Supporting Information for

Synthesis of Phosphorus Amidite Ligand and investigation of its Flexibility impact on rhodium-catalyzed hydroformylation of 1-octene

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2. Experimental

General Information

Solvent were dried with standard procedures and degassed with N_2. The ^{1}H, ^{13}C, and ^{31}P NMR spectra were recorded on a Bruker ARX 400 NMR instrument. Mass spectra were recorded with an AMD 40223 (Interambulacra) spectrometer. The hydroformylation products were analyzed by Agilent GC-6890N with a FID detector and a capillary column (φ0.25m×30mm, SE-30).

Hydroformylation

The hydroformylation of olefins was carried out in a 60 ml stainless steel autoclave equipped with a magnetic stirrer. The aqueous solution of $Rh(acac)(CO)_2$, a certain amount of ligands, and olefins were introduced in autoclave. Then it was evacuated and purged five times by syngas. And the autoclave was pressurized to each desired pressere with syngas. The reaction mixture was stirred at a constant speed of 10 rps when the temperature reached the desired value. After the reaction was completed, the autoclave was quickly cooled in an ice-water bath and carefully depressurized. The reaction mixture was immediately analyzed by GC to determine the activity and regioselectivity.

Synthesis of diphenic acid (B)

The mixture of phenanthrene (8.9g, 50mmol) and glacial acetic (100ml) was heated to 85℃, adding 30% H_2O_2 solution (34.5ml) drop-wise in 40 minutes. The whole mixture was stirred for 4 h at 80℃.Then, subjecting the resulting mixture to distillation under reduced pressure to make the volume half and cooling the mixture until diphenic acid crystallises out. Yellow solid crude product was obtained by filtering the cooled mixture. The crude product was dissolved in 10% sodium carbonate solution and heating the mixture to 100℃. After addition of activated charcoal for decolouration and acidifying the filtrate with HCl to maintain a pH of 4-5. Cooling the solution until diphenic acid crystallizes out. Obtained 9.1g pure product and the yield is 90.0%.

^{1}H NMR (400 MHz, CD_3OD): δ=8.00 (dd, *J*=7.8, 1.4 Hz, 2H), 7.55 (td, *J*=7.5, 1.4 Hz, 2H), 7.44 (td, *J*=7.6, 1.3 Hz, 2H), 7.19 (dd, *J*=7.6, 1.2 Hz, 2H).

Synthesis of C

A solution of $BF_3{\cdot}Et_2O$ (2.7ml，0.19mmol) in THF (15 mL) was added slowly to a room temperature solution of $NaBH_4$ (1.78g，0.44mol) and carboxylic acids (3.8g，0.016mol) in THF (25 mL) under an inert atmosphere. The mixture was heated to reflux until TLC monitoring showed complete consumption of the substrate. The reaction mixture was cooled to 0 ºC, quenched with water (caution: vigorous gas evolution) keeping the temperature below 10 ºC. The THF was removed under reduced pressure, CH_2Cl_2 (or Et_2O) was added, and the stirring was continued for another 1 h. The organic layer was separated, washed with brine, dried over $MgSO_4$, and

the solvent was removed under reduced pressure. Purification of the residue by SiO_2 chromatography gave pure alcohol . Obtained pure product 3.0g and the yield is 90.0%.

^{1}H NMR (400 MHz, d_6-DMSO)： δ=7.61-7.53 (m, 2H), 7.39 (td, *J*=7.5, 1.3 Hz, 2H), 7.29 (td, *J*= 7.4, 1.2 Hz, 2H), 7.06 (dd, *J*=7.5, 1.2 Hz, 2H), 5.04 (t, *J* =5.4 Hz, 2H), 4.16 (qd, *J*=13.6, 5.4 Hz, 4H).

Synthesis of Ligand L1

To a solution of backbone C (3.27 mmol, 0.700g), DMAP (0.65 mmol, 80.0mmg) and chlorodipyrrolylphosphine (7.26mmol, 1.43ml) in THF (40 ml) was added dropwise a solution of triethylamine (2ml) in 15ml THF at -15℃ in 30 minutes.The triethylamine HCl salts were formed immediately after the addition. The reaction mixture was stirred for 1.5h at room temperature. The triethylamine HCl salts were then filtered off, and the solvent was removed under vacuum. The crude product was extracted by pentane (10 ml), to afford white oil products 0.73g and the yield is 41.1%.

^{1}H NMR (400 MHz, $CDCl_3$): δ=7.38 (d, *J*=4.1 Hz, 4H), 7.17 (dd, *J*=5.9, 1.9 Hz, 2H), 7.10 (d, *J*=7.5 Hz, 2H), 6.84-6.76 (m, 8H), 6.29-6.22 (m, 8H), 4.56-4.43 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ=67.20(d, J_{PC}=20Hz), 112.16(d，J_{PC}=4Hz), 121.34(d，J_{PC}=16Hz), 128.37（d，J_{PC}=21Hz），129.29,130.02,134.72(d, J_{PC}=9Hz),139.58; ^{31}P NMR (166 MHz, $CDCl_3$): δ=112.34. HRMS (ES+) Calcd. For $C_{30}H_{28}N_4O_2P_2Na$ [M+ Na^+] 538.1687，Found: 538.1674

Synthesis of Ligand L2

To a solution of backbone C (3.27 mmol, 0.700g), DMAP (0.65 mmol, 80.0mmg) and chlorodiphenylphosphane (7.26mmol, 1.30ml) in THF (40 ml) was added dropwise a solution of triethylamine (2ml) in 15ml THF at -15℃ in 30 minutes.The triethylamine HCl salts were formed immediately after the addition. The reaction mixture was stirred for 1.5h at room temperature. The triethylamine HCl salts were then filtered off, and the solvent was removed under vacuum. The crude product was extracted by n-hexane (10 ml), to afford white oil products 0.86g and the yield is 45.0%.

