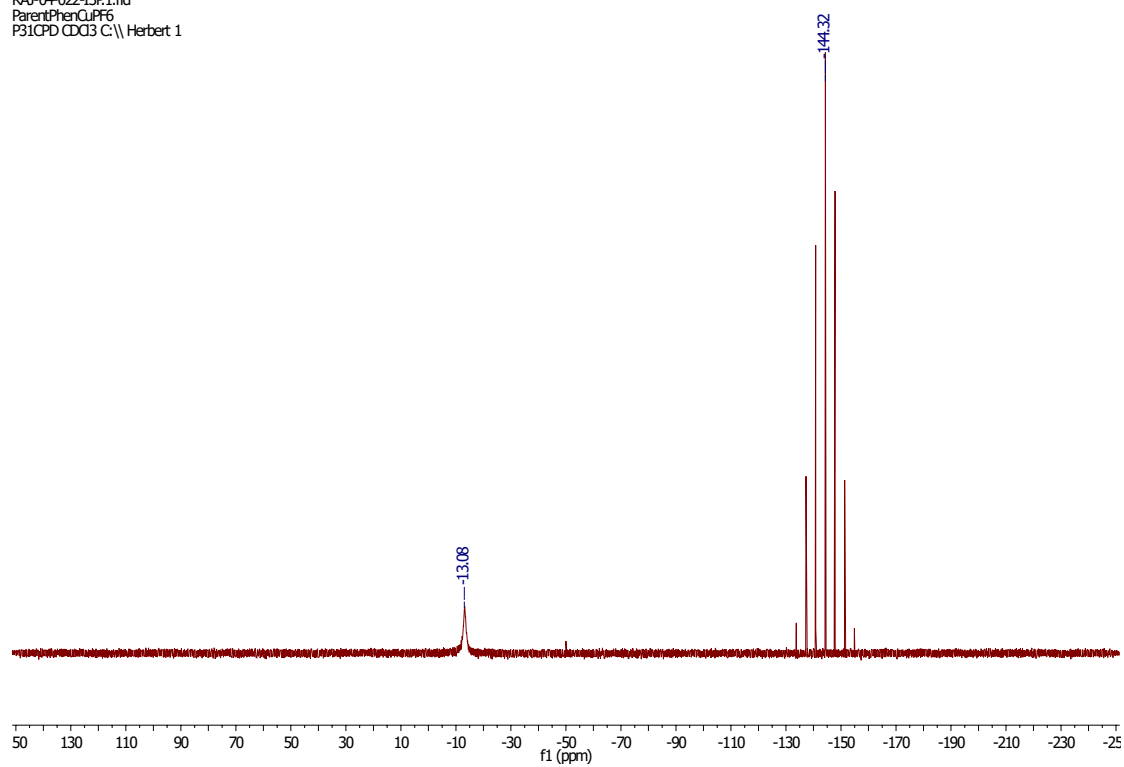


Figure S4.3. $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, 22°C) NMR spectrum of **(L1)CuPF₆** in CDCl_3 .

RAJ-04-022-13F1.fid
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F19CPD CDCl3 C\\ Herbert 1

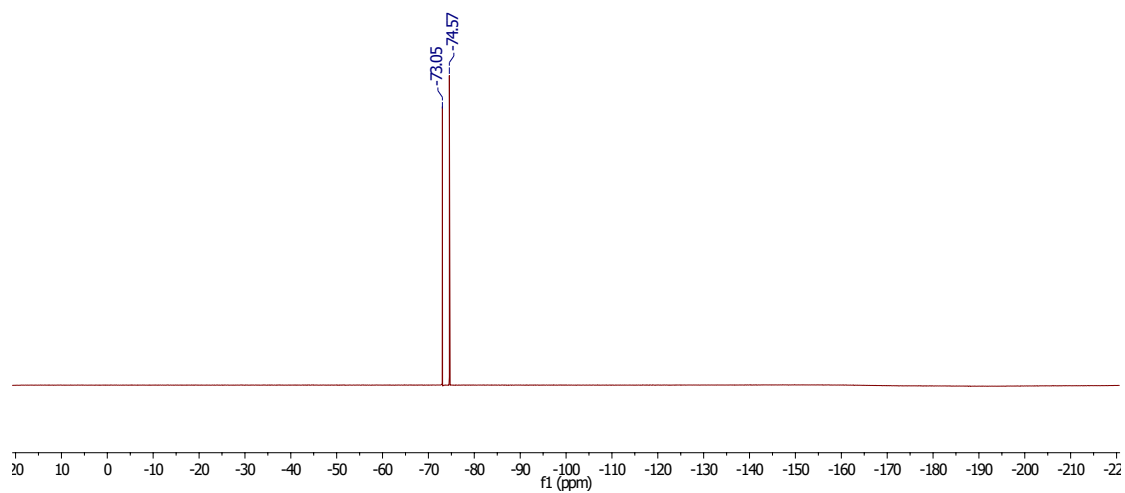


Figure S4.4. ^{19}F NMR (282 MHz, 22°C) spectrum of **(L1)CuPF₆** in CDCl_3 .

RAJ-04-021-ESH.2.fid
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PROTON CDCl3 C:\\\ Herbert 1

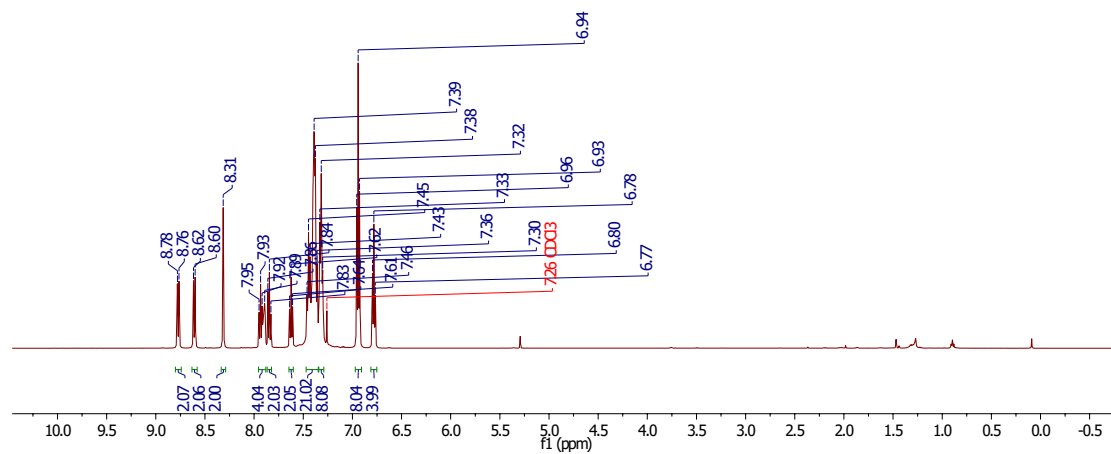


Figure S4.5. ¹H NMR (500 MHz, 22°C) spectrum of (L1)CuBPh₄ in CDCl₃.

RAJ-04-021-ESC.1.fid
 ParentPNCuBPh4
 C13CPD CDCl3 C\\ Herbert 1

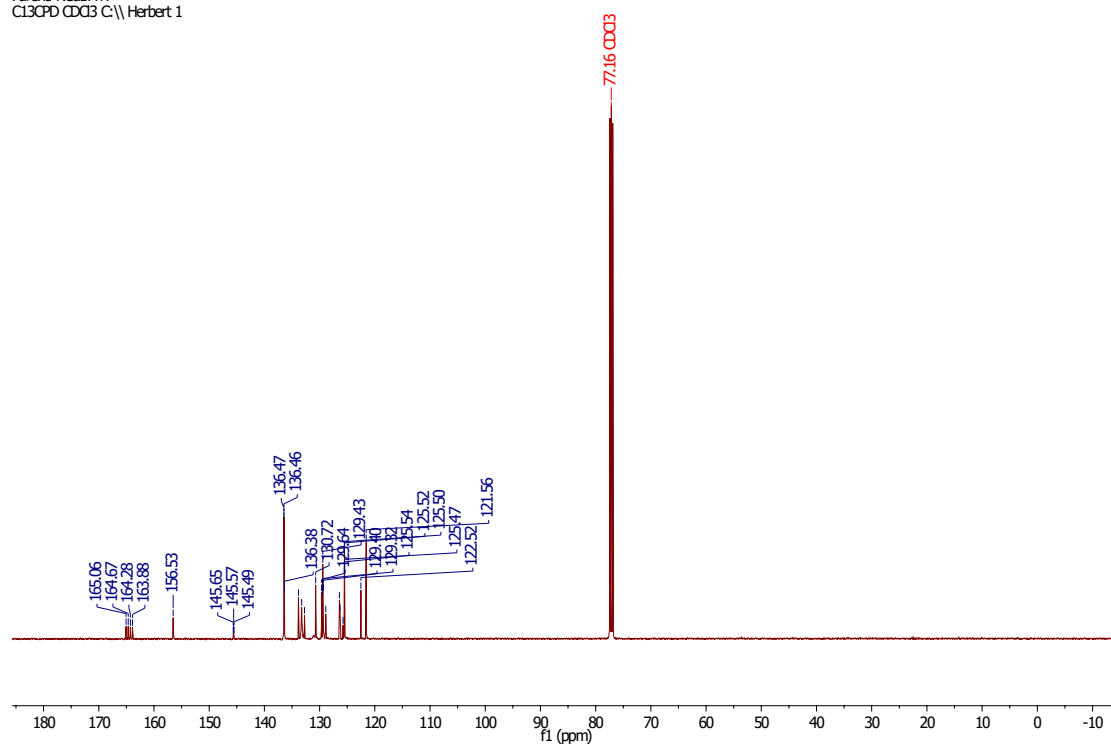


Figure S4.6. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, 22°C) spectrum of **(L1)CuBPh₄** in CDCl_3 .

RAJ-04-021-ESP1.fid
ParentPNCuBPh4
P31CPD CDCl3 C\\ Herbert 1

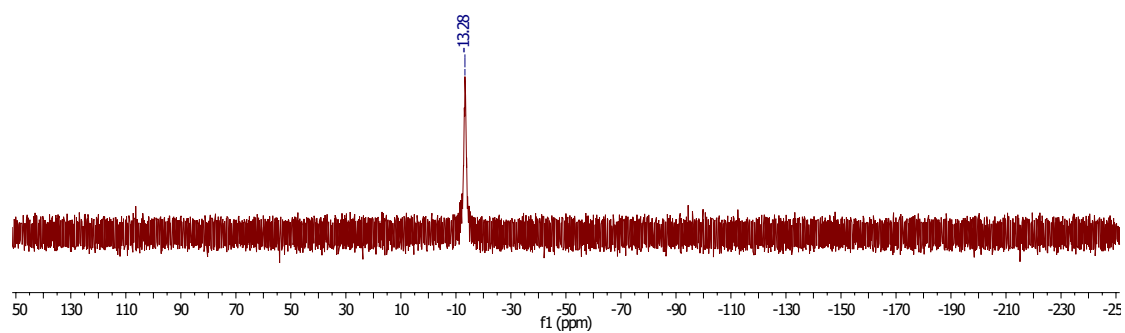


Figure S4.7. $^{31}\text{P}\{^1\text{H}\}$ (202 MHz, 22°C) NMR spectrum of **(L1)CuBPh₄** in CDCl_3 .

RAJ-04-021-D3H.1.fid
MePNCuPF6
PROTON CDCl3 C:\Herbert 2

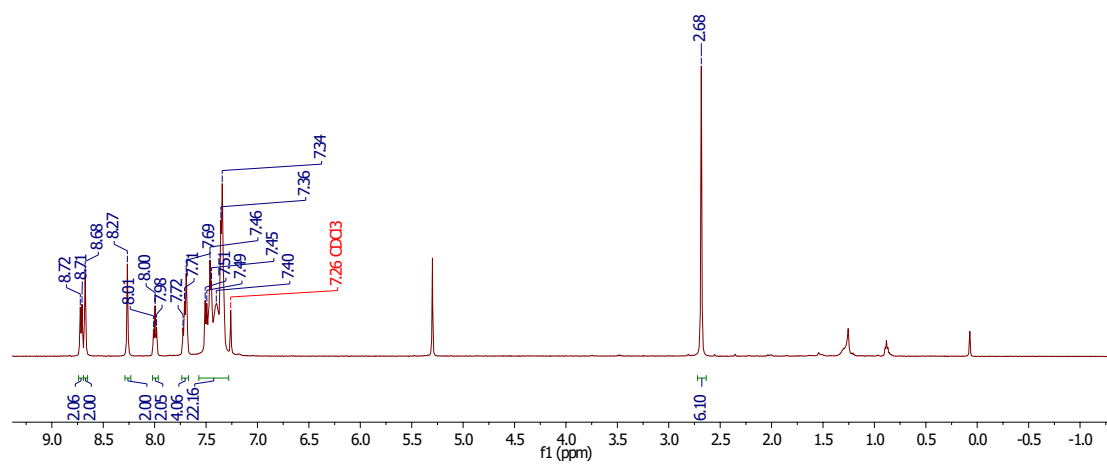


Figure S4.8. ^1H NMR (300 MHz, 22°C) spectrum of $(\text{L2})\text{CuPF}_6$ in CDCl_3 .

RAJ-04-021-A3Cl.1.fid
MePNCuPF₆
Cl₃CPD CDCl₃ C:\\ Herbert 1

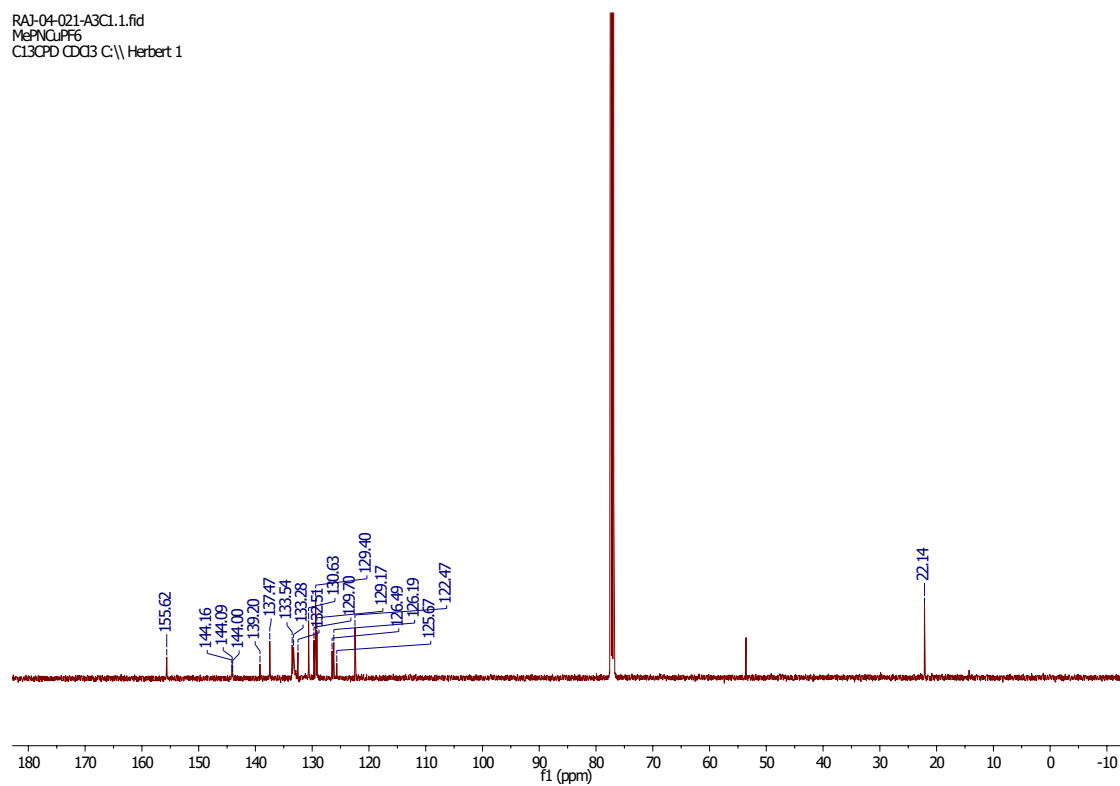


Figure S4.9. ¹³C{¹H} NMR (75 MHz, 22°C) spectrum of (L2)CuPF₆ in CDCl₃.

RAJ-04-021-D3P1.fid
MePNCuPF₆
P31CPD CDCl₃ C:\\ Herbert 2

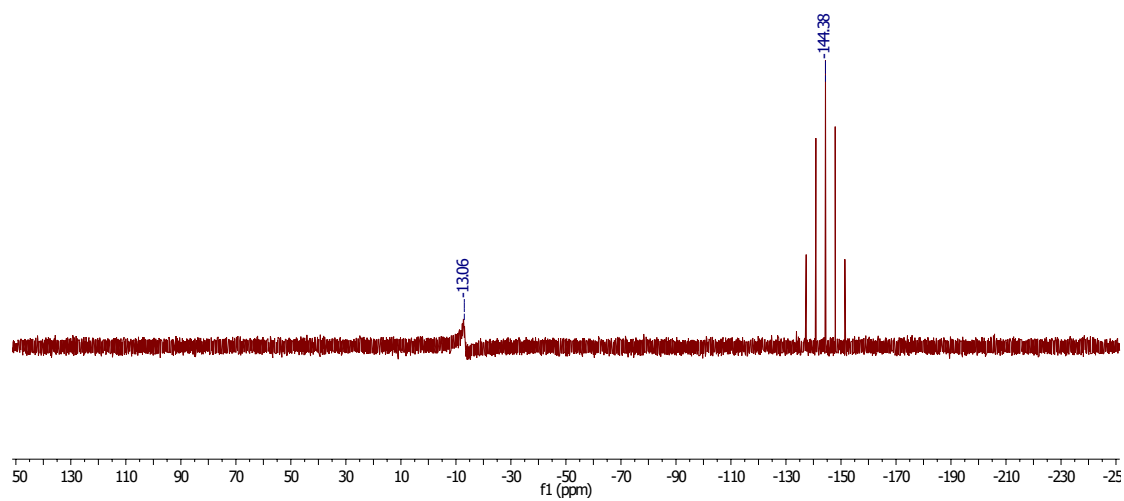


Figure S4.10. $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, 22°C) NMR spectrum of **(L2)CuPF₆** in CDCl₃.