^{1}H NMR (400 MHz, d_6-DMSO): δ=7.55 (d, *J*=7.4 Hz, 2H), 7.44-7.39 (m, 2H), 7.37-7.26 (m, 22H), 7.15 (d, *J*=7.4 Hz, 2H), 4.58-4.44 (m, 4H). ^{13}C NMR (101 MHz, d_6-DMSO): δ=141.79 (d, *J*=19.0 Hz), 139.50 (s), 136.55 (d, *J*=9.5 Hz), 130.25 (d, *J*=9.2 Hz), 130.14 (s), 130.03 (d, *J*= 9.1 Hz), 129.82 (d, *J*= 5.6 Hz), 129.30 (s), 128.86 (dd, *J*= 6.8, 1.2 Hz), 128.23 (d, *J*= 19.0 Hz), 69.36 (d, *J*= 20.3 Hz). ^{31}P NMR (162 MHz, d_6-DMSO): δ=112.04 (s).HRMS (ES+) Calcd.

For $C_{30}H_{28}N_4O_2P_2Na$ [M+ Na^+] 582.1878，Found：582.1858

Synthesis of Ligand L3

A solution of 2,2′-dihydroxy-1,1′- biphenyl (1,7g，9.0mmol) in 25mL of THF was added dropwise to a solution of chlorodipyrrolylphosphine (3mL, 18.0mmol) and triethylamine (6.0ml，43.0mmol) in 30 mL of THF at 0℃. The triethylamine, HCl salts were filtered off after 12 h of stirring at room temperature and the solvent was removed under vacuum to get yellow oily product. The crude product was recrystallize by ethyl alcohol (10ml) to get white solid 1.94g and the yield is 42.4%.

^{1}H NMR (400 MHz, $CDCl_3$): δ=7.20 (dd, *J*=12.3, 5.0 Hz, 4H), 7.09 (t, *J*=7.4 Hz, 2H), 6.78 (d, *J*=8.0 Hz, 2H), 6.63 (s, 8H), 6.16 (s, 8H).^{31}P NMR (162 MHz, CDCl3) δ=108.31 (s).

Synthesis of Ligand L4

To a solution of backbone C (1,7g，9.0mmol) chlorodiphenylphosphane (3.3mL, 18.0mmol) in THF (25mL) was added dropwise a solution of triethylamine (6.0 ml，43mmol) in THF (30mL) at -15℃ in 30 minutes. The triethylamine HCl salts were formed immediately after the addition. The reaction mixture was stirred overnight at room temperature. The triethylamine HCl salts were then filtered off, and the solvent was removed under vacuum. The crude product was extracted by n-hexane (10 ml), to afford white oil products 1.85g and the yield is 37.1%.

^{1}H NMR (400 MHz, $CDCl_3$): δ=7.21 (ddd, *J*=7.6, 4.3, 1.5 Hz, 10H), 7.16 (ddd, *J*=9.6, 5.5, 3.5 Hz, 6H), 7.13-7.06 (m, 10H), 6.97 (td, *J* = 7.4, 0.9 Hz, 2H). ^{31}P NMR (162 MHz, $CDCl_3$) δ=111.81 (s).

Synthesis of Ligand L5

Triphenylphosphine (5.2g，19.8mmol), THF (30ml) and lithium (0.45g, 64.8mmol) were added respectively in100 ml three flask. Then reaction was stirred overnight at room temperature and the lithium was dissolved. The flask was cooled to 10℃, and tertiary butyl chloride (2.0 ml，18.4 mmol) was added over 1 h while the temperature was held below 30℃ with a water bath. After the addition, the reaction was heated to 40℃ for 0.5 h and then cooled to -10℃. 2,2'-Bis(chloromethy)-1,1'-biphenyl (3.0g, 8.8mmol) in THF (15ml) was added dropwise to the solution of the anion and heated to reflux for 0.5 h after the addition.The solvent was removed under vacuum and then added dichloromethane (20ml) and deionized water (20ml). The organic layer was separated and dried by $MgSO_4$. Cooling the solution, After added ethyl alcohol to oil generation and then cooled it, the solution pure BISBI crystallizes out.

Obtained 3.9g pure product and the yield is 70.0%.

^{1}H NMR (400 MHz, $CDCl_3$): δ=7.36-7.27 (m, 12H), 7.22 (d, *J*=7.3 Hz, 4H), 7.14-7.08 (m, 8H), 7.03 (dd, *J*=5.3, 3.5 Hz, 2H), 6.94-6.87 (m, 2H), 3.21 (dd, *J*=49.6, 13.5 Hz, 4H). ^{31}P NMR (162 MHz, $CDCl_3$): δ=-10.53 (s).

3. Table 3 Optimization of reaction conditions for the hydroformylation of 1-octenewith Rh/L2

Entry	P/Rh	P(Mpa）	T（^{o}C）	Con. %[a]	Aldehyde %[b]	Oct.%[c]	Iso. %[d]	n/i
1	0	2.0	100.0	97.6	23.6	46.4	30.0	0.7
2	5	2.0	100.0	64.4	65.4	8.7	25.2	1.2
3	10	2.0	100.0	83.0	68.4	5.2	14.3	1.5
4	15	2.0	100.0	97.7	98.0	0.4	1.5	3.7
5	20	2.0	100.0	89.6	96.4	1.2	2.5	4.7
6	25	2.0	100.0	90.6	97.0	1.0	1.9	5.8
7	30	2.0	100.0	57.6	93.8	3.6	2.8	5.2
8	20	2.0	60.0	51.0	96.9	1.2	1.0	5.0
9	20	2.0	80.0	98.3	94.7	3.6	2.6	4.4
10	20	2.0	100.0	98.7	96.9	2.0	1.0	4.3
12	20	0.5	100.0	85.8	88.7	5.5	5.7	9.1
13	20	1.0	100.0	98.4	96.0	1,9	2.0	7.1
14	20	1.5	100.0	98.4	96.7	1.5	1.6	6.9
15	20	2.0	100.0	98.9	97.0	1.4	1.5	5.9
16	20	3.0	100.0	97.3	97.6	1.1	1.2	5.1

Reaction conditions: S/C=1000, [Rh]=1.60mM, toluene 3ml, 1h

[a]The conversion of 1-octene ; [b] Selectivity for aldehyde in all product; [c] Selectivity for octane in all product; [d] Selectivity for 2-octene in all product; [e]Molar ratio of linear to branched aldehyde. The products were analyzed by GC.

4. 1H, 13C and 31P NMR spectra

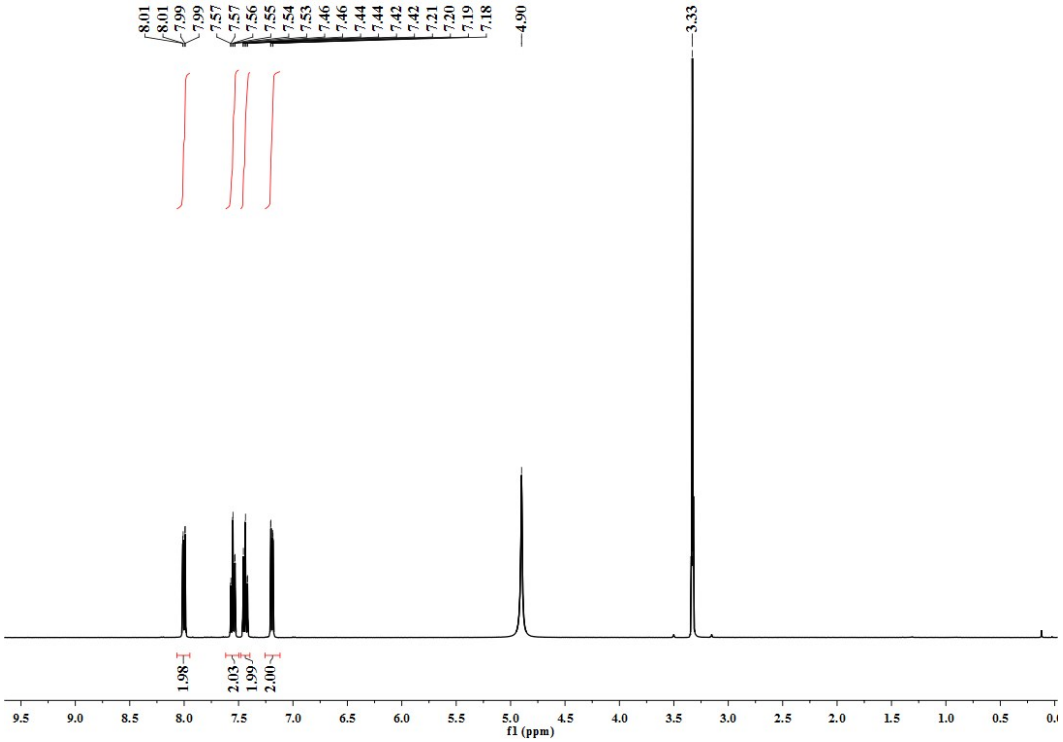


Figure S1: 1H NMR spectrum of compound **B** in CD_3OD.