RAJ-04-021-D3F1.fid
MePNCuPF₆
F19CPD CDCl₃ C\\ Herbert 2

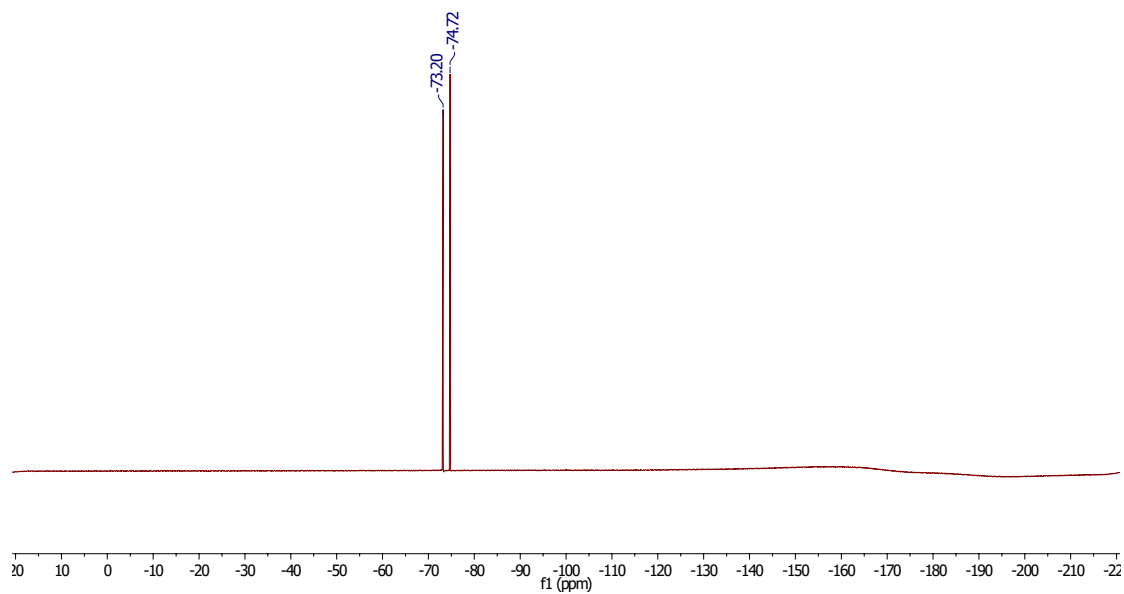


Figure S4.11. ¹⁹F NMR (282 MHz, 22°C) spectrum of **(L2)CuPF₆** in CDCl₃.

RAJ-04-021-B5H.2.fid
MePNCuBPh4
PROTON CDCl3 C:\ Herbert 1

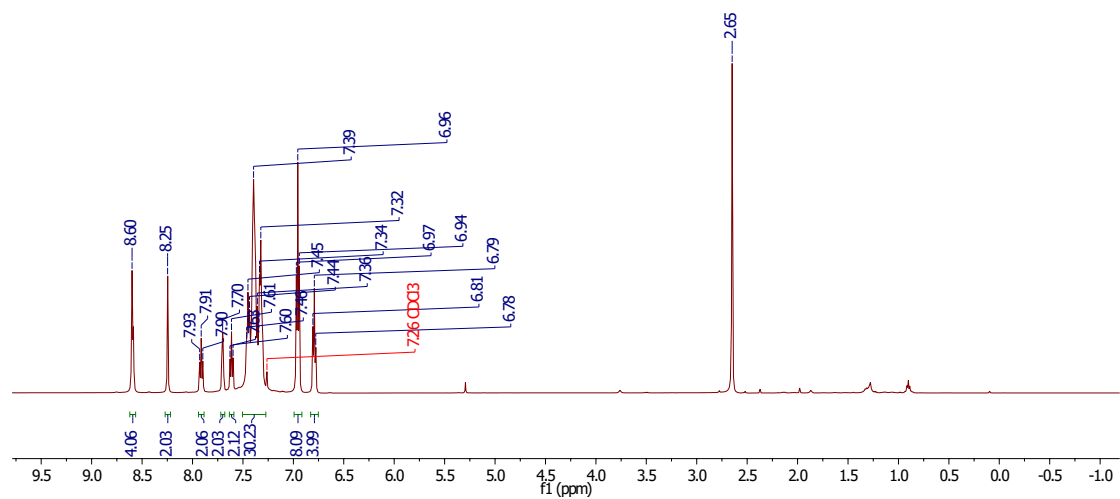


Figure S4.12. ^1H NMR (500 MHz, 22°C) spectrum of $(\text{L2})\text{CuBPh}_4$ in CDCl_3 .

RAJ-04-021-B5C.2.fid
MePNCuBPh4
Cl3CPD CDCl3 C\\ Herbert 1

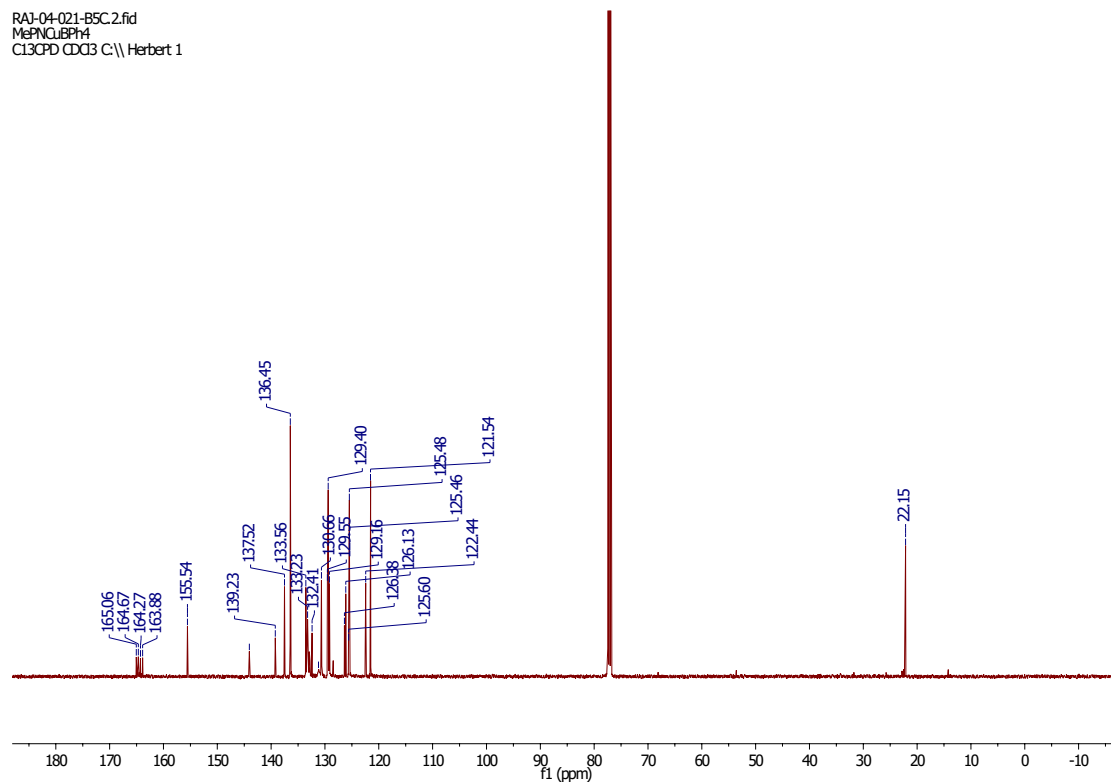


Figure S4.13. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, 22°C) spectrum of **(L2)CuBPh₄** in CDCl_3 .

KAP-UP-021-0041.100
MePNCuBPh₄
P31CPD CDCl₃ C\\ Herbert 1

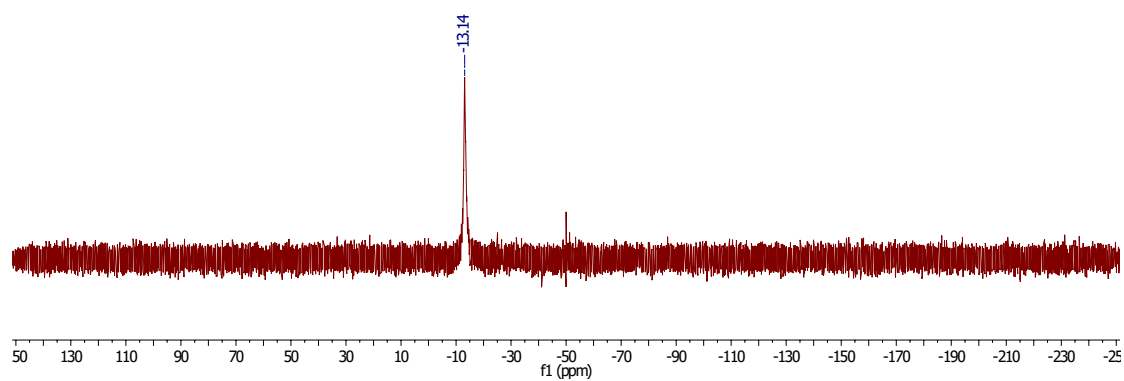


Figure S4.14. $^{31}\text{P}\{^1\text{H}\}$ (202 MHz, 22°C) NMR spectrum of **(L2)CuBPh₄** in CDCl_3 .

RAJ-04-061-C3H.1.fid
 Acyl, MePNCuBr
 PROTON CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 18

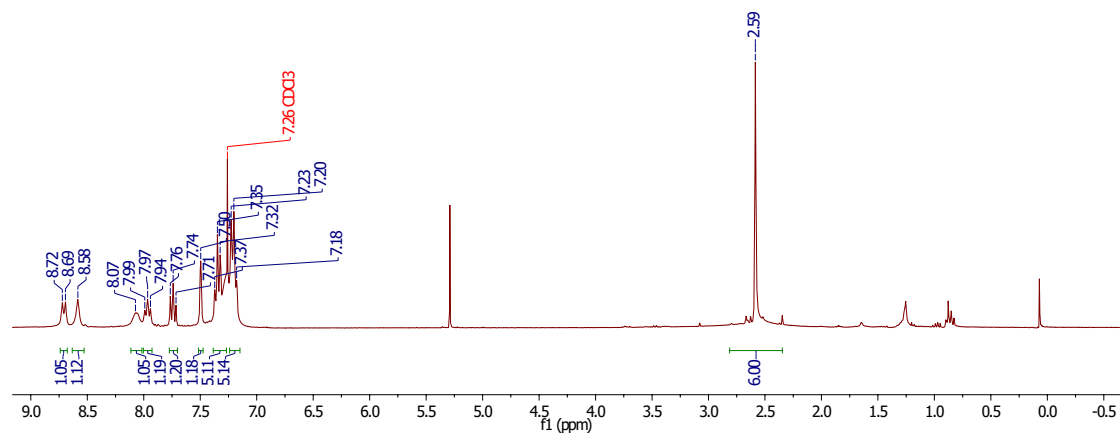


Figure S4.15. ^1H NMR (300 MHz, 22°C) spectrum of $(\text{L3})_2\text{Cu}_2(\mu\text{-Br})_2$ in CDCl_3 .

RAJ-02-061-ESC.1.fid
 Acyl, MePNCuBr
 C13CPD CDCl3 C\\ Herbert 2

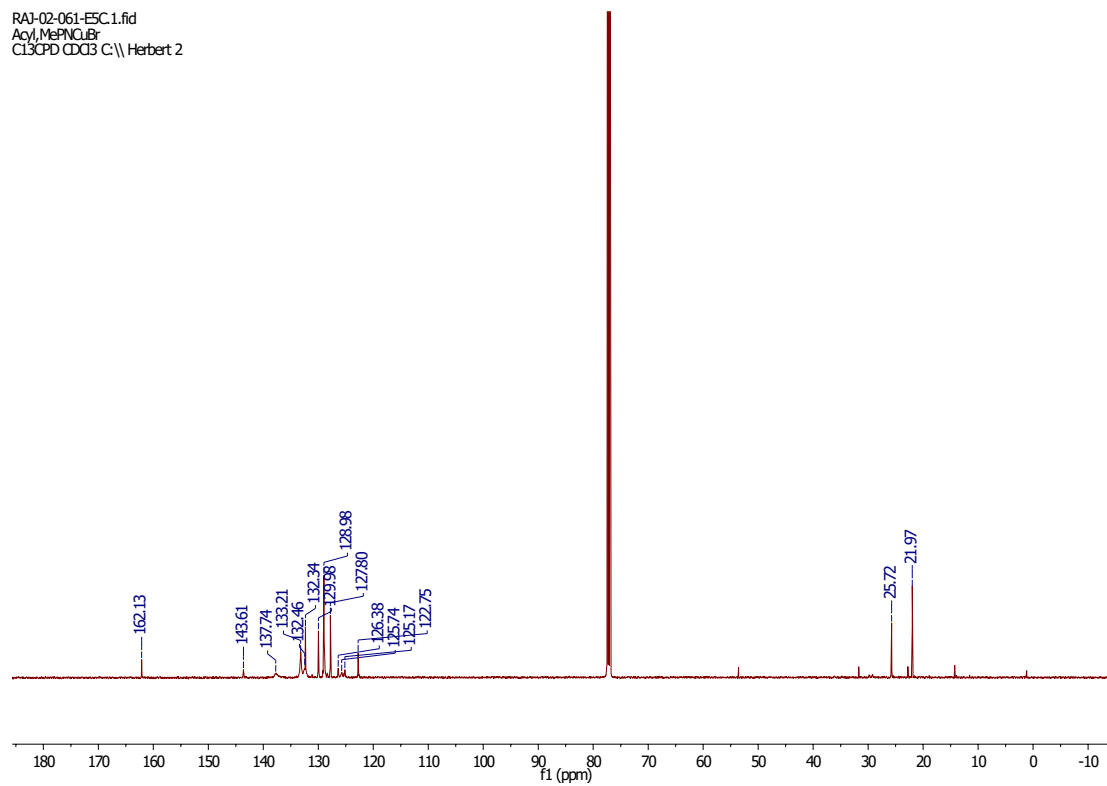


Figure S4.16. $^{13}\text{C}\{^1\text{H}\}$ NMR (75 MHz, 22°C) spectrum of $(\text{L3})_2\text{Cu}_2(\mu\text{-Br})_2$ in CDCl_3 .

RAJ-04-051-D5P2.fid
Acyl₁MePNCuBr
P31CPD CDCl₃ C:\\ Herbert 2

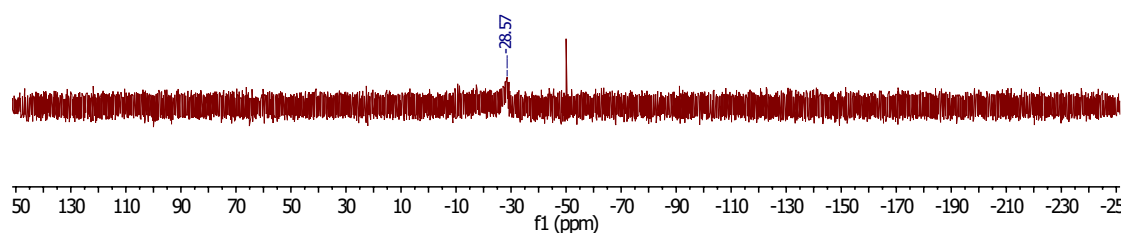


Figure S4.17. $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, 22°C) NMR spectrum of $(\text{L}3)_2\text{Cu}_2(\mu\text{-Br})_2$ in CDCl_3 .

RAJ-04-021-ASH.2.fid
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PROTON CDCl3 C:\Herbert 1

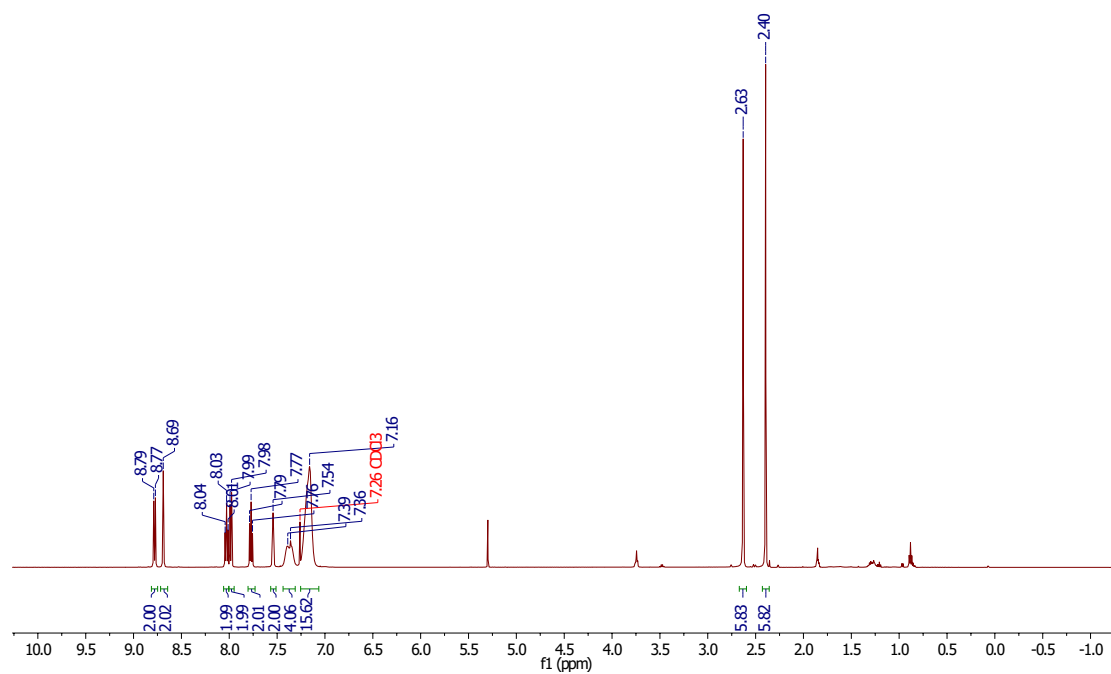


Figure S4.18. ¹H NMR (500 MHz, 22°C) spectrum of (L5)CuPF₆ in CDCl₃.

RAJ-04-021-ASC.1.fid
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 C13CPD CDCl₃ C\\ Herbert 1

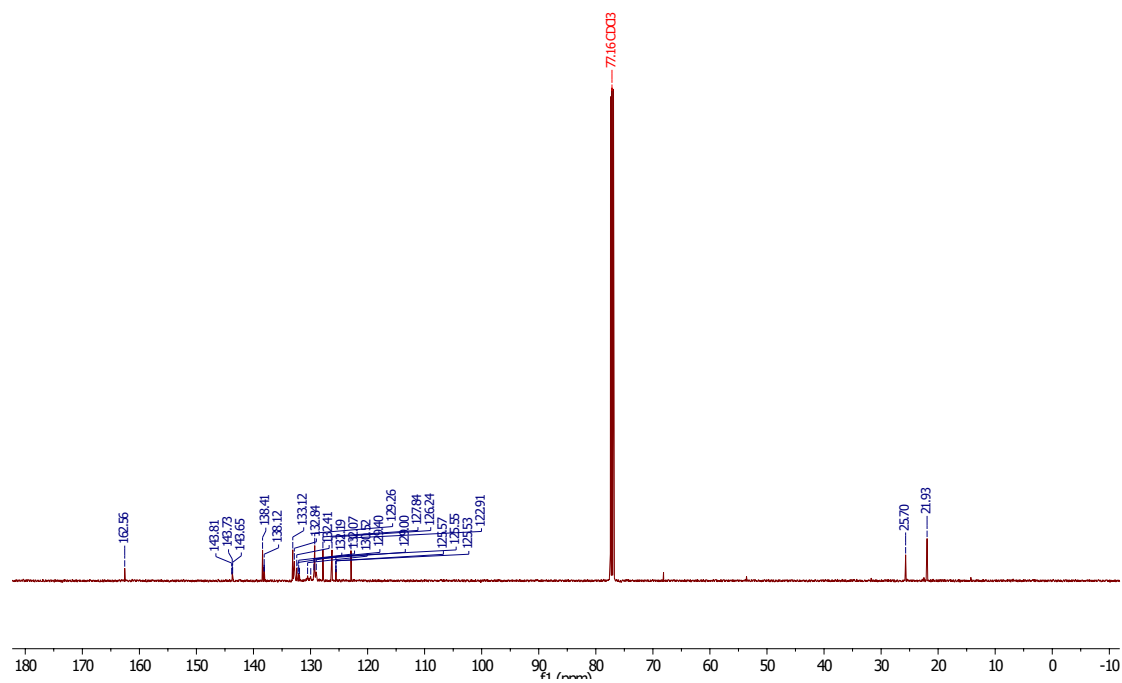


Figure S4.19. ¹³C{¹H} NMR (126 MHz, 22°C) spectrum of (L5)CuPF₆ in CDCl₃.

KAU-UPHRS-C3F2.n0
acyl,MePNCuPF6 2nd batch as -04-048-B3h is actually bromide counter ion
P31CPD CDCl3 C:\\ Herbert 2

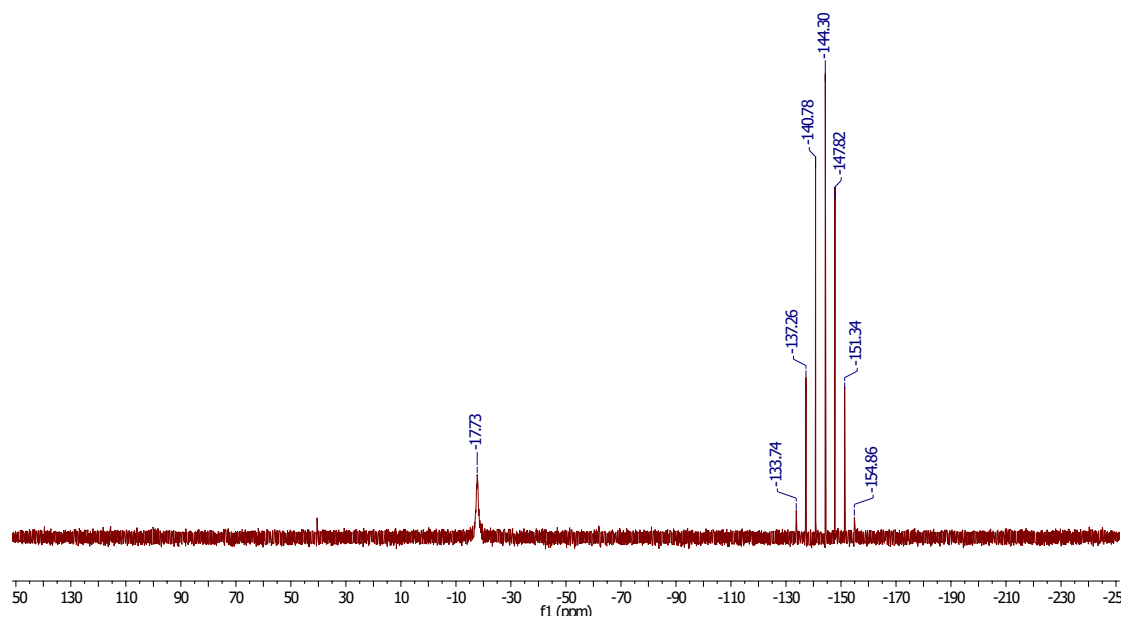


Figure S4.20. $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, 22°C) NMR spectrum of $(\text{L5})\text{CuPF}_6$ in CDCl_3 .

RAJ-04-048-C3E2.fid
acyl,MePNCuPF6 2nd batch as -04-048-B3h is actually bromide counter ion
F19CPD CDCl3 C:\\ Herbert 2

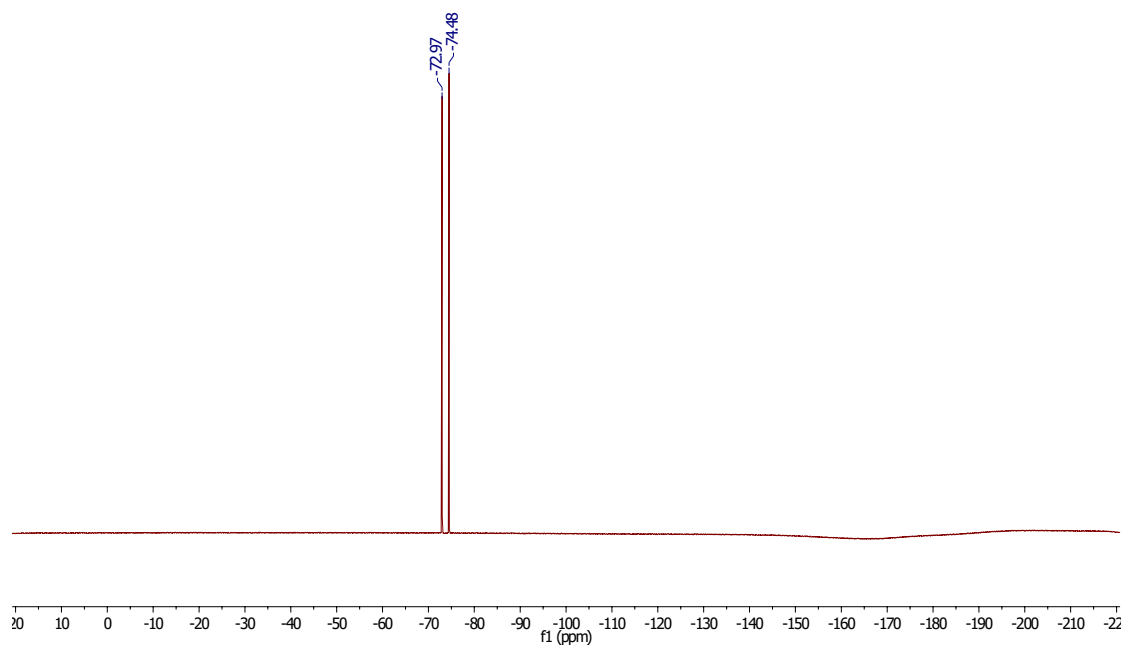


Figure S4.21. ^{19}F NMR(282 MHz, 22°C) NMR spectrum of **(L5)CuPF₆** in CDCl_3 .

RAJ-04-048-ESH.2.fid
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PROTON CD2Cl2 C:\\ Herbert 1

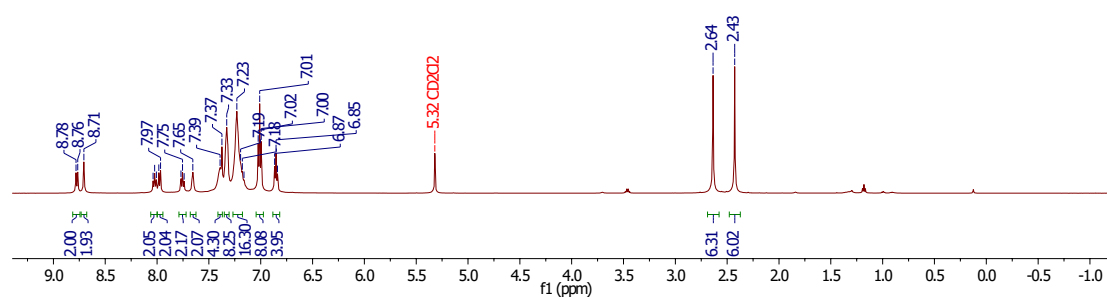


Figure S4.22. ^1H NMR (500 MHz, 22°C) spectrum of $(\text{L5})\text{CuBPh}_4$ in CDCl_3 .

RAJ-04-048-ESC.1.fid
 Acyl, MePNCuBPh₄
 C13CPD CD2Cl2 C:\\ Herbert 1

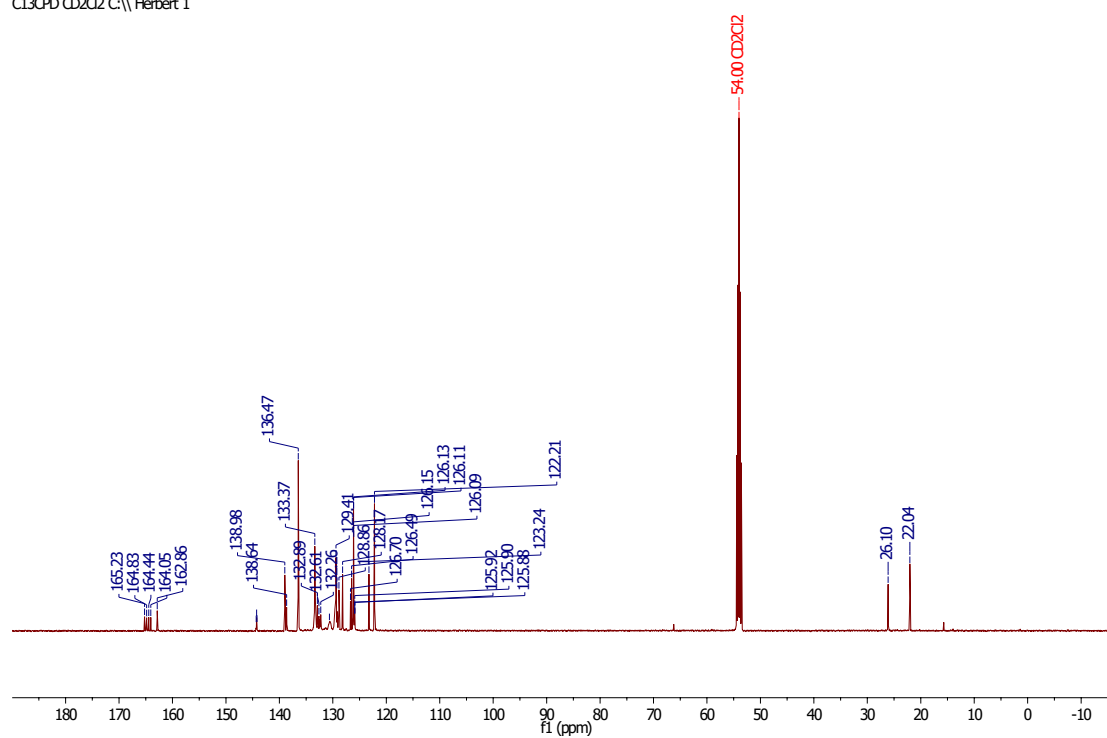


Figure S4.23. ¹³C{¹H} NMR (126 MHz, 22°C) spectrum of (L5)CuBPh₄ in CDCl₃.

RAJ-03-012-A3P1.fid
Acyl, MeCuBph4 crystal
P31CPD CDCl3 {C:\Bruker\TOPSPIN1.3} Herbert 7

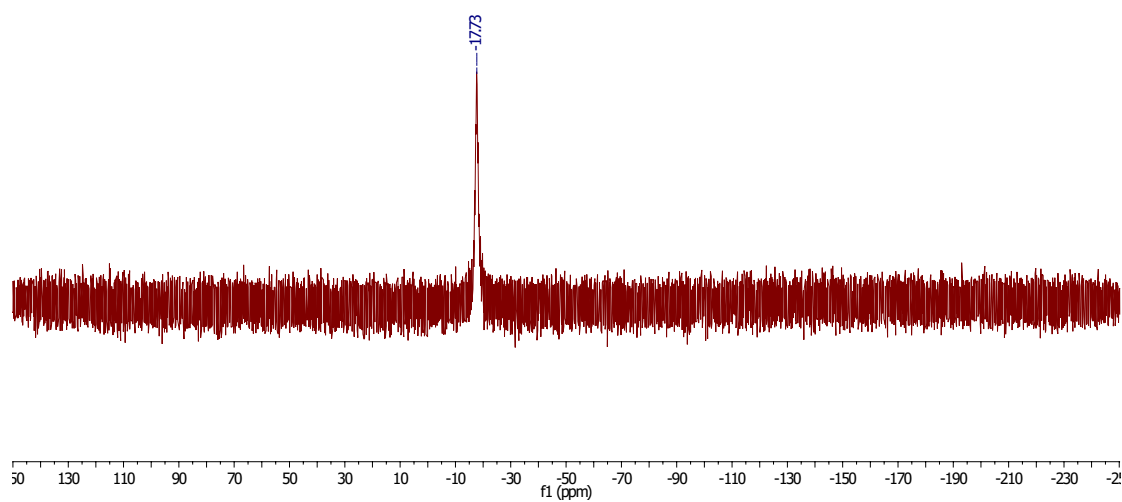


Figure S4.24. $^{31}\text{P}\{^1\text{H}\}$ (121 MHz, 22°C) NMR spectrum of **(L5)CuBPh₄** in CDCl_3 .

Computational Details

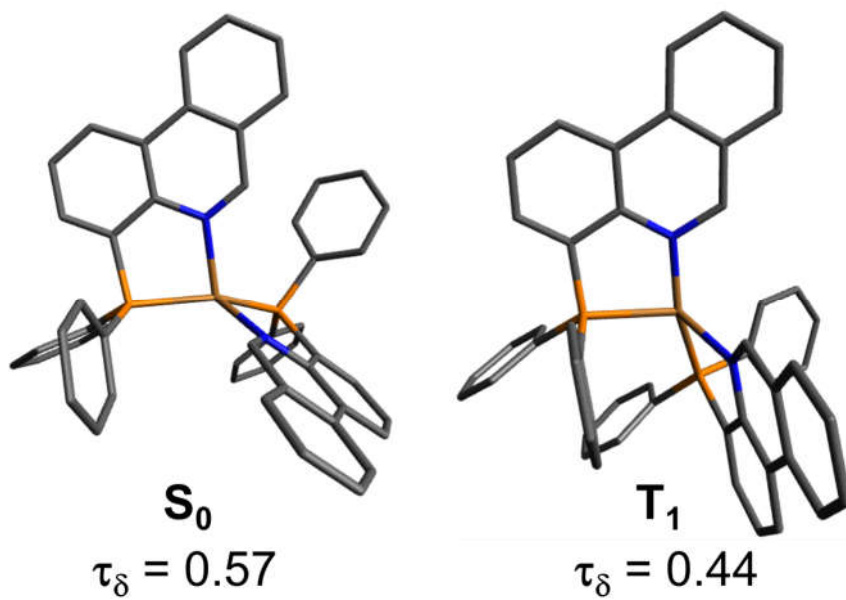


Figure S4.25. Alternate view of DFT optimized structures of (a) S₀ and (b) T₁ states for (L1)Cu⁺.

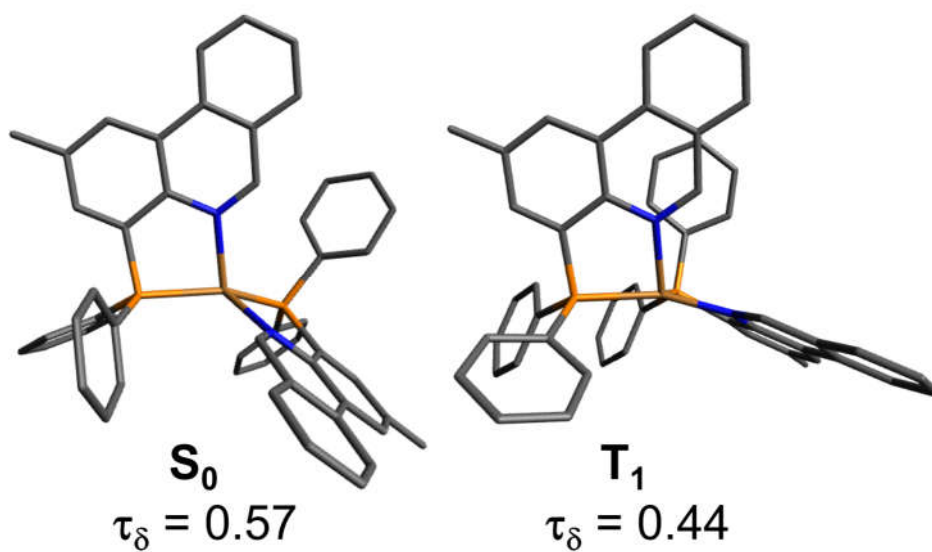


Figure S4.26. Alternate view of DFT optimized structures of (a) S₀ and (b) T₁ states for (L2)Cu⁺.

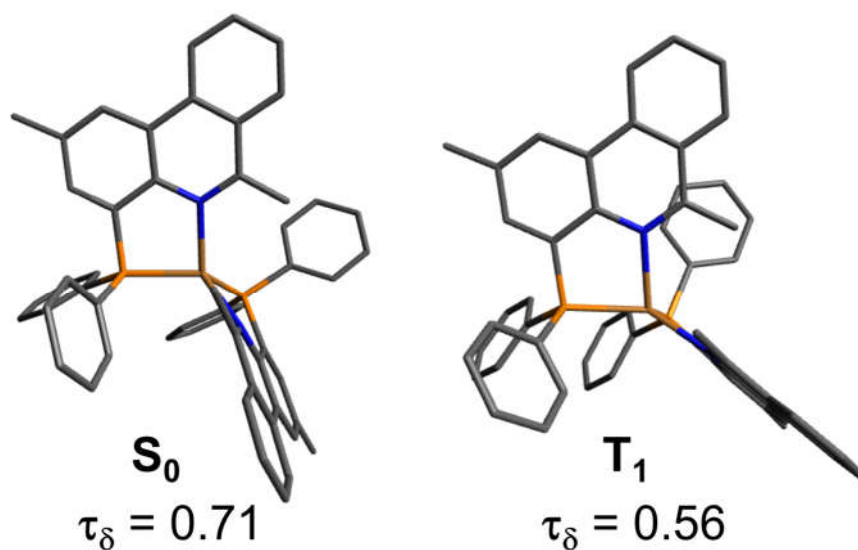


Figure S4.27. Alternate view of DFT optimized structures of (a) S₀ and (b) T₁ states for (L5)Cu⁺.

Table S11. Selected bond distances [Å] and angles [°] for the DFT-optimized S₀ and T₁ state structures of (L1)Cu⁺, (L2)Cu⁺, and (L5)Cu⁺.

	1⁺		2⁺		3⁺	
Bond (Å)	S₀	T₁	S₀	T₁	S₀	T₁
Cu-N1	2.104	1.921	2.102	2.097	2.146	2.185
Cu-N2	2.104	2.098	2.102	1.920	2.121	1.945
Cu-P1	2.238	2.297	2.238	2.299	2.244	2.262
Cu-P2	2.237	2.271	2.238	2.272	2.257	2.290
Angle (°)	S₀	T₁	S₀	T₁	S₀	T₁
N1-Cu-N2	109.2	105.6	109.2	105.8	118.5	120.9
N1-Cu-P1	85.7	84.4	115.5	114.7	86.0	84.1
N1-Cu-P2	115.5	159.0	85.8	84.2	114.5	113.2
N2-Cu-P1	115.4	115.0	85.8	84.4	124.2	144.9
N2-Cu-P2	85.7	84.1	115.5	159.0	86.4	85.9
P1-Cu-P2	144.3	108.7	144.1	108.6	130.6	107.7

Table S12. Geometric indices (τ_8)¹ of **(L1)₂CuX**, **(L2)₂CuX**, and **(L5)₂CuX** (X = PF₆ or BPh₄) crystal structures, and DFT optimized S₀ and T₁ structures of (L1)Cu⁺, (L2)Cu⁺, and (L5)Cu⁺.

τ_8	PF ₆	BPh ₄	S ₀	T ₁
1X	0.56	0.64	0.57	0.44
2X	0.54	0.64	0.57	0.44
3X	0.70	0.72	0.71	0.56

Table S13. Calculated photophysical parameters for L1Cu⁺, L2Cu⁺ and L5Cu⁺ complexes.

<i>E</i> (eV)	L1 ⁺	L2 ⁺	L5 ⁺
ΔE (S ₁ -TD)	3.110	3.172	3.158
ΔE (S ₁ -T ₁)	0.863	0.901	0.721
ΔE (adiab)	2.247	2.272	2.436
ΔE (phos)	1.444	1.477	1.691
λ_T	0.803	0.795	0.745

Table S14. First four TD-DFT calculated electronic transitions for L1⁺, L2⁺ and L5⁺ with the corresponding oscillators strengths and MO characters.