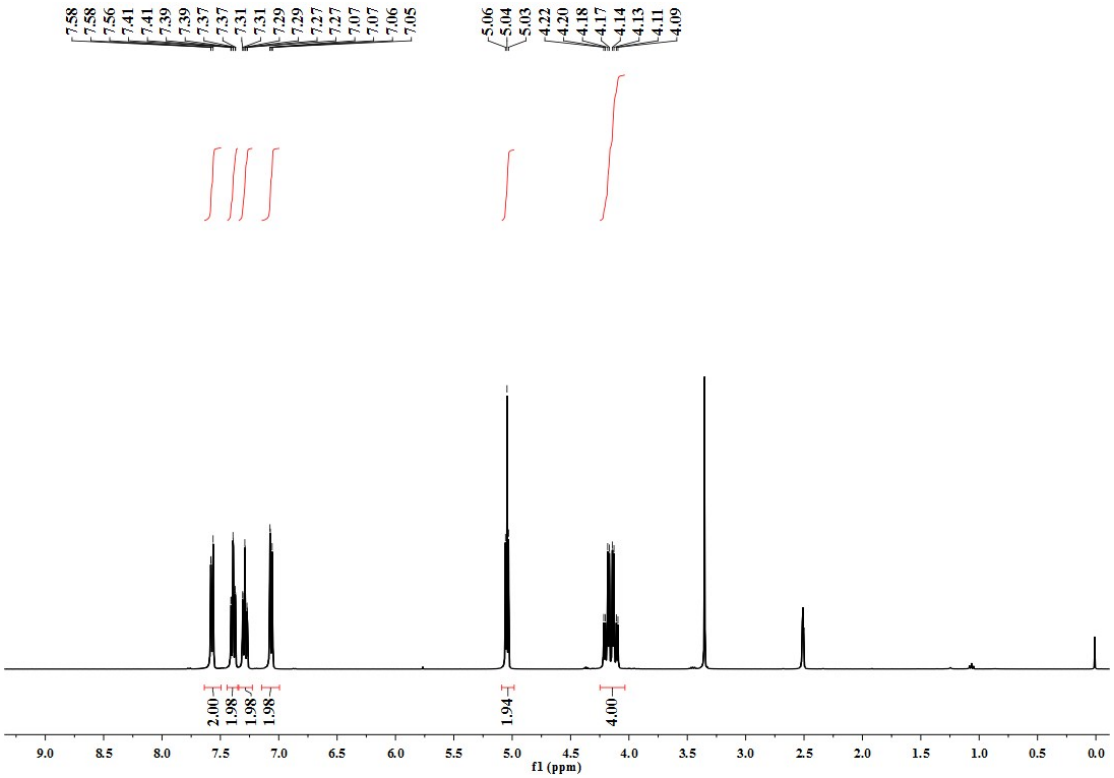


Figure S2: 1H NMR spectrum of compound **C** in d_6-DMSO.

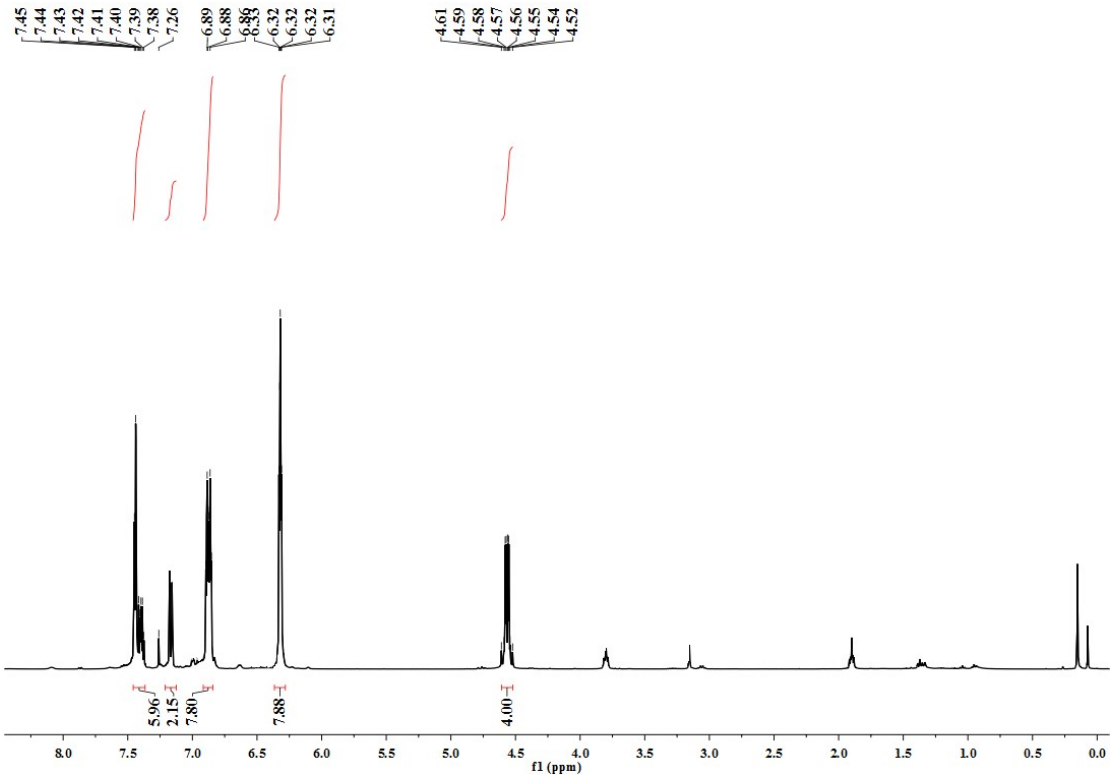


Figure S3: ^{1}H NMR spectrum of ligand **L1** in $CDCl_3$.