Complex	State	Calc. $\lambda_{\text{abs.}}$ (nm)	Oscillator strength	MO character	% Contribution
1⁺	S ₁	398.70	0.0046	HOMO → LUMO	49%
				HOMO-1 → LUMO+1	47%
	S ₂	398.13	0.0011	HOMO-1 → LUMO	54%
				HOMO → LUMO+1	41%
	S ₃	376.85	0.0494	HOMO-1 → LUMO+1	50%
				HOMO → LUMO	48%
	S ₄	375.85	0.0142	HOMO → LUMO+1	55%
				HOMO-1 → LUMO	42%
2⁺	S ₁	390.87	0.0049	HOMO → LUMO	49%
				HOMO-1 → LUMO+1	47%
	S ₂	390.30	0.0013	HOMO-1 → LUMO	55%
				HOMO → LUMO+1	41%
	S ₃	369.80	0.528	HOMO-1 → LUMO+1	51%
				HOMO → LUMO	47%
	S ₄	368.87	0.0132	HOMO → LUMO+1	55%
				HOMO-1 → LUMO	42%
5⁺	S ₁	392.65	0.0180	HOMO → LUMO	85%
	S ₂	387.03	0.0148	HOMO → LUMO+1	84%
				HOMO-1 → LUMO+1	10%
	S ₃	358.16	0.0299	HOMO-1 → LUMO+1	58%
				HOMO-1 → LUMO	29%
	S ₄	357.43	0.0100	HOMO-1 → LUMO	58%
				HOMO-1 → LUMO+1	27%

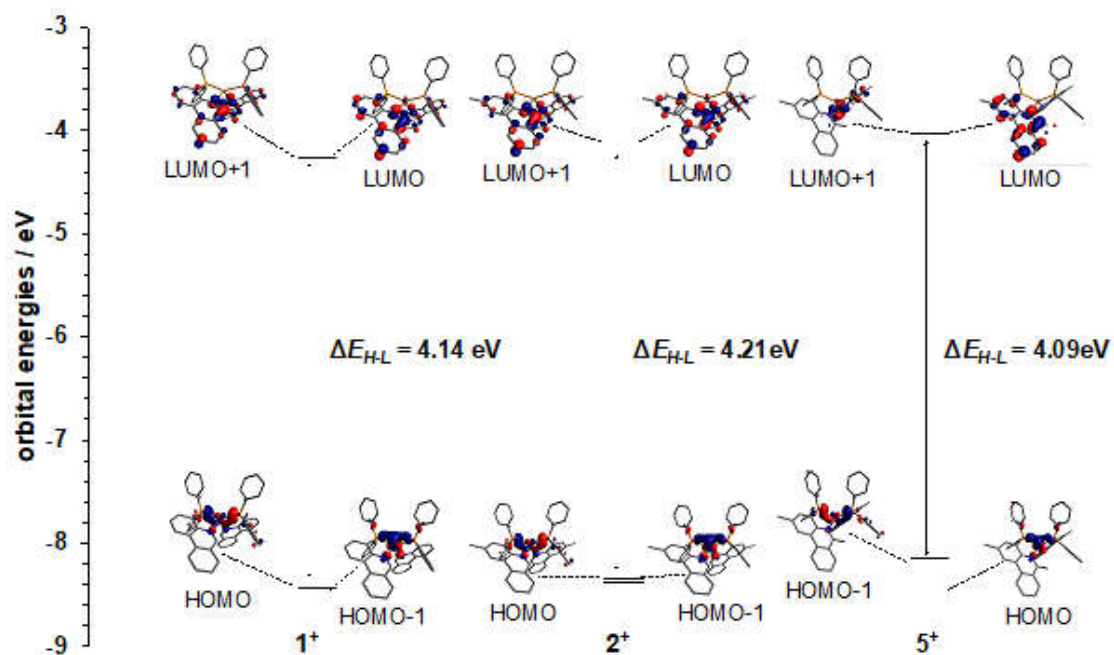


Figure S4.28. TD-DFT orbital energies, HOMO-LUMO gap (ΔE_{H-L}), and frontier molecular orbital (MO; isosurface value = 0.05) diagrams of 1^+ , 2^+ , and 5^+ .

Table S15. Fragment contributions to the two highest occupied MOs and two lowest unoccupied MOs of 1⁺. Fragment contributions >10% are in bold.

Fragment	HOMO-1	HOMO	LUMO	LUMO+1
Cu	36.2	26.6	0.9	0.5
P ₁	9.0	13.5	0.4	0.5
Ph _{1a}	7.8	5.6	0.7	0.4
Ph _{1b}	2.0	8.4	2.0	1.3
(HC=N) ₁ ^a	5.2	3.2	19.8	15.7
(Ar _{phenan}) ₁ ^b	7.8	6.2	33.7	24.8
P ₂	9.1	13.4	0.4	0.5
Ph _{2a}	7.8	5.5	0.6	0.5
Ph _{2b}	2.0	8.3	2.2	1.2
(HC=N) ₂ ^a	5.3	3.2	14.5	20.9
(Ar _{phenan}) ₂ ^b	7.9	6.1	24.8	33.6

^a (HC=N)_n refers to the imine-bridge fragment of phenanthridine.

^b (Ar_{phenan})_n refers to the biphenyl fragment of phenanthridine.

Table S16. Fragment contributions to the two highest occupied MOs and two lowest unoccupied MOs of 2⁺. Fragment contributions >10% are in bold.

Fragment	HOMO-1	HOMO	LUMO	LUMO+1
Cu	36.2	26.7	0.9	0.5
P ₁	9.0	13.4	0.4	0.6
Ph _{1a}	7.7	5.4	0.7	0.5
Ph _{1b}	1.9	8.2	2.2	1.2
(HC=N) ₁ ^a	5.3	3.3	17.1	18.3
(Ar _{phenan}) ₁ ^b	8.0	6.2	28.9	28.8
Me ₁ ^c	0.1	0.1	0.3	0.4
P ₂	9.0	13.4	0.4	0.6
Ph _{2a}	7.7	5.4	0.7	0.5
Ph _{2b}	1.9	8.2	2.2	1.2
(HC=N) ₂ ^a	5.3	3.3	17.1	18.3
(Ar _{phenan}) ₂ ^b	8.0	6.2	28.9	28.9
Me ₂ ^c	0.1	0.1	0.3	0.45

^a (HC=N)_n refers to the imine-bridge fragment of phenanthridine.

^b (Ar_{phenan})_n refers to the biphenyl fragment of phenanthridine.

^c Me_{na} refers to the methyl substituent at the C₂-position of phenanthridine.

Table S17. Fragment contributions to the two highest occupied MOs and two lowest unoccupied MOs of 5⁺. Fragment contributions >10% are in bold.

Fragment	HOMO-1	HOMO	LUMO	LUMO+1
Cu	36.4	25.2	0.9	0.8
P ₁	7.9	13.9	0.3	0.4
(C=N) ₁ ^a	5.7	2.2	0.5	32.5
(Ar _{phenan}) ₁ ^b	7.8	5.3	0.5	54.5
Ph _{1a}	8.0	5.6	0.1	0.9
Ph _{1b}	2.1	8.6	0.5	1.0
Me _{1a} ^c	0.1	0.1	0.0	0.7
Me _{1b} ^d	1.5	0.3	1.4	3.9
P ₂	8.4	15.3	0.4	0.4
(C=N) ₂ ^a	4.5	2.8	33.2	0.3
(Ar _{phenan}) ₂ ^b	6.0	6.7	55.2	1.0
Ph _{2a}	8.2	5.9	1.1	0.4
Ph _{2b}	1.5	7.5	1.2	1.6
Me _{2a} ^c	0.1	0.1	0.7	0.0
Me _{2b} ^d	1.9	0.5	4.2	1.5

^a (C=N)_n refers to the imine-bridge fragment of phenanthridine.

^b (Ar_{phenan})_n refers to the biphenyl fragment of phenanthridine.

^c Me_{na} refers to the methyl substituent at the C₂-position of phenanthridine.

^d Me_{nb} refers to the methyl substituent at the C₆-position of phenanthridine.

Chapter 5:

RAJ-04-022-H3H.1.fid
(PN)3Fe(PF₆)₂
PROTON CD₂Cl₂ C:\ Herbert 1

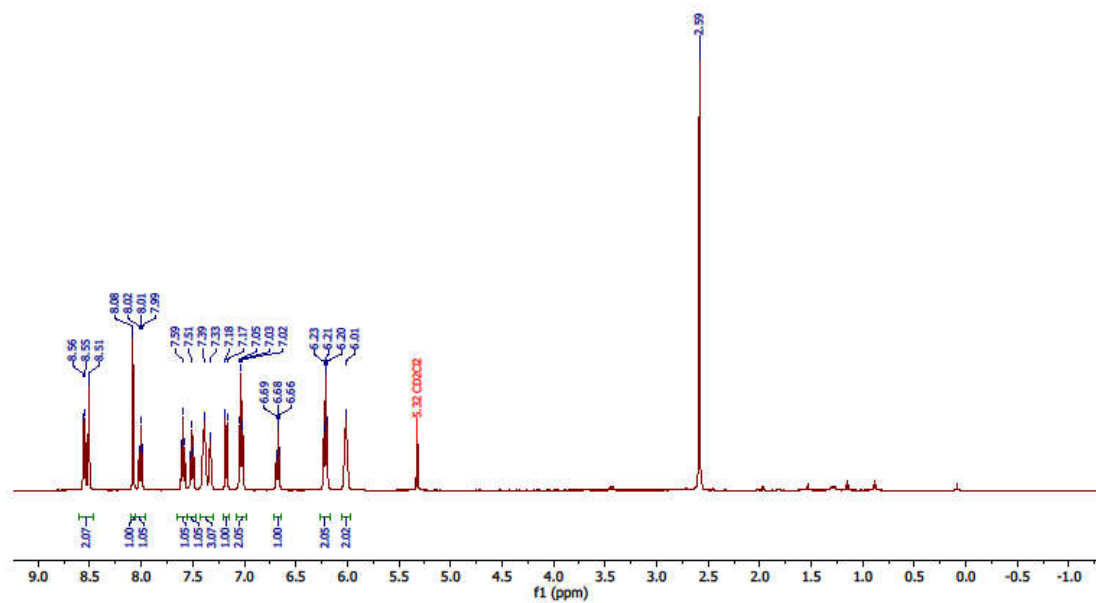


Figure S5.1. ¹H NMR (300 MHz, 22°C) spectrum of (L2)₃Fe(PF₆)₂ in CD₂Cl₂.

RAJ-04-022-H3C.1.fid
(PN)3Fe(PF6)2
C13CPD CD2Cl2 C:\Herbert.1

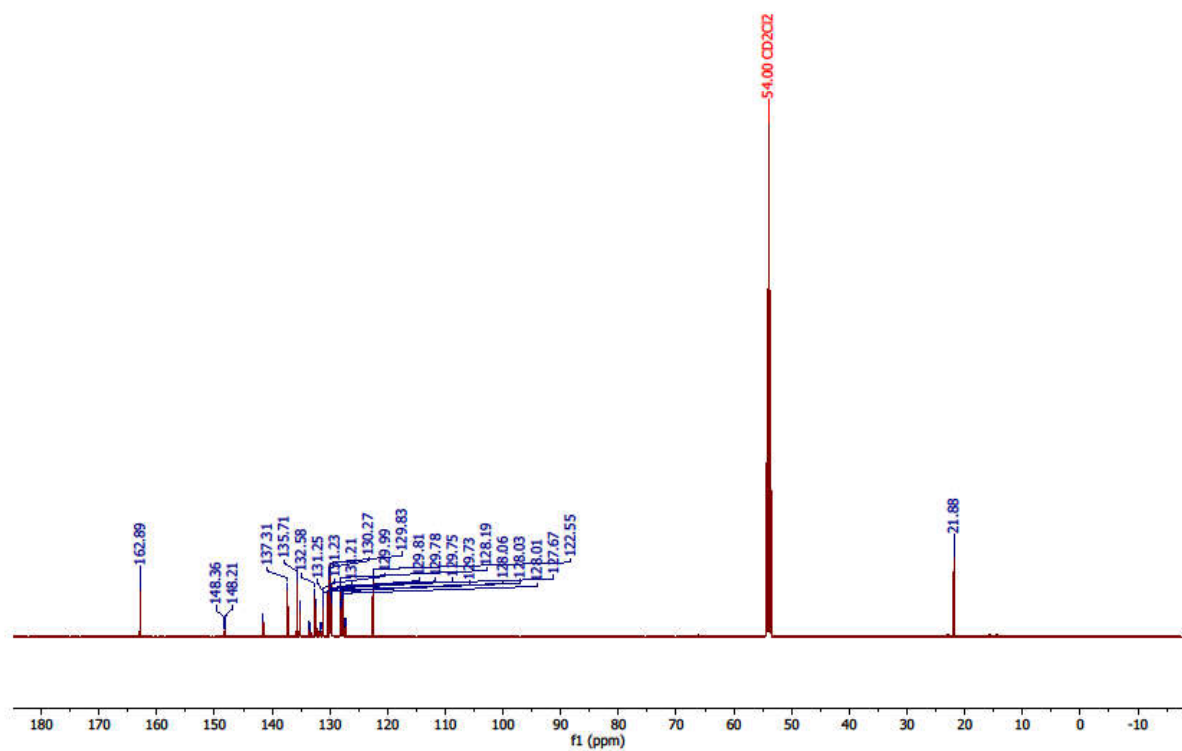


Figure S5.2. ^{13}C NMR (75 MHz, 22°C) spectrum of $(\text{L2})_3\text{Fe}(\text{PF}_6)_2$ in CD_2Cl_2 .

RAJ-04-054-NSH.2.fid
 (MePN)₃Ru(PF₆)₂
 PROTON CD₃CN C:\ Herbert 2

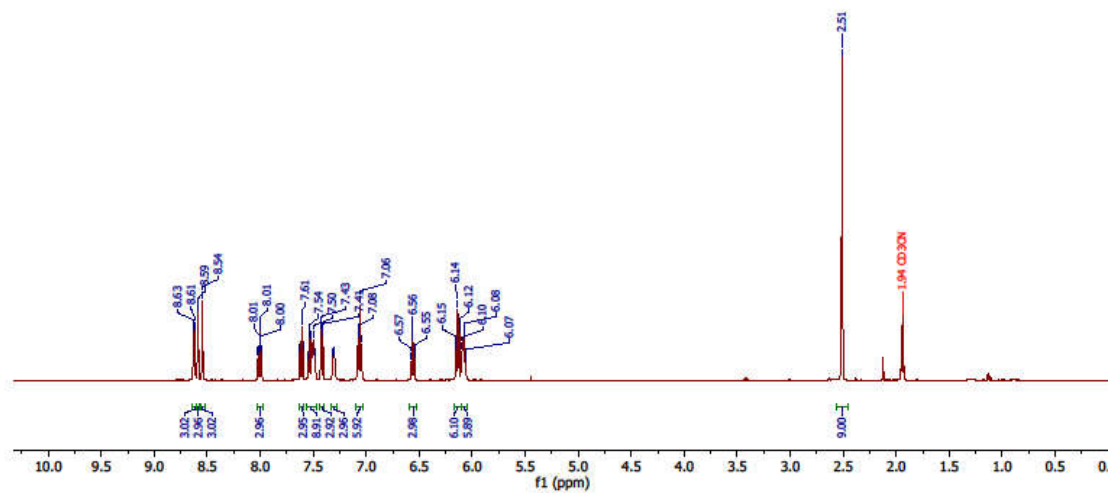


Figure S5.3. ¹H NMR (500 MHz, 22°C) spectrum of (L2)₃Ru(PF₆)₂ in CD₃CN.

RAJ-04-054-NSC.1.fid
 (MePN)₃Ru(PF₆)₂
 C13CPD CD₃CN C:\\ Herbert 2

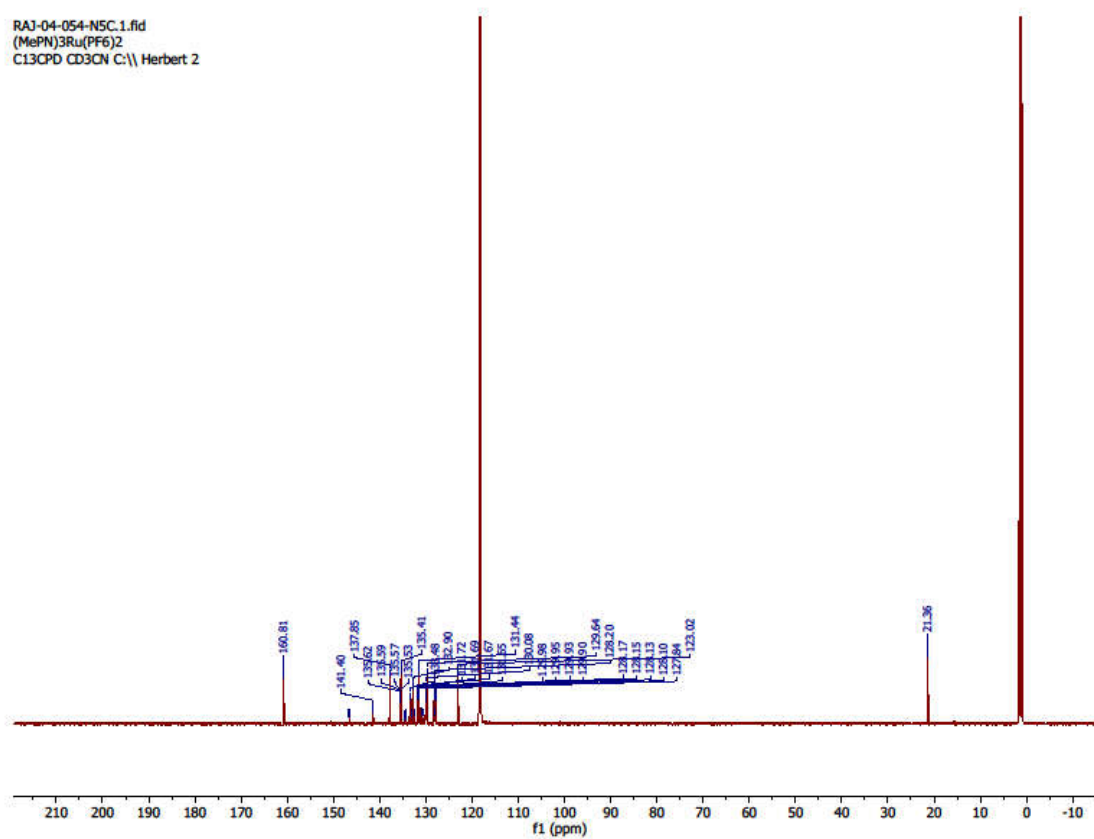


Figure S5.4. ¹³C NMR (75 MHz, 22°C) spectrum of (L2)₃Ru(PF₆)₂ in CD₃CN.