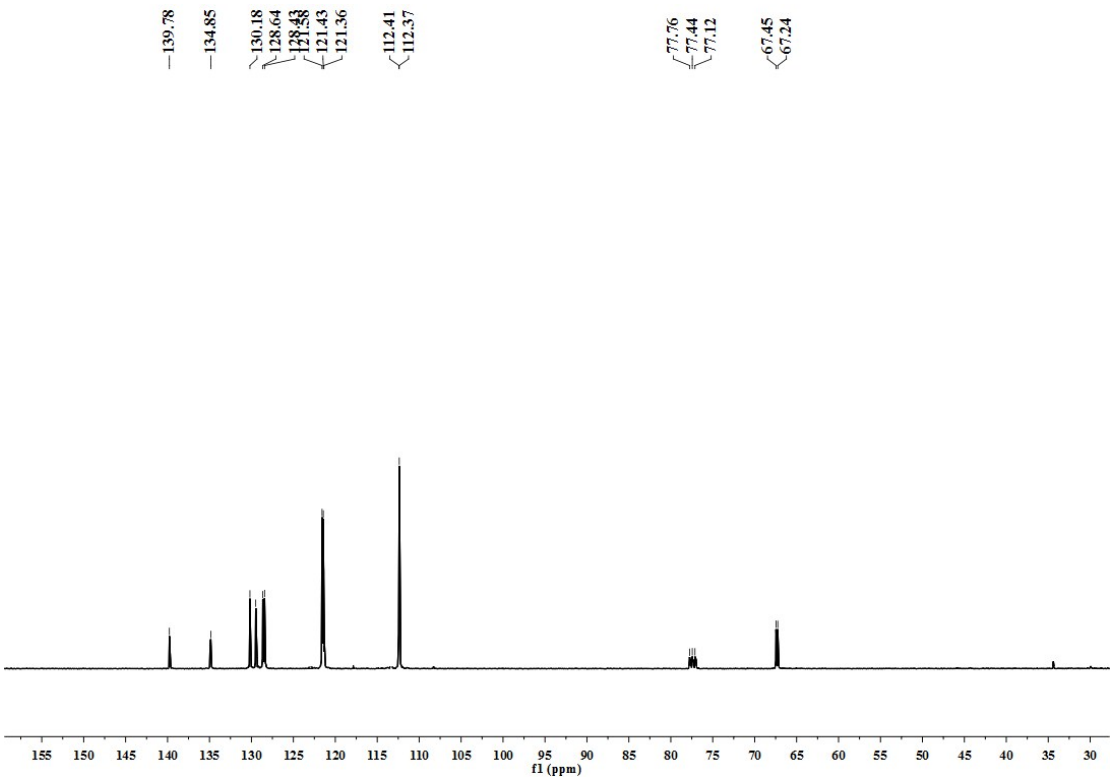


Figure S4: ^{13}C NMR spectrum of ligand **L1** in $CDCl_3$.

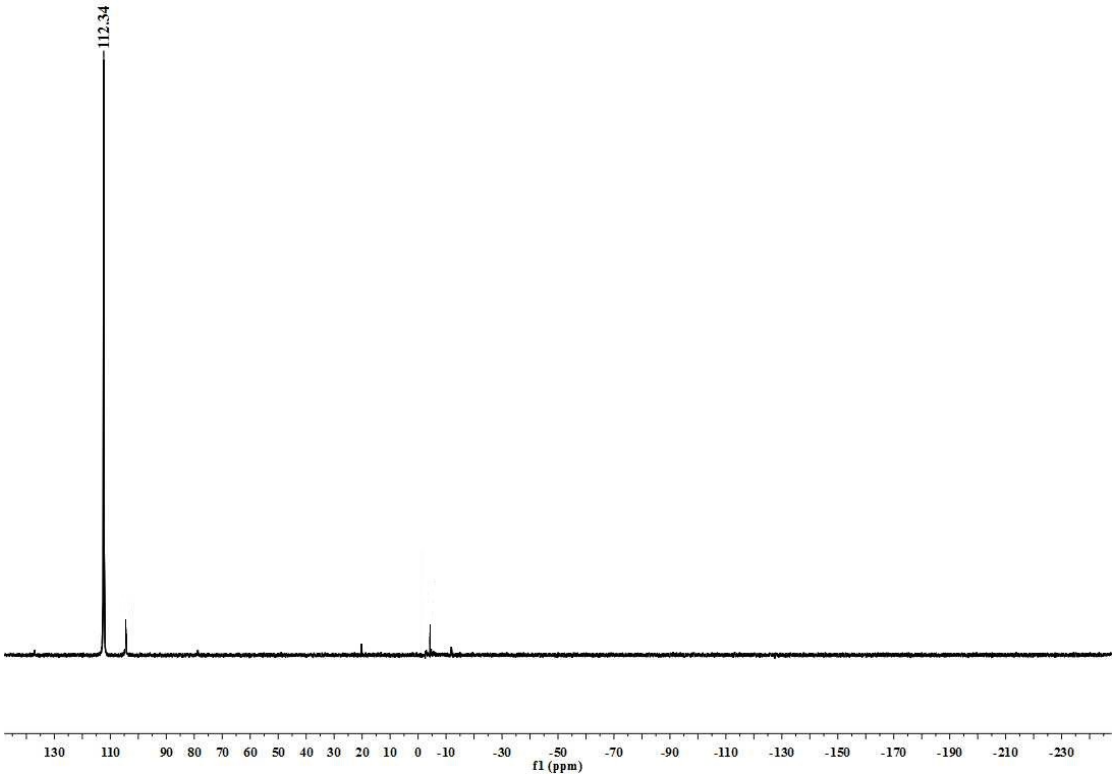


Figure S5: ^{31}P NMR spectrum of ligand **L1** in $CDCl_3$.

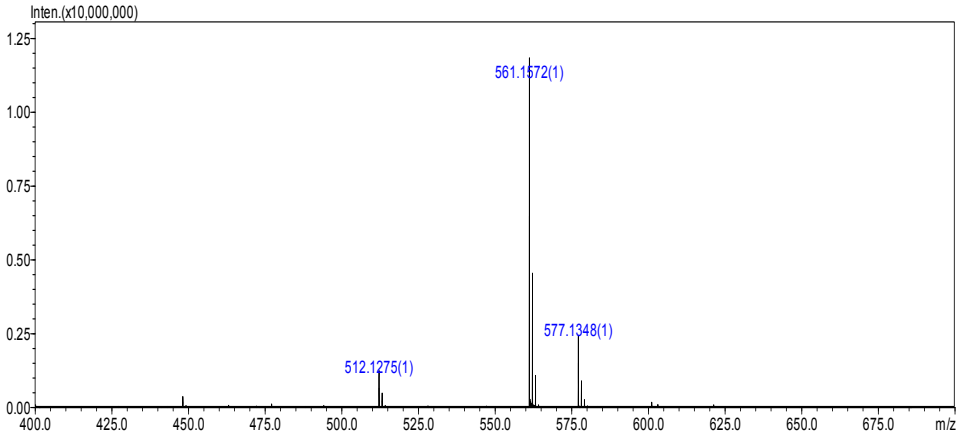


Figure S6: HRMS [M+ Na^+] of ligand **L1**

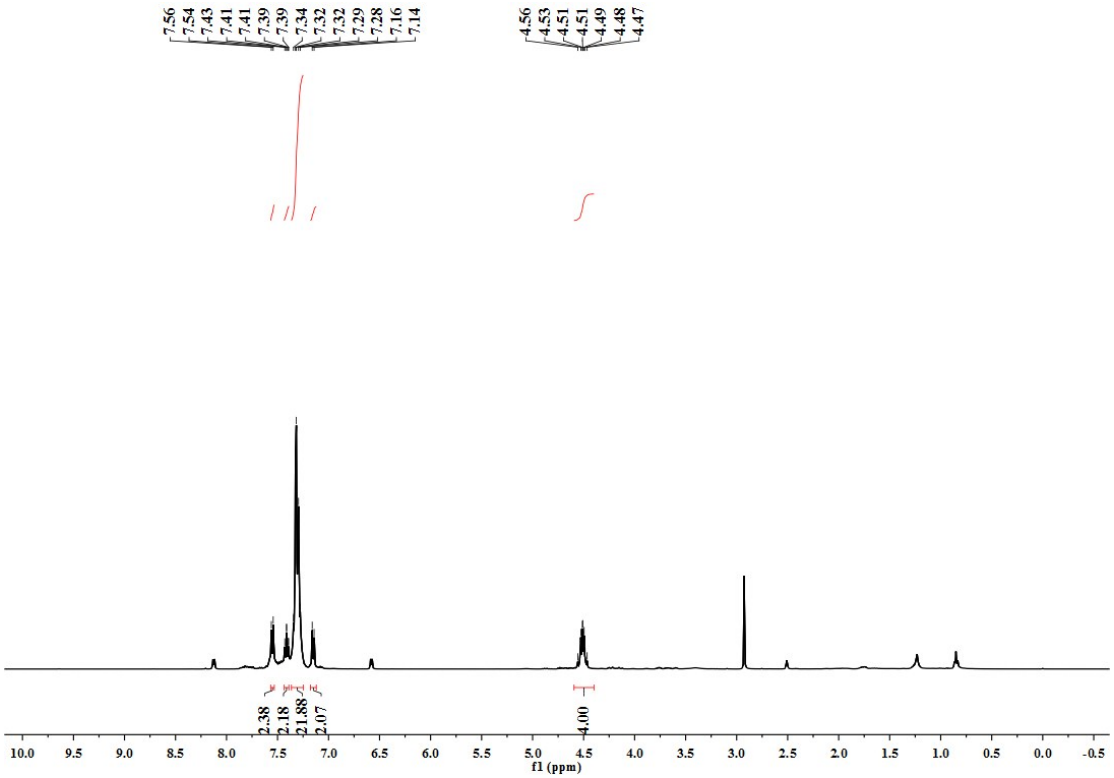


Figure S7: ^{1}H NMR spectrum of ligand **L2** in DMSO.