RAJ-04-054-NSP.1.fid
(MePN)₃Ru(PF₆)₂
P31CPD CD₃CN C:\ Herbert 2

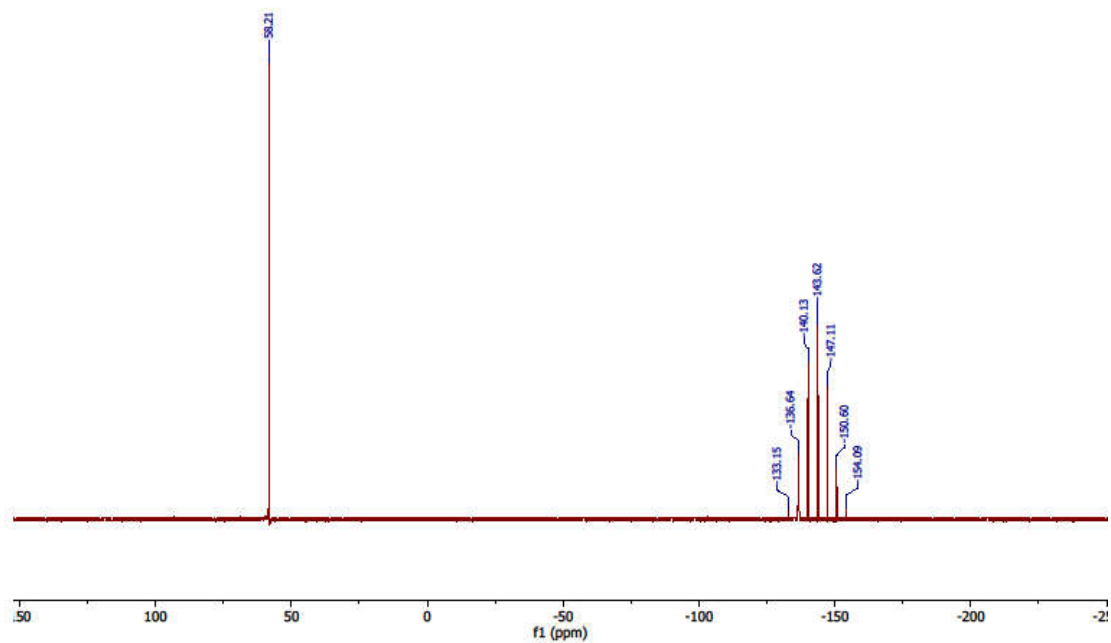


Figure S5.5. ³¹P NMR (202 MHz, 22°C) spectrum of (L2)₃Ru(PF₆)₂ in CD₃CN.

RAJ-04-074-ASH.1.fid
(quin)₃Fe(PF₆)₂
PROTON CD₂Cl₂ C:\ Herbert 1

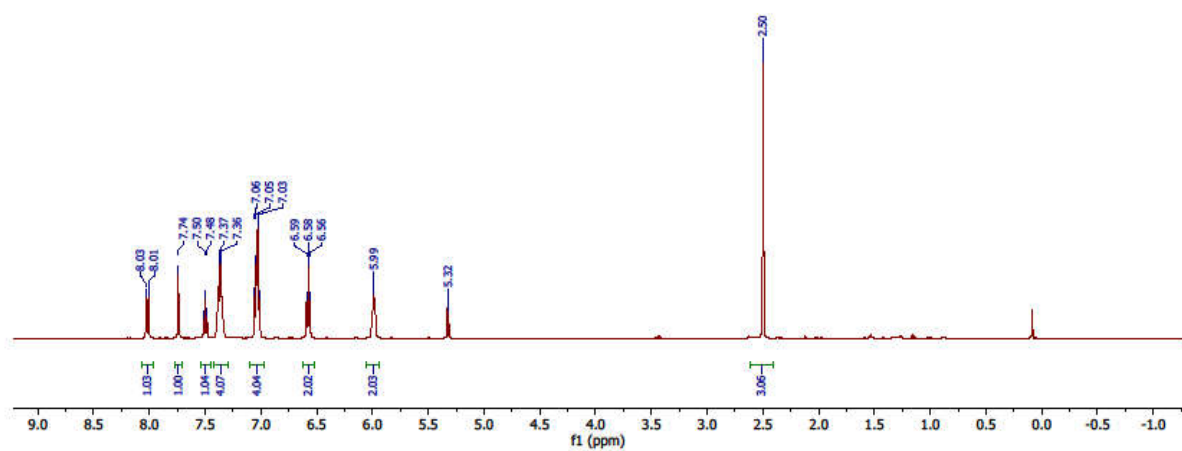


Figure S5.6. ¹H NMR (500 MHz, 22°C) spectrum of (L3)₃Fe(PF₆)₂ in CD₃CN.

RAJ-04-074-A5C.1.fid
(quin)₃Fe(PF₆)₂
C13CPD CD2Cl2 C:\ Herbert 1

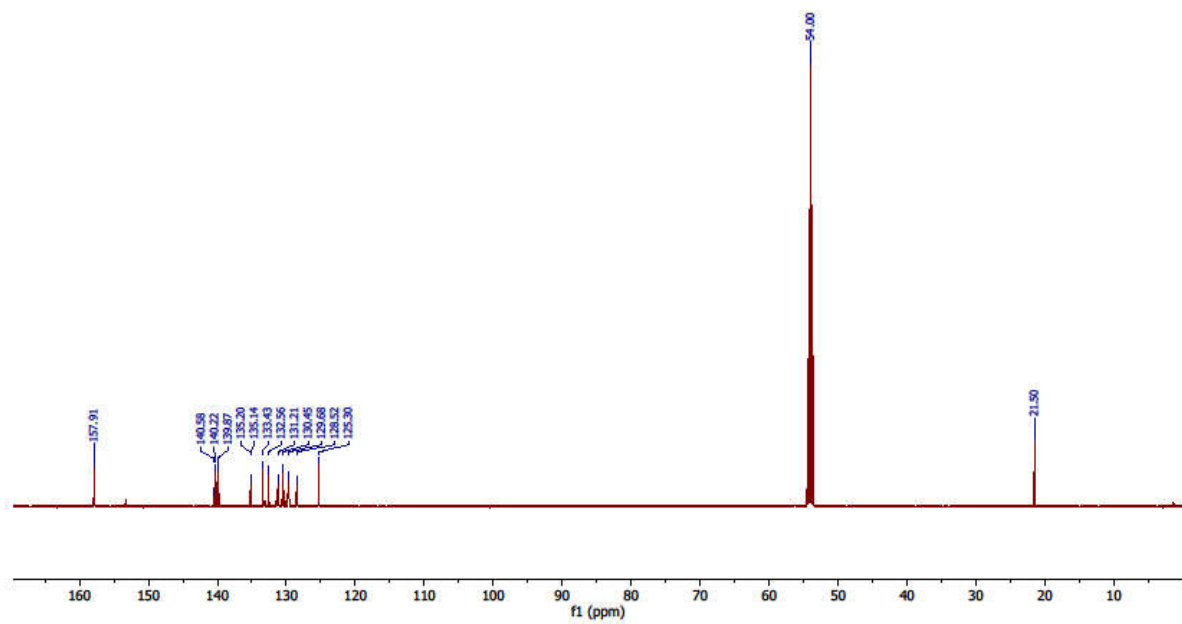


Figure S5.7. ¹³C NMR (126 MHz, 22°C) spectrum of **(L3)₃Fe(PF₆)₂** in CD₃CN.

RAJ-04-074-ASP.1.fid
(quin)₃Fe(PF₆)₂
P31CPD CD₂C₂ C:\\ Herbert 1

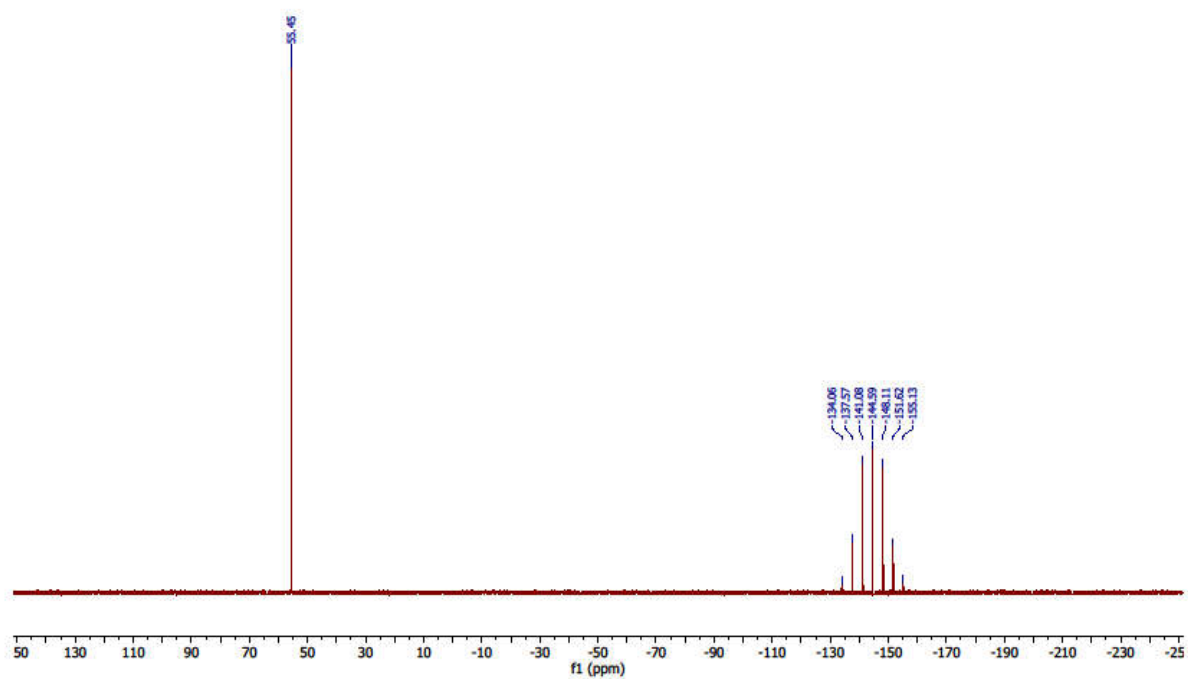


Figure S5.8. ³¹P NMR (202 MHz, 22°C) spectrum of (L3)₃Fe(PF₆)₂ in CD₃CN.

RAJ-04-074-ASF.1.fid
(quin)₃Fe(PF₆)₂
F19CPD CD₂Cl₂ C:\\ Herbert 1

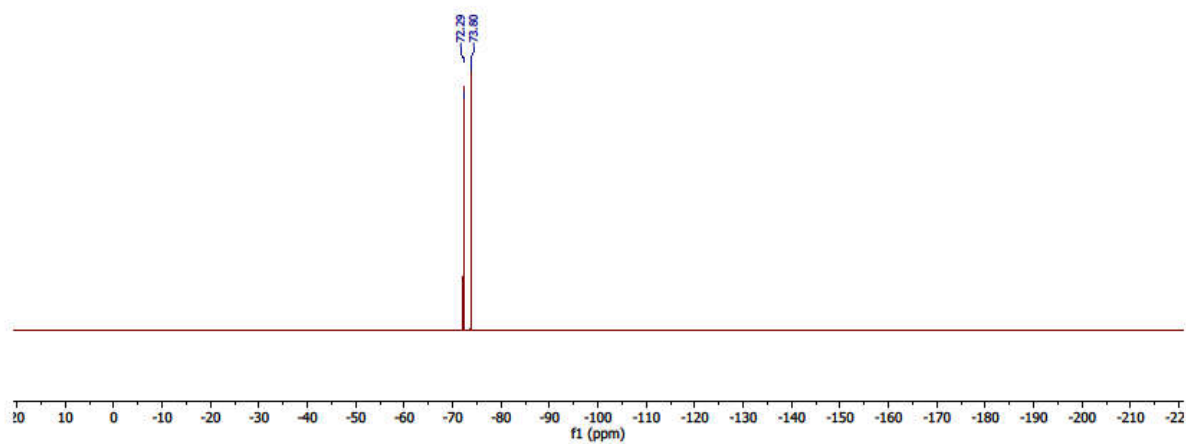


Figure S5.9. ¹⁹F NMR (282 MHz, 22°C) spectrum of (L3)₃Fe(PF₆)₂ in CD₃CN.

RAJ-04-022-B5H.2.fid
 (CN)₃Fe(PF₆)₂
 PROTON CD₃CN C:\ Herbert 1

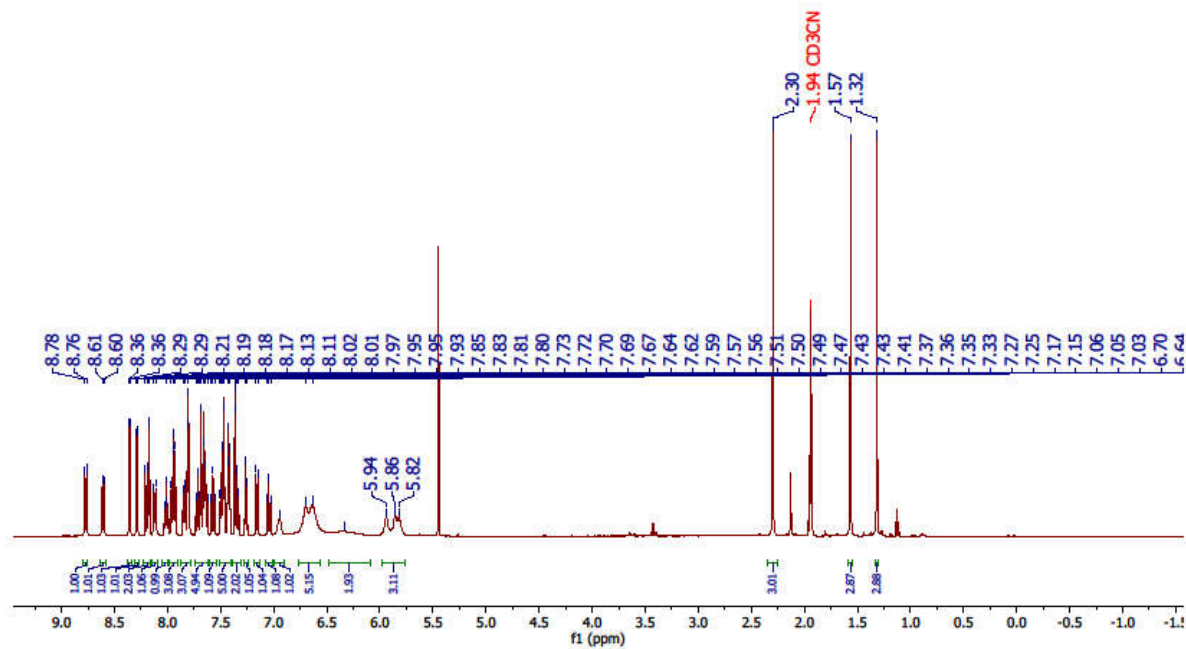


Figure S5.10. ¹H NMR (500 MHz, 22°C) spectrum of (L8)₃Fe(PF₆)₂ in CD₃CN.

RAJ-04-054-N3H2.fid
(CN)3Ru(PF6)2
PROTON CD3CN C:\ Herbert 1

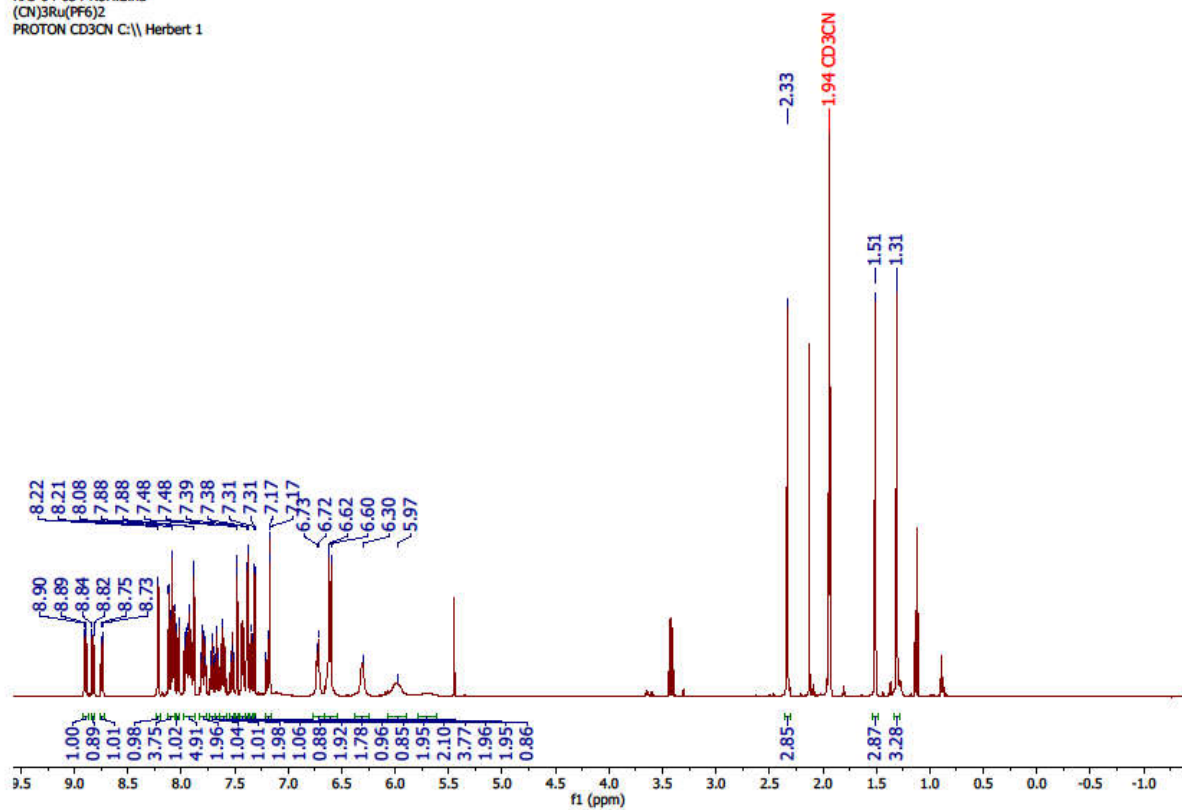


Figure S5.11. ^1H NMR (500 MHz, 22°C) spectrum of $(\text{L8})_3\text{Ru}(\text{PF}_6)_2$ in CD_3CN .

Chapter 6:

RAJ-03-080-A3Hwide.1.fid
Ph2PNCpFe(CH3CN)PF6
PROTON_wide CD3CN {C:\Bruker\TOPSPIN1.3} Herbert 33

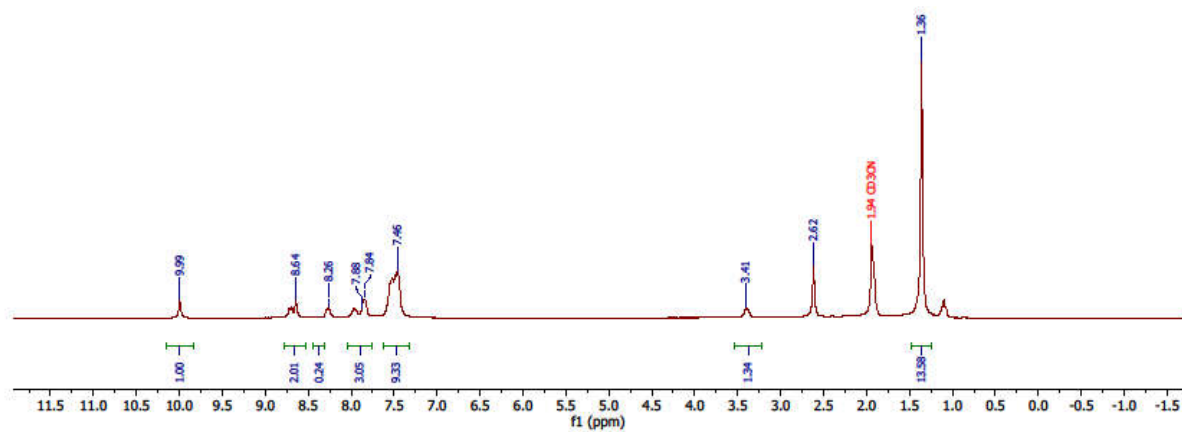


Figure S6.1. ^1H NMR (300 MHz, 22°C) spectrum of $\text{CpFeCH}_3\text{CNPF}_6$ in CD_3CN .

RAJ-03-080-A3P.1.fid
Ph2PNCpFe(CH3CN)PF6
P31CPD CD3CN {C:\Bruker\TOPSPIN1.3} Herbert 33

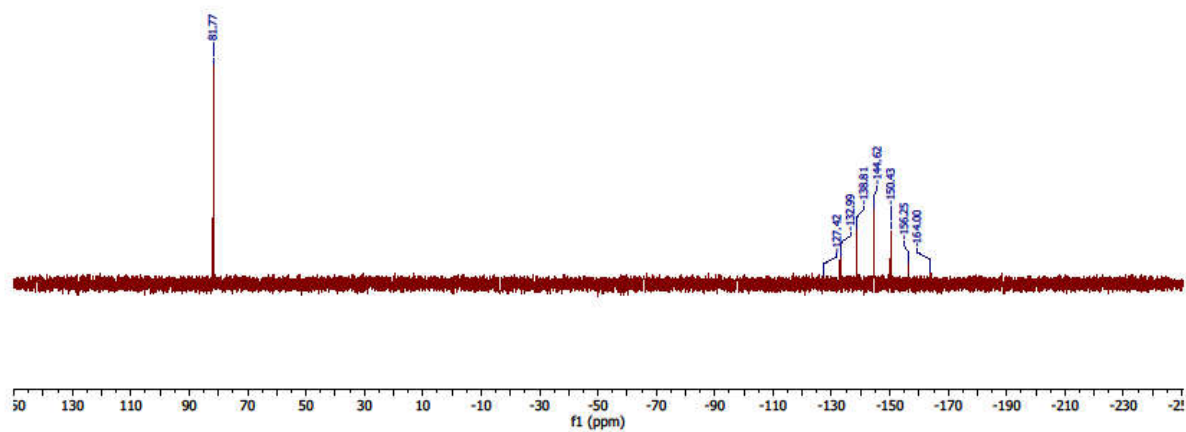


Figure S6.2. ^{31}P NMR (121 MHz, 22°C) spectrum of $\text{CpFeCH}_3\text{CNPF}_6$ in CD_3CN .

References:

- (1) Reineke, M. H.; Sampson, M. D.; Rheingold, A. L.; Kubiak, C. P. Synthesis and Structural Studies of Nickel(0) Tetracarbene Complexes with the Introduction of a New Four-Coordinate Geometric Index, T δ . *Inorg. Chem.* **2015**, *54*, 3211–3217.

Energies and Reaction Coordinates

2-I (S₀)

HF = -5794.0055983 hartrees

Zero-point correction = 0.677686 (Hartree/Particle)

Thermal correction to Gibbs Free Energy = 0.579573

Sum of electronic and zero-point Energies = -5793.327912

Sum of electronic and thermal Free Energies= -5793.426025

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	1.654559	-2.941500	-1.429459
2	1	0	0.636128	-2.720537	-1.737652
3	6	0	2.189785	-4.240490	-1.581175
4	1	0	1.581631	-5.022843	-2.022644
5	6	0	3.468830	-4.485885	-1.139924
6	1	0	3.908016	-5.477339	-1.215399
7	6	0	4.230083	-3.431400	-0.574544

8	6	0	3.623280	-2.141205	-0.499548
9	6	0	4.377176	-1.041068	0.023304
10	6	0	5.647479	-1.277550	0.510081
11	1	0	6.212082	-0.453110	0.938315
12	6	0	6.254228	-2.565325	0.475183
13	6	0	5.547926	-3.611506	-0.079192
14	1	0	5.993469	-4.602107	-0.135587
15	6	0	7.643881	-2.750020	1.033816
16	1	0	7.999795	-3.773700	0.891488
17	1	0	7.668336	-2.530695	2.107612
18	1	0	8.359368	-2.073243	0.552856
19	6	0	4.349057	1.489038	1.421369
20	6	0	5.459882	2.338074	1.298311
21	1	0	5.905004	2.513409	0.324118
22	6	0	5.994096	2.970749	2.423338
23	1	0	6.852846	3.627458	2.313229
24	6	0	5.427588	2.763096	3.681637
25	1	0	5.844181	3.256852	4.555214
26	6	0	4.316913	1.925753	3.811619
27	1	0	3.863538	1.767189	4.786042
28	6	0	3.774529	1.298499	2.690365
29	1	0	2.895616	0.667800	2.794881
30	6	0	4.288232	1.439900	-1.489760
31	6	0	5.524891	1.095336	-2.056878
32	1	0	6.111509	0.288298	-1.629992
33	6	0	6.004832	1.777019	-3.176591
34	1	0	6.962181	1.497487	-3.607977
35	6	0	5.256535	2.810921	-3.742826
36	1	0	5.630296	3.338297	-4.616045
37	6	0	4.020731	3.154545	-3.192136

38	1	0	3.424472	3.945316	-3.637991
39	6	0	3.535012	2.469051	-2.078423
40	1	0	2.555169	2.712046	-1.678820
41	29	0	1.385086	-0.103366	-0.198453
42	53	0	-0.205834	0.813646	-2.136234
43	7	0	2.332603	-1.935311	-0.904688
44	15	0	3.558065	0.622201	-0.003531
45	6	0	-1.654548	2.941493	1.429460
46	1	0	-0.636119	2.720526	1.737655
47	6	0	-2.189769	4.240486	1.581174
48	1	0	-1.581612	5.022837	2.022643
49	6	0	-3.468812	4.485886	1.139921
50	1	0	-3.907994	5.477343	1.215394
51	6	0	-4.230069	3.431404	0.574541
52	6	0	-3.623272	2.141207	0.499546
53	6	0	-4.377172	1.041073	-0.023306
54	6	0	-5.647474	1.277560	-0.510084
55	1	0	-6.212079	0.453122	-0.938319
56	6	0	-6.254217	2.565338	-0.475188
57	6	0	-5.547911	3.611516	0.079187
58	1	0	-5.993449	4.602119	0.135581
59	6	0	-7.643868	2.750038	-1.033823
60	1	0	-7.999777	3.773720	-0.891496
61	1	0	-7.668322	2.530713	-2.107620
62	1	0	-8.359359	2.073265	-0.552864
63	6	0	-4.349064	-1.489035	-1.421368
64	6	0	-5.459889	-2.338071	-1.298308
65	1	0	-5.905009	-2.513406	-0.324114
66	6	0	-5.994105	-2.970745	-2.423335
67	1	0	-6.852856	-3.627454	-2.313225

68	6	0	-5.427599	-2.763092	-3.681634
69	1	0	-5.844193	-3.256847	-4.555210
70	6	0	-4.316924	-1.925749	-3.811617
71	1	0	-3.863551	-1.767185	-4.786041
72	6	0	-3.774537	-1.298496	-2.690364
73	1	0	-2.895624	-0.667798	-2.794881
74	6	0	-4.288239	-1.439894	1.489763
75	6	0	-5.524897	-1.095325	2.056879
76	1	0	-6.111512	-0.288285	1.629992
77	6	0	-6.004841	-1.777005	3.176594
78	1	0	-6.962188	-1.497469	3.607979
79	6	0	-5.256547	-2.810909	3.742831
80	1	0	-5.630309	-3.338282	4.616051
81	6	0	-4.020743	-3.154537	3.192141
82	1	0	-3.424488	-3.945310	3.637998
83	6	0	-3.535022	-2.469047	2.078428
84	1	0	-2.555180	-2.712045	1.678825
85	29	0	-1.385086	0.103357	0.198454
86	53	0	0.205833	-0.813659	2.136233
87	7	0	-2.332597	1.935307	0.904689
88	15	0	-3.558068	-0.622200	0.003532

2-I (T₁)

HF=-5793.9394098 hartrees

Zero-point correction= 0.675397
(Hartree/Particle)

Sum of electronic and zero-point Energies= -5793.264013

Sum of electronic and thermal Energies= -5793.212911

Sum of electronic and thermal Free Energies= -5793.361762

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

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3	6	0	-0.533997	3.600870	-1.730036
4	1	0	0.291982	4.091588	-2.235204
5	6	0	-1.654780	4.329434	-1.297842
6	1	0	-1.716115	5.403018	-1.448430
7	6	0	-2.737239	3.650296	-0.683482
8	6	0	-2.621069	2.222755	-0.501798
9	6	0	-3.703268	1.521554	0.084057
10	6	0	-4.860121	2.213475	0.537773
11	1	0	-5.659466	1.657852	1.019602
12	6	0	-4.970671	3.589678	0.381788
13	6	0	-3.913319	4.289195	-0.230015
14	1	0	-3.987158	5.367846	-0.351972
15	6	0	-6.195174	4.333636	0.861122
16	1	0	-6.695240	4.856485	0.036551
17	1	0	-5.934694	5.094058	1.607639
18	1	0	-6.922685	3.655431	1.316344
19	6	0	-4.296714	-0.847602	1.687765
20	6	0	-5.240344	-1.885484	1.705396
21	1	0	-5.549673	-2.355291	0.777935
22	6	0	-5.792318	-2.313240	2.913875
23	1	0	-6.525904	-3.114418	2.914499
24	6	0	-5.408163	-1.713573	4.113708
25	1	0	-5.839172	-2.048615	5.052850
26	6	0	-4.465474	-0.682181	4.104125
27	1	0	-4.159546	-0.213585	5.034909

28	6	0	-3.908856	-0.253234	2.901451
29	1	0	-3.174345	0.546019	2.901206
30	6	0	-4.434758	-1.039830	-1.231417
31	6	0	-5.439895	-0.346380	-1.922430
32	1	0	-5.680920	0.673723	-1.641380
33	6	0	-6.122156	-0.965591	-2.970266
34	1	0	-6.899210	-0.422523	-3.500663
35	6	0	-5.806385	-2.274936	-3.338753
36	1	0	-6.337136	-2.752154	-4.157698
37	6	0	-4.799236	-2.966224	-2.662024
38	1	0	-4.538807	-3.978815	-2.955699
39	6	0	-4.109169	-2.350557	-1.617859
40	1	0	-3.310249	-2.884654	-1.111763
41	29	0	-1.216444	-0.324220	-0.290754
42	53	0	0.070578	-1.569831	-2.418407
43	7	0	-1.483598	1.553971	-0.886028
44	15	0	-3.506615	-0.256635	0.146433
45	6	0	3.040163	-3.544492	-0.097312
46	1	0	2.052008	-3.950526	-0.294008
47	6	0	4.156684	-4.398360	0.041479
48	1	0	4.023721	-5.471448	-0.042622
49	6	0	5.391507	-3.840634	0.272794
50	1	0	6.277113	-4.461856	0.377940
51	6	0	5.518472	-2.431567	0.372235
52	6	0	4.334915	-1.642213	0.233080
53	6	0	4.431888	-0.217322	0.331451
54	6	0	5.674413	0.352768	0.531650
55	1	0	5.757694	1.435474	0.582460
56	6	0	6.862118	-0.416848	0.669065
57	6	0	6.764152	-1.790581	0.592831

58	1	0	7.653843	-2.407683	0.694528
59	6	0	8.182833	0.278861	0.888992
60	1	0	9.003813	-0.437690	0.972874
61	1	0	8.411935	0.959809	0.061377
62	1	0	8.165464	0.881278	1.804464
63	6	0	3.370242	1.992561	-1.175768
64	6	0	3.954889	3.235962	-0.889729
65	1	0	4.102635	3.542925	0.140943
66	6	0	4.327582	4.094457	-1.925319
67	1	0	4.774124	5.056948	-1.691472
68	6	0	4.123464	3.721660	-3.255516
69	1	0	4.411118	4.393222	-4.059401
70	6	0	3.538674	2.487984	-3.548662
71	1	0	3.365605	2.196089	-4.580336
72	6	0	3.158884	1.629413	-2.516123
73	1	0	2.681558	0.681144	-2.750252
74	6	0	2.730679	1.771043	1.661352
75	6	0	3.438172	1.480466	2.836340
76	1	0	4.172224	0.682101	2.847585
77	6	0	3.201956	2.211307	4.003207
78	1	0	3.757059	1.972708	4.906110
79	6	0	2.259890	3.239266	4.011169
80	1	0	2.078068	3.806253	4.919622
81	6	0	1.544467	3.530508	2.846755
82	1	0	0.802054	4.323227	2.844660
83	6	0	1.769513	2.798958	1.682068
84	1	0	1.194430	3.027626	0.788462
85	29	0	1.430072	-0.962620	-0.242152
86	53	0	-0.264612	-1.648121	1.775697
87	7	0	3.118938	-2.227238	-0.006018

88	15	0	2.877801	0.775912	0.120996
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3-1 (S₀)

HF=-6101.2997378 hartrees

Zero-point correction= 0.771426

(Hartree/Particle)

Sum of electronic and zero-point Energies= -6100.528311

Sum of electronic and thermal Energies=-6100.471601

Sum of electronic and thermal Free Energies= -6100.632200

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	-3.148443	-2.825437	-0.718143
2	1	0	-2.227348	-3.226966	-1.137083
3	6	0	-4.264383	-3.695867	-0.503129
4	6	0	-4.195192	-5.063097	-0.852251
5	1	0	-3.282730	-5.444379	-1.302308
6	6	0	-5.271199	-5.896159	-0.619512
7	1	0	-5.220412	-6.947181	-0.886489
8	6	0	-6.439884	-5.374849	-0.029023
9	1	0	-7.286253	-6.030410	0.154705
10	6	0	-6.524465	-4.038630	0.320830
11	1	0	-7.438548	-3.669381	0.772139
12	6	0	-5.439517	-3.162238	0.092255

13	6	0	-5.447178	-1.746773	0.418648
14	6	0	-4.290844	-0.980000	0.111351
15	6	0	-4.278866	0.422537	0.365592
16	6	0	-5.375454	1.006844	0.977951
17	1	0	-5.356917	2.069577	1.205242
18	6	0	-6.521526	0.255833	1.326828
19	6	0	-6.543783	-1.096600	1.028078
20	1	0	-7.430505	-1.668645	1.281438
21	6	0	-7.686819	0.932478	2.007763
22	1	0	-8.055266	1.780109	1.418859
23	1	0	-7.395155	1.326473	2.988286
24	1	0	-8.519706	0.240784	2.159292
25	6	0	-3.266048	2.123375	-1.767902
26	6	0	-4.582215	2.487401	-2.094927
27	1	0	-5.387721	2.305812	-1.390543
28	6	0	-4.868279	3.072181	-3.329094
29	1	0	-5.891537	3.345593	-3.571727
30	6	0	-3.844481	3.300045	-4.251814
31	1	0	-4.070126	3.751849	-5.213760
32	6	0	-2.534907	2.932617	-3.940224
33	1	0	-1.736546	3.089521	-4.659598
34	6	0	-2.247025	2.341259	-2.709039
35	1	0	-1.234258	2.018633	-2.487346
36	6	0	-2.737901	2.772634	1.027510
37	6	0	-2.276113	2.508510	2.331065
38	1	0	-1.973453	1.500299	2.602991
39	6	0	-2.188001	3.534546	3.271361
40	1	0	-1.832068	3.313347	4.273524
41	6	0	-2.543926	4.841073	2.924112
42	1	0	-2.470442	5.639965	3.656679

43	6	0	-2.988761	5.114722	1.629696
44	1	0	-3.265305	6.127955	1.350639
45	6	0	-3.086475	4.088197	0.685702
46	1	0	-3.433409	4.314516	-0.317138
47	6	0	1.464165	2.372382	0.535541
48	1	0	0.452034	2.180244	0.885426
49	6	0	1.897321	3.723980	0.349126
50	6	0	1.038190	4.807030	0.643564
51	1	0	0.045222	4.603142	1.034138
52	6	0	1.462024	6.104162	0.433043
53	1	0	0.804970	6.938584	0.658224
54	6	0	2.753391	6.342358	-0.078746
55	1	0	3.085205	7.363403	-0.244495
56	6	0	3.606289	5.293001	-0.373068
57	1	0	4.594538	5.510651	-0.762465
58	6	0	3.202430	3.954641	-0.164724
59	6	0	4.037905	2.795950	-0.428677
60	6	0	3.510458	1.506817	-0.144412
61	6	0	4.326721	0.349999	-0.315972
62	6	0	5.600075	0.496358	-0.840738
63	1	0	6.215344	-0.384997	-1.001296
64	6	0	6.125869	1.764725	-1.179465
65	6	0	5.347654	2.887474	-0.951499
66	1	0	5.760662	3.862121	-1.190595
67	6	0	7.511401	1.871852	-1.769518
68	1	0	7.564289	1.369025	-2.742193
69	1	0	8.257783	1.396527	-1.123014
70	1	0	7.806642	2.914442	-1.914905
71	6	0	4.298258	-1.545065	1.885388
72	6	0	3.608880	-2.441718	2.718643

73	1	0	2.693138	-2.906594	2.366024
74	6	0	4.076065	-2.716224	4.003910
75	1	0	3.530575	-3.410345	4.636627
76	6	0	5.227043	-2.086429	4.481323
77	1	0	5.585137	-2.293223	5.486015
78	6	0	5.909198	-1.179807	3.668044
79	1	0	6.799791	-0.678681	4.037562
80	6	0	5.449215	-0.910400	2.377516
81	1	0	5.985030	-0.199471	1.756673
82	6	0	4.510648	-2.488807	-0.856103
83	6	0	5.684320	-3.143771	-0.450902
84	1	0	6.105368	-2.945984	0.529794
85	6	0	6.311192	-4.059198	-1.299101
86	1	0	7.217456	-4.561846	-0.972161
87	6	0	5.775333	-4.330135	-2.559126
88	1	0	6.263650	-5.044034	-3.216721
89	6	0	4.603387	-3.688750	-2.966622
90	1	0	4.173630	-3.903613	-3.940920
91	6	0	3.969121	-2.779749	-2.119975
92	1	0	3.043572	-2.303325	-2.431432
93	29	0	-1.312903	-0.406849	-0.256131
94	29	0	1.383874	-0.684875	0.106713
95	53	0	0.234802	-0.953876	-2.355586
96	53	0	-0.285812	-1.194600	2.132231
97	7	0	-3.148859	-1.553790	-0.425759
98	7	0	2.207534	1.326639	0.295630
99	15	0	-2.770175	1.359853	-0.161345
100	15	0	3.601447	-1.276911	0.196476

3-I (T₁)

HF=-6101.2295931 hartrees

Zero-point correction= 0.769210
(Hartree/Particle)