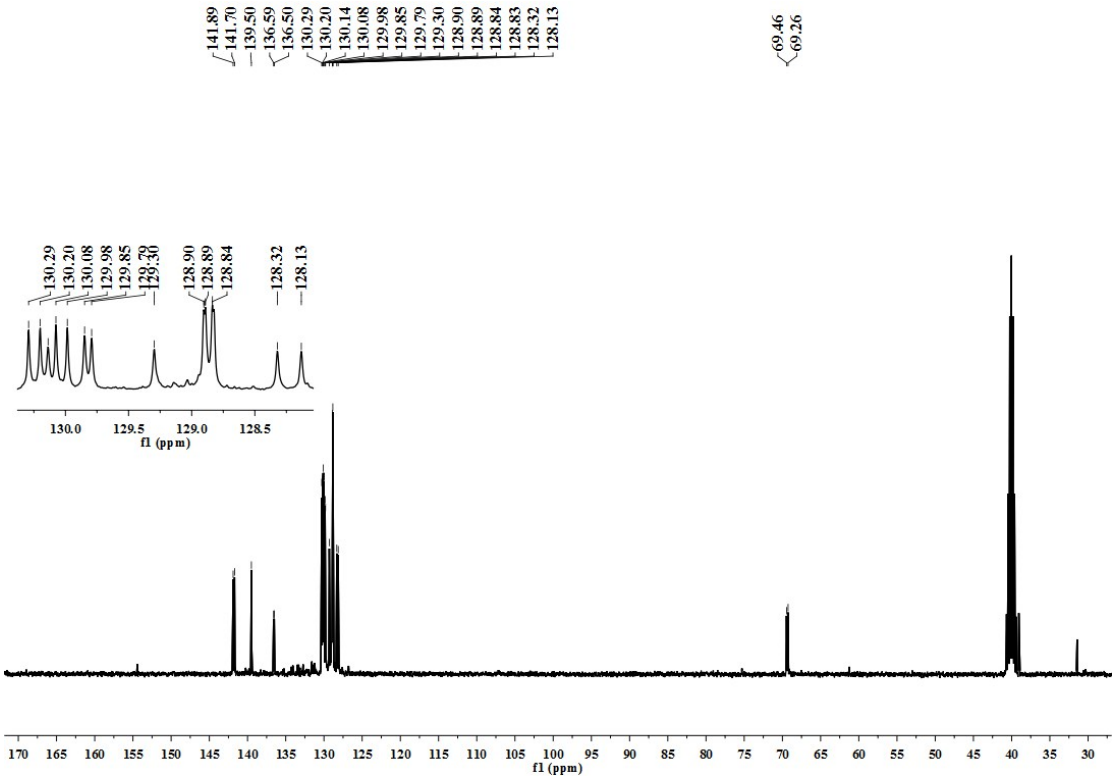


Figure S8: ^{13}C NMR spectrum of ligand **L2** in DMSO.

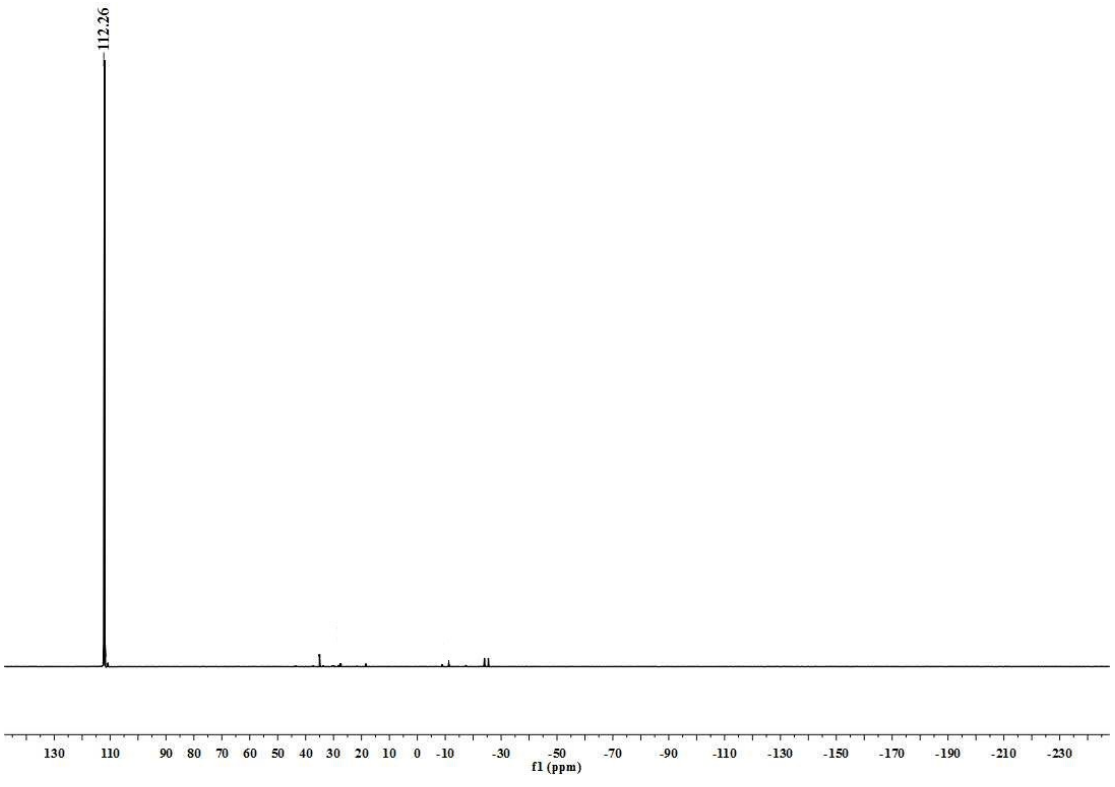


Figure S9: ^{31}P NMR spectrum of ligand **L2** in DMSO.