Sum of electronic and zero-point Energies= -6100.460383

Sum of electronic and thermal Energies= -6100.403777

Sum of electronic and thermal Free Energies= -6100.564789

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	3.620144	-2.543713	-0.685025
2	1	0	2.792257	-3.109965	-1.107269
3	6	0	4.911217	-3.150846	-0.587508
4	6	0	5.122410	-4.476909	-1.027182
5	1	0	4.286821	-5.031435	-1.445078
6	6	0	6.372709	-5.052372	-0.922550
7	1	0	6.539068	-6.071027	-1.258565
8	6	0	7.436747	-4.308651	-0.373741
9	1	0	8.420245	-4.761899	-0.290216
10	6	0	7.247343	-3.008444	0.060726
11	1	0	8.088279	-2.466043	0.477687
12	6	0	5.978653	-2.393033	-0.035391
13	6	0	5.692696	-1.032654	0.387458
14	6	0	4.365061	-0.540188	0.239719
15	6	0	4.057507	0.795794	0.630108
16	6	0	5.064793	1.597003	1.143705
17	1	0	4.838526	2.620829	1.428511
18	6	0	6.385634	1.126751	1.308627
19	6	0	6.673814	-0.174624	0.929713
20	1	0	7.689952	-0.535327	1.050225

21	6	0	7.446181	2.036929	1.879148
22	1	0	7.184466	2.364202	2.891901
23	1	0	7.560563	2.940361	1.269538
24	1	0	8.418169	1.539263	1.928168
25	6	0	1.843619	2.223589	1.926957
26	6	0	2.412710	1.873647	3.160649
27	1	0	3.237361	1.170147	3.201099
28	6	0	1.923345	2.424532	4.346794
29	1	0	2.375961	2.144241	5.293816
30	6	0	0.859756	3.326437	4.317820
31	1	0	0.481322	3.754326	5.241736
32	6	0	0.277529	3.669295	3.095256
33	1	0	-0.558392	4.361723	3.061061
34	6	0	0.758207	3.118454	1.908097
35	1	0	0.281606	3.382194	0.968515
36	6	0	2.618402	2.804088	-0.833962
37	6	0	2.531001	2.509353	-2.204279
38	1	0	2.240345	1.512182	-2.524600
39	6	0	2.795185	3.494595	-3.157562
40	1	0	2.722345	3.252753	-4.213839
41	6	0	3.134921	4.787128	-2.753466
42	1	0	3.332448	5.555873	-3.495096
43	6	0	3.208233	5.092239	-1.392380
44	1	0	3.460460	6.099438	-1.072659
45	6	0	2.954042	4.107683	-0.436923
46	1	0	2.998095	4.361396	0.617524
47	6	0	-1.365811	2.176503	-1.140452
48	1	0	-0.432557	1.875461	-1.598082
49	6	0	-1.782133	3.515825	-1.156648
50	6	0	-0.968056	4.546039	-1.720733

51	1	0	-0.009458	4.274457	-2.153416
52	6	0	-1.387026	5.859535	-1.717405
53	1	0	-0.752151	6.628737	-2.149882
54	6	0	-2.632743	6.211210	-1.157189
55	1	0	-2.959418	7.246628	-1.154091
56	6	0	-3.446754	5.221753	-0.612631
57	1	0	-4.406004	5.511044	-0.194642
58	6	0	-3.057933	3.873433	-0.597434
59	6	0	-3.890721	2.791218	-0.064039
60	6	0	-3.368411	1.452900	-0.098347
61	6	0	-4.189464	0.395407	0.388357
62	6	0	-5.455160	0.655001	0.949100
63	1	0	-6.043277	-0.170547	1.341398
64	6	0	-5.955418	1.948784	1.008114
65	6	0	-5.158768	2.990961	0.489136
66	1	0	-5.556574	4.000473	0.534774
67	6	0	-7.308469	2.248862	1.607698
68	1	0	-7.226206	2.910880	2.478904
69	1	0	-7.810966	1.333677	1.934207
70	1	0	-7.966481	2.751429	0.888010
71	6	0	-4.240098	-2.032298	-1.307237
72	6	0	-3.628471	-3.174282	-1.851318
73	1	0	-2.728301	-3.578150	-1.396987
74	6	0	-4.165749	-3.784802	-2.984018
75	1	0	-3.685284	-4.665825	-3.399111
76	6	0	-5.304705	-3.252660	-3.592899
77	1	0	-5.716174	-3.723866	-4.480967
78	6	0	-5.906178	-2.108207	-3.066563
79	1	0	-6.786878	-1.686891	-3.542757
80	6	0	-5.377937	-1.497169	-1.928530

81	1	0	-5.843683	-0.604487	-1.524092
82	6	0	-4.069129	-2.253704	1.609975
83	6	0	-4.802287	-3.440223	1.460513
84	1	0	-5.070448	-3.793596	0.470727
85	6	0	-5.196759	-4.169137	2.583990
86	1	0	-5.768344	-5.083915	2.455662
87	6	0	-4.863055	-3.724498	3.863385
88	1	0	-5.170485	-4.293996	4.735803
89	6	0	-4.129431	-2.545353	4.019554
90	1	0	-3.862006	-2.196056	5.012484
91	6	0	-3.730407	-1.815482	2.902463
92	1	0	-3.154080	-0.904777	3.032147
93	29	0	1.381538	-0.541687	-0.340432
94	29	0	-1.307479	-0.609511	-0.237601
95	53	0	0.038351	-1.945187	1.587841
96	53	0	0.141557	-1.211053	-2.555454
97	7	0	3.353100	-1.326770	-0.294999
98	7	0	-2.116231	1.173414	-0.580996
99	15	0	2.329483	1.416916	0.348931
100	15	0	-3.505934	-1.253526	0.184131

Energies and Reaction Coordinates

$I^+(S_0)$

HF = -4356.9073317 hartrees

Zero-point correction=

0.726635

(Hartree/Particle)

Thermal correction to Gibbs Free Energy=

0.643816

Sum of electronic and zero-point Energies=

-4356.180696

Sum of electronic and thermal Free Energies=

-4356.263515

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	-0.000323	-0.001770	0.293419
2	15	0	-1.424963	1.580375	0.981777
3	6	0	-1.703381	1.100502	3.680063
4	1	0	-1.300317	0.117489	3.423255
5	6	0	-1.866131	2.064262	2.678354

6	6	0	-2.045838	1.392564	4.995802
7	1	0	-1.919225	0.634959	5.771636
8	6	0	-2.691484	3.621264	4.332030
9	1	0	-3.072313	4.611703	4.588600
10	6	0	-2.539580	2.654010	5.322518
11	1	0	-2.801947	2.886585	6.356439
12	6	0	-2.357669	3.329636	3.012114
13	1	0	-2.472536	4.094051	2.240865
14	7	0	-1.579286	-0.672258	-0.924114
15	6	0	-2.848194	-0.185388	-0.644317
16	6	0	-1.434762	-1.646843	-1.767167
17	1	0	-0.417031	-2.003523	-1.953867
18	6	0	-2.519097	-2.286778	-2.442835
19	6	0	-4.000912	-0.743935	-1.243796
20	6	0	-3.833474	-1.840780	-2.181472
21	6	0	-5.260822	-0.215279	-0.895510
22	1	0	-6.163204	-0.631113	-1.342497
23	6	0	-2.283681	-3.354306	-3.333868
24	1	0	-1.256884	-3.684116	-3.504973
25	6	0	-5.374506	0.817444	0.009761
26	1	0	-6.359722	1.205677	0.273014
27	6	0	-4.898057	-2.487623	-2.840513
28	1	0	-5.926278	-2.172715	-2.666416
29	6	0	-3.340659	-3.969482	-3.964511
30	1	0	-3.167649	-4.795993	-4.655595
31	6	0	-4.652785	-3.527765	-3.713200
32	1	0	-5.490284	-4.016509	-4.214730
33	6	0	-1.150038	3.141794	0.074088
34	6	0	-0.014227	3.890526	0.414090
35	1	0	0.610238	3.579953	1.255880
36	6	0	0.330834	5.020269	-0.316641
37	1	0	1.214894	5.597429	-0.039149
38	6	0	-1.922790	3.537606	-1.019889
39	1	0	-2.806837	2.964487	-1.302933
40	6	0	-1.568217	4.666610	-1.758644
41	1	0	-2.181641	4.968804	-2.609856
42	6	0	-0.444701	5.408961	-1.409270
43	1	0	-0.171315	6.294438	-1.986449
44	6	0	-2.971813	0.895130	0.271172
45	6	0	-4.227189	1.373854	0.594894
46	1	0	-4.328690	2.189557	1.313268
47	15	0	1.428066	-1.581852	0.978015
48	6	0	1.708787	-1.105715	3.676705
49	1	0	1.303227	-0.123184	3.422002
50	6	0	1.872350	-2.067496	2.673239
51	6	0	2.053589	-1.399150	4.991533
52	1	0	1.926296	-0.643083	5.768755
53	6	0	2.703318	-3.625341	4.323311
54	1	0	3.086677	-4.615341	4.577792
55	6	0	2.550549	-2.660017	5.315560
56	1	0	2.814774	-2.893682	6.348763
57	6	0	2.367139	-3.332324	3.004313
58	1	0	2.482683	-4.095239	2.231679
59	7	0	1.575635	0.670666	-0.928010
60	6	0	2.845898	0.186616	-0.649554
61	6	0	1.428114	1.644862	-1.770967
62	1	0	0.409408	1.999287	-1.956648

63	6	0	2.510339	2.287182	-2.447773
64	6	0	3.996771	0.747591	-1.250288
65	6	0	3.825967	1.844108	-2.187734
66	6	0	5.258166	0.221524	-0.903442
67	1	0	6.159186	0.639242	-1.351422
68	6	0	2.271680	3.354205	-3.338541
69	1	0	1.243999	3.681769	-3.508612
70	6	0	5.374989	-0.811054	0.001593
71	1	0	6.361295	-1.197312	0.263666
72	6	0	4.888458	2.493329	-2.847812
73	1	0	5.917546	2.180694	-2.674742
74	6	0	3.326661	3.971767	-3.970196
75	1	0	3.151123	4.797917	-4.661076
76	6	0	4.640015	3.532967	-3.720203
77	1	0	5.475929	4.023591	-4.222542
78	6	0	1.153696	-3.142321	0.068484
79	6	0	0.020738	-3.894382	0.410637
80	1	0	-0.601485	-3.587242	1.255340
81	6	0	-0.324338	-5.023159	-0.321588
82	1	0	-1.206123	-5.602967	-0.042380
83	6	0	1.923566	-3.533855	-1.029062
84	1	0	2.805394	-2.958129	-1.313748
85	6	0	1.568954	-4.661893	-1.769270
86	1	0	2.180132	-4.960731	-2.623278
87	6	0	0.448275	-5.407548	-1.417811
88	1	0	0.174892	-6.292296	-1.996111
89	6	0	2.972789	-0.893656	0.265760
90	6	0	4.229485	-1.369890	0.587982
91	1	0	4.333477	-2.185473	1.306128

$I^+(T_1)$

HF = -4356.8225394 hartrees

Zero-point correction=

0.723727

(Hartree/Particle)

Thermal correction to Gibbs Free Energy=

0.640649

Sum of electronic and zero-point Energies=

-4356.098813

Sum of electronic and thermal Free Energies=

-4356.181890

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	-0.212856	0.260850	0.586020
2	15	0	-0.101624	1.462900	-1.368231
3	6	0	1.729102	3.488725	-1.080677
4	1	0	1.337808	3.553310	-0.062660
5	6	0	1.213019	2.538138	-1.971114
6	6	0	2.739328	4.348179	-1.489943
7	1	0	3.137644	5.087815	-0.793552
8	6	0	2.742372	3.311777	-3.671077
9	1	0	3.135659	3.246918	-4.687312
10	6	0	3.248331	4.258645	-2.784910
11	1	0	4.044321	4.933760	-3.105181
12	6	0	1.724534	2.450913	-3.269240
13	1	0	1.324888	1.715973	-3.969872
14	7	0	-2.048276	0.826179	0.608131

15	6	0	-2.492918	1.842692	-0.188983
16	6	0	-2.881197	0.283973	1.562799
17	1	0	-2.486035	-0.549578	2.147297
18	6	0	-4.173898	0.780106	1.799107
19	6	0	-3.791946	2.409349	-0.035012
20	6	0	-4.672685	1.859783	1.006398
21	6	0	-4.145850	3.466375	-0.872070
22	1	0	-5.128157	3.924896	-0.757908
23	6	0	-5.010544	0.227049	2.805466
24	1	0	-4.628964	-0.597606	3.412215
25	6	0	-3.284999	3.978034	-1.851025
26	1	0	-3.606789	4.811970	-2.475844
27	6	0	-5.964887	2.334017	1.249132
28	1	0	-6.362614	3.156250	0.653504
29	6	0	-6.279701	0.718991	3.017849
30	1	0	-6.908813	0.282505	3.796487
31	6	0	-6.767307	1.780299	2.238669
32	1	0	-7.771954	2.170288	2.408062
33	6	0	-0.339601	0.080545	-2.526400
34	6	0	0.719044	-0.804461	-2.772251
35	1	0	1.713911	-0.590583	-2.377331
36	6	0	0.508724	-1.964319	-3.507334
37	1	0	1.339508	-2.647892	-3.691786
38	6	0	-1.611703	-0.216097	-3.024150
39	1	0	-2.442478	0.464901	-2.830751
40	6	0	-1.818261	-1.381868	-3.758007
41	1	0	-2.814008	-1.605741	-4.145329
42	6	0	-0.763536	-2.258276	-3.996464
43	1	0	-0.931846	-3.175373	-4.564039
44	6	0	-1.640853	2.351002	-1.203837
45	6	0	-2.030662	3.419166	-2.020015
46	1	0	-1.347734	3.800904	-2.781978
47	15	0	1.898632	-0.113991	1.332131
48	6	0	3.862645	0.654676	-0.500487
49	1	0	3.458545	-0.120647	-1.153169
50	6	0	3.347951	0.830271	0.789592
51	6	0	4.900643	1.457820	-0.956060
52	1	0	5.294370	1.313569	-1.963450
53	6	0	4.919411	2.631384	1.150034
54	1	0	5.333914	3.403926	1.800330
55	6	0	5.431174	2.446960	-0.130979
56	1	0	6.247376	3.076892	-0.489450
57	6	0	3.878891	1.829827	1.611108
58	1	0	3.485253	1.981309	2.617831
59	7	0	-0.266206	-1.822039	0.342917
60	6	0	0.944941	-2.493683	0.280701
61	6	0	-1.348361	-2.389438	-0.097251
62	1	0	-2.271612	-1.803273	-0.048235
63	6	0	-1.383864	-3.705926	-0.645649
64	6	0	1.032475	-3.805526	-0.235766
65	6	0	-0.178624	-4.438891	-0.726226
66	6	0	2.298550	-4.424329	-0.276212
67	1	0	2.390797	-5.438822	-0.662587
68	6	0	-2.593348	-4.251223	-1.123321
69	1	0	-3.508592	-3.660103	-1.049705
70	6	0	3.430069	-3.766863	0.157194
71	1	0	4.400391	-4.263644	0.112026

72	6	0	-0.221022	-5.727052	-1.294063
73	1	0	0.685861	-6.325348	-1.373515
74	6	0	-2.607920	-5.510994	-1.676254
75	1	0	-3.539137	-5.941043	-2.048162
76	6	0	-1.411847	-6.247622	-1.758603
77	1	0	-1.425751	-7.247819	-2.195901
78	6	0	1.942011	-0.190040	3.145775
79	6	0	0.817378	0.245813	3.852812
80	1	0	-0.050381	0.643604	3.319020
81	6	0	0.797193	0.180899	5.243811
82	1	0	-0.083105	0.524127	5.789985
83	6	0	3.047956	-0.692028	3.842034
84	1	0	3.933369	-1.032459	3.301510
85	6	0	3.024282	-0.754113	5.229384
86	1	0	3.888032	-1.144973	5.770255
87	6	0	1.898996	-0.318901	5.930210
88	1	0	1.884533	-0.369898	7.020632
89	6	0	2.115936	-1.819038	0.717147
90	6	0	3.341059	-2.456346	0.648596
91	1	0	4.247967	-1.935629	0.961496

2⁺ (S₀)

HF = -4435.4439075 hartrees

Zero-point correction=

0.781268

(Hartree/Particle)

Thermal correction to Gibbs Free Energy=

0.693458

Sum of electronic and zero-point Energies=

-4434.662640

Sum of electronic and thermal Free Energies=

-4434.750450

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	0.000000	0.000005	0.274723
2	15	0	1.672241	-1.318644	0.964243
3	15	0	-1.672249	1.318655	0.964222
4	7	0	-1.440128	-0.928098	-0.943276
5	7	0	1.440141	0.928096	-0.943273
6	6	0	-2.191360	1.727176	2.658853
7	6	0	2.771433	0.663072	-0.661150
8	6	0	-3.079772	0.378415	0.256009
9	6	0	3.079772	-0.378410	0.256036
10	6	0	3.816955	1.402369	-1.256022
11	6	0	-1.667104	2.900809	0.050649
12	6	0	1.135732	1.862882	-1.789018
13	1	0	0.073274	2.043946	-1.978902
14	6	0	-2.771423	-0.663073	-0.661166
15	6	0	2.100996	2.672912	-2.462910
16	6	0	3.471055	2.453423	-2.196971
17	6	0	-1.135710	-1.862896	-1.789004
18	1	0	-0.073249	-2.043966	-1.978870
19	6	0	-0.677969	3.835487	0.388369
20	1	0	-0.011608	3.641436	1.232935
21	6	0	2.191339	-1.727156	2.658880
22	6	0	5.454861	0.098894	0.005763
23	6	0	5.146814	1.093529	-0.902496

24	1	0	5.963433	1.658618	-1.351808
25	6	0	2.634993	4.466242	-3.987173
26	1	0	2.328273	5.250683	-4.680917
27	6	0	-2.891999	2.891393	2.987205
28	1	0	-3.133584	3.622252	2.212719
29	6	0	-2.100966	-2.672939	-2.462890
30	6	0	4.001923	4.250551	-3.731396
31	1	0	4.747474	4.871212	-4.232158
32	6	0	-2.961774	2.202735	5.299892
33	1	0	-3.262146	2.390848	6.332531
34	6	0	-4.395346	0.634864	0.579882
35	1	0	-4.628219	1.423036	1.299964
36	6	0	4.414456	3.268000	-2.855412
37	1	0	5.480177	3.129238	-2.677642
38	6	0	1.667097	-2.900801	0.050675
39	6	0	-3.816938	-1.402380	-1.256038
40	6	0	-6.873722	0.211076	0.389917
41	1	0	-7.117513	1.264421	0.184313
42	1	0	-7.032342	0.047247	1.466831
43	1	0	-7.588768	-0.416673	-0.157621
44	6	0	1.693946	3.684530	-3.357654
45	1	0	0.627012	3.837798	-3.532524
46	6	0	-1.869388	0.808751	3.664599
47	1	0	-1.304390	-0.092240	3.412139
48	6	0	-1.693906	-3.684575	-3.357610
49	1	0	-0.626969	-3.837847	-3.532466
50	6	0	-5.454858	-0.098898	0.005721
51	6	0	4.395343	-0.634859	0.579922
52	1	0	4.628208	-1.423027	1.300011
53	6	0	-2.259711	1.042673	4.978659
54	1	0	-2.007700	0.320345	5.757559
55	6	0	-4.001878	-4.250604	-3.731367
56	1	0	-4.747423	-4.871276	-4.232125
57	6	0	-3.273716	3.126565	4.305451
58	1	0	-3.817989	4.038734	4.557616
59	6	0	-2.634946	-4.466299	-3.987125
60	1	0	-2.328218	-5.250753	-4.680851
61	6	0	-3.471028	-2.453447	-2.196970
62	6	0	-2.492829	3.151768	-1.047497
63	1	0	-3.263673	2.433000	-1.329182
64	6	0	1.869360	-0.808724	3.664618
65	1	0	1.304365	0.092266	3.412148
66	6	0	-0.529808	5.003553	-0.348569
67	1	0	0.241326	5.725395	-0.072940
68	6	0	6.873722	-0.211080	0.389971
69	1	0	7.588774	0.416659	-0.157569
70	1	0	7.117510	-1.264429	0.184382
71	1	0	7.032335	-0.047239	1.466885
72	6	0	2.259672	-1.042640	4.978683
73	1	0	2.007655	-0.320306	5.757576
74	6	0	2.891974	-2.891372	2.987244
75	1	0	3.133564	-3.622235	2.212764
76	6	0	-5.146801	-1.093541	-0.902526
77	1	0	-5.963415	-1.658638	-1.351837
78	6	0	-4.414421	-3.268038	-2.855405
79	1	0	-5.480144	-3.129276	-2.677646
80	6	0	0.677946	-3.835466	0.388381

81	1	0	0.011576	-3.641408	1.232938
82	6	0	2.961731	-2.202701	5.299928
83	1	0	3.262095	-2.390809	6.332570
84	6	0	-1.356935	5.246943	-1.445349
85	1	0	-1.237486	6.162658	-2.027716
86	6	0	3.273679	-3.126537	4.305495
87	1	0	3.817949	-4.038705	4.557669
88	6	0	2.335025	-4.320522	-1.792527
89	1	0	2.987963	-4.507594	-2.647442
90	6	0	-2.335028	4.320525	-1.792558
91	1	0	-2.987959	4.507592	-2.647479
92	6	0	1.356916	-5.246928	-1.445331
93	1	0	1.237462	-6.162640	-2.027703
94	6	0	2.492831	-3.151767	-1.047462
95	1	0	3.263684	-2.433006	-1.329139
96	6	0	0.529779	-5.003529	-0.348562
97	1	0	-0.241368	-5.725362	-0.072943

2⁺ (T₁)

HF = -4435.3578597 hartrees

Zero-point correction=

0.778441

(Hartree/Particle)

Thermal correction to Gibbs Free Energy=

0.690788

Sum of electronic and zero-point Energies=

-4434.579419

Sum of electronic and thermal Energies=

-4434.531124

Sum of electronic and thermal Enthalpies=

-4434.530180

Sum of electronic and thermal Free Energies=

-4434.667072

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	-0.269426	0.067860	0.677863
2	15	0	-0.807926	1.354251	-1.150476
3	15	0	1.859994	0.553026	1.302636
4	7	0	0.520516	-1.819518	0.220069
5	7	0	-2.167004	-0.182424	0.825046
6	6	0	2.742121	2.058298	0.808564
7	6	0	-3.044770	0.616414	0.146077
8	6	0	2.711978	-0.848075	0.500226
9	6	0	-2.557962	1.506350	-0.840878
10	6	0	-4.447900	0.582923	0.396960
11	6	0	2.079184	0.356008	3.094559
12	6	0	-2.636378	-1.092608	1.745844
13	1	0	-1.895936	-1.734387	2.228083
14	6	0	1.891014	-1.911247	0.039609
15	6	0	-3.998115	-1.192826	2.073379
16	6	0	-4.949897	-0.357855	1.409195
17	6	0	-0.259009	-2.751083	-0.239545
18	1	0	-1.335389	-2.616185	-0.093273
19	6	0	0.937495	0.218495	3.889541
20	1	0	-0.057529	0.255137	3.437113
21	6	0	-0.102176	2.923635	-1.687900
22	6	0	-4.775340	2.362291	-1.282513
23	6	0	-5.259811	1.456245	-0.320436
24	1	0	-6.333245	1.452850	-0.125040

25	6	0	-5.802653	-2.211032	3.350965
26	1	0	-6.141397	-2.926677	4.103113
27	6	0	2.876239	3.118664	1.710441
28	1	0	2.535501	3.009963	2.741681
29	6	0	0.215265	-3.906953	-0.928532
30	6	0	-6.735667	-1.388450	2.698588
31	1	0	-7.796906	-1.461809	2.940478
32	6	0	3.893465	4.466777	-0.013820
33	1	0	4.345871	5.407074	-0.334266
34	6	0	4.078005	-0.904631	0.314452
35	1	0	4.705911	-0.075187	0.648443
36	6	0	-6.302178	-0.479251	1.742493
37	1	0	-7.042247	0.148814	1.245597
38	6	0	-0.543342	0.095549	-2.437210
39	6	0	2.478043	-3.010823	-0.620151
40	6	0	6.180339	-2.040187	-0.490663
41	1	0	6.684799	-2.073413	0.487250
42	1	0	6.540445	-1.139466	-1.010199
43	1	0	6.502887	-2.917770	-1.065689
44	6	0	-4.462561	-2.117769	3.047582
45	1	0	-3.735399	-2.755675	3.555655
46	6	0	3.179999	2.218961	-0.511489
47	1	0	3.080751	1.401349	-1.227019
48	6	0	-0.690286	-4.869444	-1.420911
49	1	0	-1.759591	-4.729468	-1.249083
50	6	0	4.688071	-2.005902	-0.321353
51	6	0	-3.412776	2.373672	-1.535029
52	1	0	-2.999577	3.058662	-2.279359
53	6	0	3.754846	3.416444	-0.918380
54	1	0	4.091487	3.532107	-1.949873
55	6	0	1.160830	-6.115891	-2.318022
56	1	0	1.530171	-6.986128	-2.864014
57	6	0	3.453621	4.316305	1.297936
58	1	0	3.561935	5.136288	2.010275
59	6	0	-0.222762	-5.964078	-2.110689
60	1	0	-0.916577	-6.713391	-2.494899
61	6	0	1.606015	-4.051831	-1.133850
62	6	0	3.346714	0.312106	3.687230
63	1	0	4.245534	0.421483	3.077161
64	6	0	0.029989	3.934413	-0.726851
65	1	0	-0.284486	3.753054	0.303622
66	6	0	1.060436	0.038607	5.265112
67	1	0	0.165228	-0.066717	5.880378
68	6	0	-5.723454	3.281379	-2.001995
69	1	0	-6.502496	2.715498	-2.535918
70	1	0	-5.197857	3.905797	-2.737183
71	1	0	-6.238655	3.953504	-1.298077
72	6	0	0.561436	5.166558	-1.081999
73	1	0	0.661625	5.951216	-0.330328
74	6	0	0.311183	3.156154	-3.002887
75	1	0	0.207362	2.375458	-3.758166
76	6	0	3.879152	-3.030483	-0.776340
77	1	0	4.347279	-3.877142	-1.278343
78	6	0	2.058792	-5.183092	-1.840805
79	1	0	3.123033	-5.332196	-2.019027
80	6	0	0.763351	-0.253269	-2.804941
81	1	0	1.610978	0.315728	-2.418618

82	6	0	0.973699	5.395619	-2.394119
83	1	0	1.393361	6.364446	-2.672028
84	6	0	2.322499	-0.004060	5.848374
85	1	0	2.420104	-0.144498	6.926608
86	6	0	0.849287	4.392278	-3.350978
87	1	0	1.164811	4.574182	-4.380066
88	6	0	-1.383183	-1.738176	-3.769239
89	1	0	-2.226681	-2.318928	-4.147262
90	6	0	3.465146	0.133786	5.059554
91	1	0	4.454396	0.101047	5.519693
92	6	0	-0.083021	-2.081266	-4.128625
93	1	0	0.096327	-2.936935	-4.782227
94	6	0	-1.616844	-0.655257	-2.924873
95	1	0	-2.636533	-0.394135	-2.636019
96	6	0	0.991136	-1.332284	-3.649679
97	1	0	2.012884	-1.597681	-3.927283

3⁺ (S₀)

HF = -4513.9891121 hartrees

Zero-point correction=

0.837257

(Hartree/Particle)

Thermal correction to Gibbs Free Energy=

0.747345

Sum of electronic and zero-point Energies=

-4513.151856

Sum of electronic and thermal Free Energies=

-4513.241767

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	0.063161	0.159798	-0.055000
2	15	0	-1.350116	1.713916	0.734603
3	15	0	1.186358	-1.474578	1.011409
4	7	0	-1.588033	-0.524066	-1.242595
5	7	0	1.896672	0.600474	-1.026300
6	6	0	-2.910801	0.935506	0.169101
7	6	0	-2.832535	-0.133105	-0.765753
8	6	0	3.031392	0.032123	-0.461144
9	6	0	2.882187	-0.982275	0.524941
10	6	0	0.900058	-3.120235	0.275631
11	6	0	-1.666755	2.044586	2.499334
12	6	0	4.328005	0.432589	-0.843001
13	6	0	-1.298937	3.351930	-0.066859
14	6	0	-4.021142	-0.761961	-1.189660
15	6	0	1.882806	-3.868755	-0.375169
16	6	0	1.334629	-1.763783	2.805480
17	6	0	-4.139085	1.330640	0.659716
18	6	0	-2.634890	-2.186025	-2.634541
19	6	0	1.993569	1.497775	-1.968885
20	6	0	-2.239116	3.775233	-1.007870
21	6	0	4.000973	-1.536416	1.114620
22	6	0	-1.481565	-1.463821	-2.141269
23	6	0	3.274970	1.984229	-2.432345
24	6	0	-2.042581	3.294919	2.996812
25	6	0	3.364480	2.982559	-3.427744
26	6	0	4.590165	3.448238	-3.846721
27	6	0	5.698798	1.951942	-2.307978

28	6	0	5.303495	-1.142669	0.750782
29	6	0	5.439927	-0.172317	-0.222923
30	6	0	-2.150242	2.381359	5.230017
31	6	0	1.548959	-5.066037	-1.005749
32	6	0	-3.916635	-1.847282	-2.148003
33	6	0	5.764784	2.925970	-3.280756
34	6	0	-5.252791	-0.317879	-0.667857
35	6	0	-5.335961	0.712443	0.248634
36	6	0	-5.030881	-2.574202	-2.614915
37	6	0	4.455678	1.459166	-1.861408
38	6	0	-2.281185	3.459919	4.359519
39	6	0	-1.530007	0.966105	3.380469
40	6	0	1.465901	-0.638130	3.628098
41	6	0	-6.651547	1.173929	0.808189
42	6	0	-0.184572	4.160113	0.197722
43	6	0	-0.420721	-3.589604	0.288264
44	6	0	-1.775423	1.132131	4.738246
45	6	0	-4.876502	-3.594622	-3.528343
46	6	0	-3.601291	-3.929958	-4.012399
47	6	0	0.732266	2.022281	-2.585505
48	6	0	1.305596	-3.035467	3.382176
49	6	0	-2.498302	-3.234408	-3.571251
50	6	0	-0.122487	-1.789970	-2.680136
51	6	0	-0.022939	5.374550	-0.457547
52	6	0	-2.067943	4.987807	-1.674220
53	6	0	6.493537	-1.770498	1.419052
54	6	0	-0.963746	5.788717	-1.400916
55	6	0	-0.750331	-4.788479	-0.332550
56	6	0	0.235263	-5.526668	-0.987065
57	6	0	1.578251	-0.783902	5.005159
58	6	0	1.409949	-3.177640	4.764700
59	6	0	1.548029	-2.055764	5.576291
60	1	0	-1.201948	-3.000428	0.775615
61	1	0	-1.783056	-5.141976	-0.318738
62	1	0	-0.022994	-6.463915	-1.483857
63	1	0	2.913059	-3.511733	-0.405473
64	1	0	2.323203	-5.642120	-1.516304
65	1	0	0.636425	-1.174923	-2.188769
66	1	0	-0.087632	-1.598297	-3.763436
67	1	0	0.127124	-2.847642	-2.521644
68	1	0	-3.486389	-4.739585	-4.734923
69	1	0	-1.511144	-3.502047	-3.945170
70	1	0	-6.029925	-2.335262	-2.253617
71	1	0	-5.751905	-4.145844	-3.876838
72	1	0	-6.175380	-0.798544	-0.992055
73	1	0	-4.187203	2.140169	1.392139
74	1	0	-6.817769	2.241289	0.597343
75	1	0	-6.676397	1.053302	1.902008
76	1	0	-7.492672	0.609287	0.385114
77	1	0	-3.108214	3.154711	-1.230898
78	1	0	-2.807451	5.308405	-2.410652
79	1	0	0.844976	5.999381	-0.237718
80	1	0	-0.834461	6.739542	-1.921579
81	1	0	0.567402	3.831665	0.920322
82	1	0	-2.147037	4.145889	2.321394
83	1	0	-2.337567	2.515301	6.297244
84	1	0	-2.572516	4.439907	4.742526

85	1	0	-1.222491	-0.009455	2.998478
86	1	0	-1.661842	0.283743	5.415930
87	1	0	-0.135939	1.497609	-2.174788
88	1	0	0.747172	1.880123	-3.675959
89	1	0	0.611328	3.097856	-2.391577
90	1	0	2.456335	3.393983	-3.866355
91	1	0	4.650146	4.220815	-4.614957
92	1	0	6.624375	1.565446	-1.884219
93	1	0	6.737412	3.294286	-3.612308
94	1	0	3.875383	-2.295795	1.890602
95	1	0	6.445034	0.133550	-0.511740
96	1	0	6.494740	-2.862339	1.280411
97	1	0	6.478189	-1.582879	2.503572
98	1	0	7.437326	-1.376584	1.019883
99	1	0	1.473096	0.361074	3.185633
100	1	0	1.680472	0.100314	5.637296
101	1	0	1.200128	-3.920841	2.752961
102	1	0	1.630920	-2.171101	6.658769
103	1	0	1.385357	-4.174751	5.208596

3⁺ (T₁)

HF = -4513.8961241 hartrees

Zero-point correction=

0.834299

(Hartree/Particle)

Thermal correction to Gibbs Free Energy=

0.743587

Sum of electronic and zero-point Energies=

-4513.061825

Sum of electronic and thermal Free Energies=

-4513.152537

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	29	0	0.293930	0.118028	0.446381
2	15	0	-1.374506	-1.158246	1.286455
3	15	0	0.944130	-0.809408	-1.543839
4	7	0	-1.274557	1.623177	0.223877
5	7	0	2.156683	0.640063	0.651299
6	6	0	-2.816715	-0.120603	0.915680
7	6	0	-2.581559	1.186459	0.408623
8	6	0	3.096217	0.161155	-0.215311
9	6	0	2.699460	-0.611288	-1.336048
10	6	0	0.304013	0.385761	-2.752117
11	6	0	-1.830416	-2.837508	0.774103
12	6	0	4.492011	0.396316	-0.027353
13	6	0	-1.135807	-1.189455	3.088203
14	6	0	-3.691361	1.991024	0.078541
15	6	0	1.167475	1.220502	-3.466381
16	6	0	0.591147	-2.478102	-2.132375
17	6	0	-4.107797	-0.587407	1.075457
18	6	0	-2.100862	3.712989	-0.647844
19	6	0	2.526623	1.403423	1.747991
20	6	0	-2.187290	-1.054456	3.999950
21	6	0	3.639657	-1.166374	-2.222621
22	6	0	-1.033733	2.806087	-0.278987
23	6	0	3.885014	1.668596	2.018964
24	6	0	-1.587516	-3.937191	1.600346

25	6	0	4.284715	2.421780	3.159580
26	6	0	5.613622	2.694100	3.404695
27	6	0	6.241377	1.484116	1.417052
28	6	0	4.991328	-0.942075	-2.041379
29	6	0	5.383570	-0.157017	-0.938409
30	6	0	-2.444790	-5.413284	-0.106298
31	6	0	0.647245	2.206959	-4.301616
32	6	0	-3.441995	3.310779	-0.470348
33	6	0	6.606575	2.227981	2.531456
34	6	0	-4.990598	1.482285	0.276160
35	6	0	-5.223841	0.211940	0.767108
36	6	0	-4.471853	4.198810	-0.840938
37	6	0	4.904489	1.188090	1.137759
38	6	0	-1.895083	-5.221571	1.156972
39	6	0	-2.372963	-3.037116	-0.501747
40	6	0	0.974532	-3.544692	-1.307708
41	6	0	-6.613654	-0.321550	0.967775
42	6	0	0.173786	-1.348293	3.558914
43	6	0	-1.082331	0.553251	-2.877912
44	6	0	-2.683948	-4.318335	-0.935524
45	6	0	-4.178704	5.437912	-1.368440
46	6	0	-2.844361	5.837759	-1.546508
47	6	0	1.434304	1.909915	2.639621
48	6	0	-0.036250	-2.735527	-3.354335
49	6	0	-1.822388	4.986957	-1.191128
50	6	0	0.383395	3.231543	-0.499000
51	6	0	0.424727	-1.391694	4.926733
52	6	0	-1.930193	-1.090626	5.366243
53	6	0	6.026067	-1.511126	-2.971876
54	6	0	-0.627061	-1.262084	5.829965
55	6	0	-1.596332	1.538261	-3.710993
56	6	0	-0.730182	2.369786	-4.421547
57	6	0	0.741041	-4.852384	-1.708415
58	6	0	-0.269365	-4.050347	-3.749456
59	6	0	0.118361	-5.106472	-2.930195
60	1	0	-1.765985	-0.079643	-2.307134
61	1	0	-2.676636	1.667032	-3.799310
62	1	0	-1.133847	3.148368	-5.071646
63	1	0	2.247327	1.102048	-3.360654
64	1	0	1.325981	2.853770	-4.860760
65	1	0	1.083800	2.437815	-0.229014
66	1	0	0.618035	4.123626	0.100125
67	1	0	0.541017	3.488601	-1.555593
68	1	0	-2.619075	6.820618	-1.963359
69	1	0	-0.790594	5.304427	-1.331241
70	1	0	-5.514769	3.913858	-0.712120
71	1	0	-4.989921	6.112602	-1.648200
72	1	0	-5.849293	2.104337	0.026032
73	1	0	-4.269836	-1.606944	1.433827
74	1	0	-6.802575	-0.538045	2.030405
75	1	0	-6.758839	-1.262059	0.415240
76	1	0	-7.374560	0.393573	0.629280
77	1	0	-3.209244	-0.911942	3.645904
78	1	0	-2.752997	-0.981921	6.075182
79	1	0	1.447628	-1.516530	5.286476
80	1	0	-0.430201	-1.288372	6.903437
81	1	0	1.005704	-1.427700	2.853919

82	1	0	-1.165758	-3.794289	2.596576
83	1	0	-2.688547	-6.420678	-0.448949
84	1	0	-1.709170	-6.076373	1.809848
85	1	0	-2.561499	-2.186252	-1.159376
86	1	0	-3.107552	-4.465080	-1.930187
87	1	0	0.438325	1.681571	2.233426
88	1	0	1.483379	3.002727	2.775053
89	1	0	1.474902	1.461508	3.646896
90	1	0	3.528095	2.789381	3.852629
91	1	0	5.892664	3.275479	4.286076
92	1	0	7.025998	1.127421	0.749507
93	1	0	7.658249	2.444031	2.724841
94	1	0	3.294492	-1.776950	-3.060651
95	1	0	6.451904	0.007299	-0.791949
96	1	0	5.563749	-2.100542	-3.775395
97	1	0	6.727942	-2.167720	-2.434392
98	1	0	6.625285	-0.714693	-3.440095
99	1	0	1.463827	-3.346608	-0.351122
100	1	0	1.042215	-5.679551	-1.063604
101	1	0	-0.331268	-1.911690	-4.006006
102	1	0	-0.063468	-6.135878	-3.245108
103	1	0	-0.748883	-4.249078	-4.709807