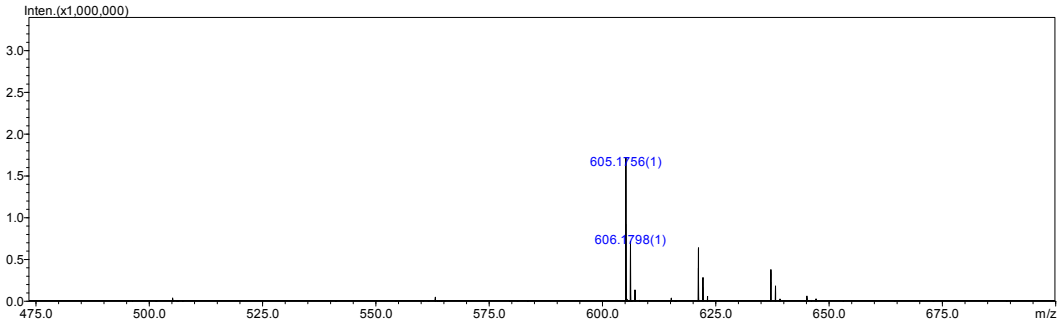


Figure S10: HRMS [M+ Na^+] of ligand **L2**

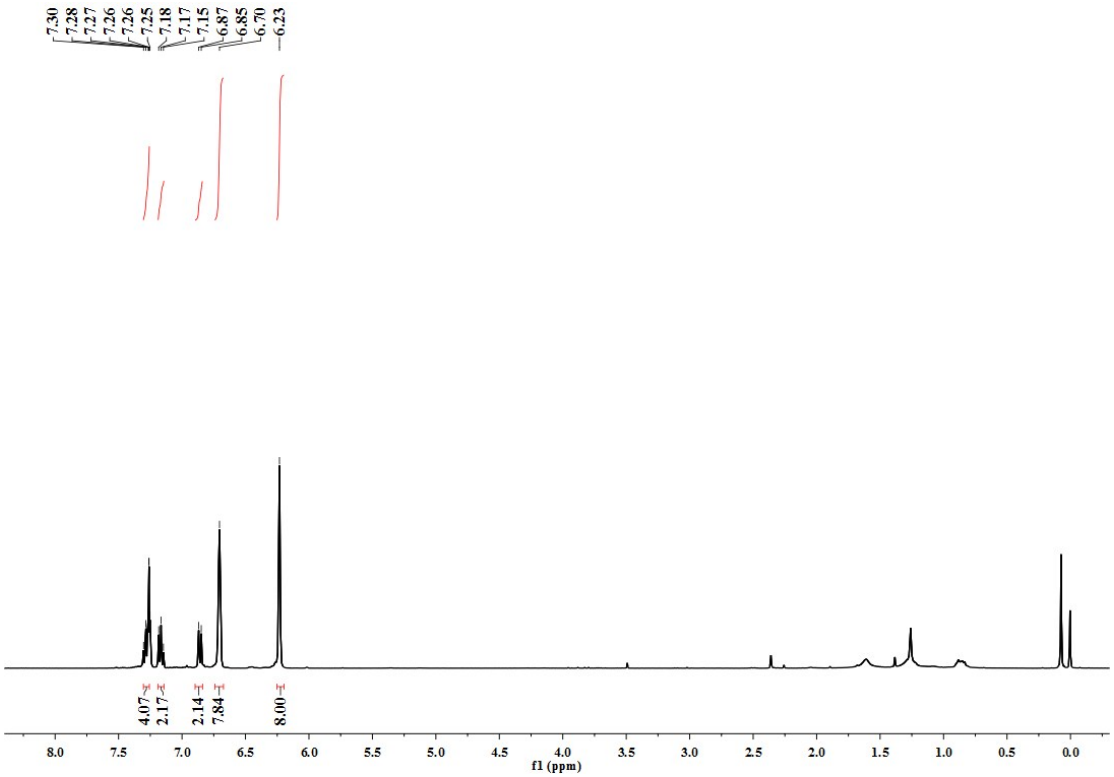


Figure S11: ^1H NMR spectrum of ligand **L3** in $CDCl_3$.

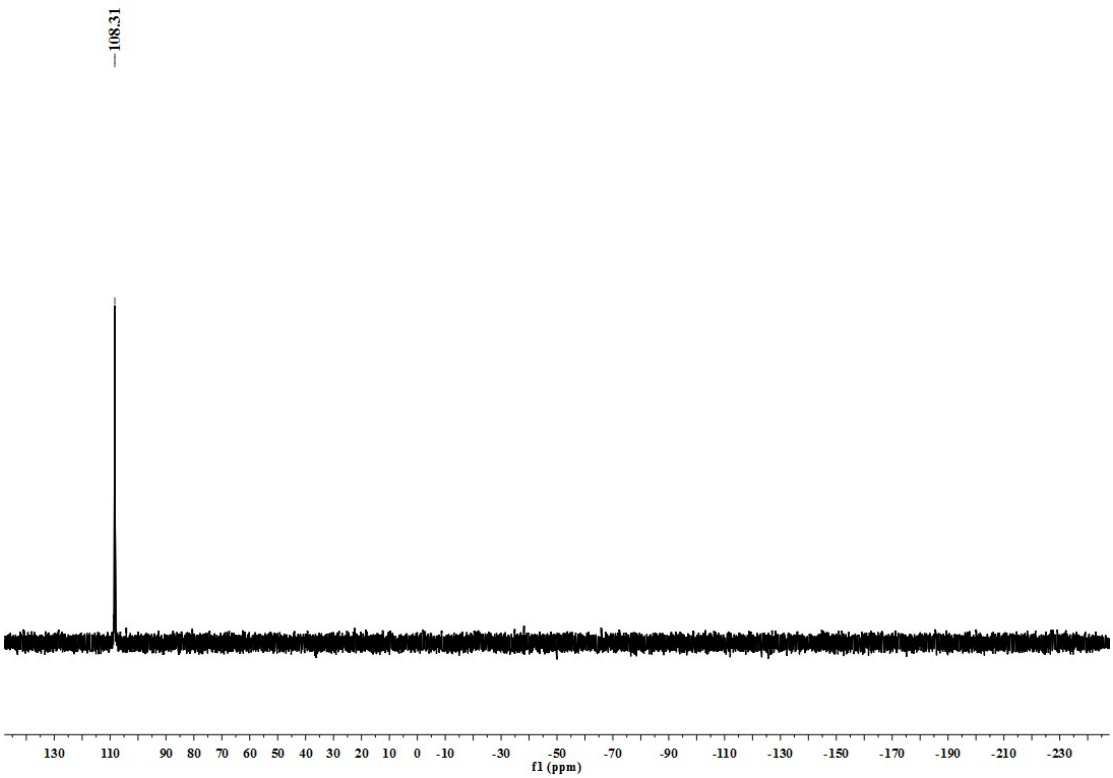


Figure S12: ^{31}P NMR spectrum of ligand L**3** in $CDCl_3$.

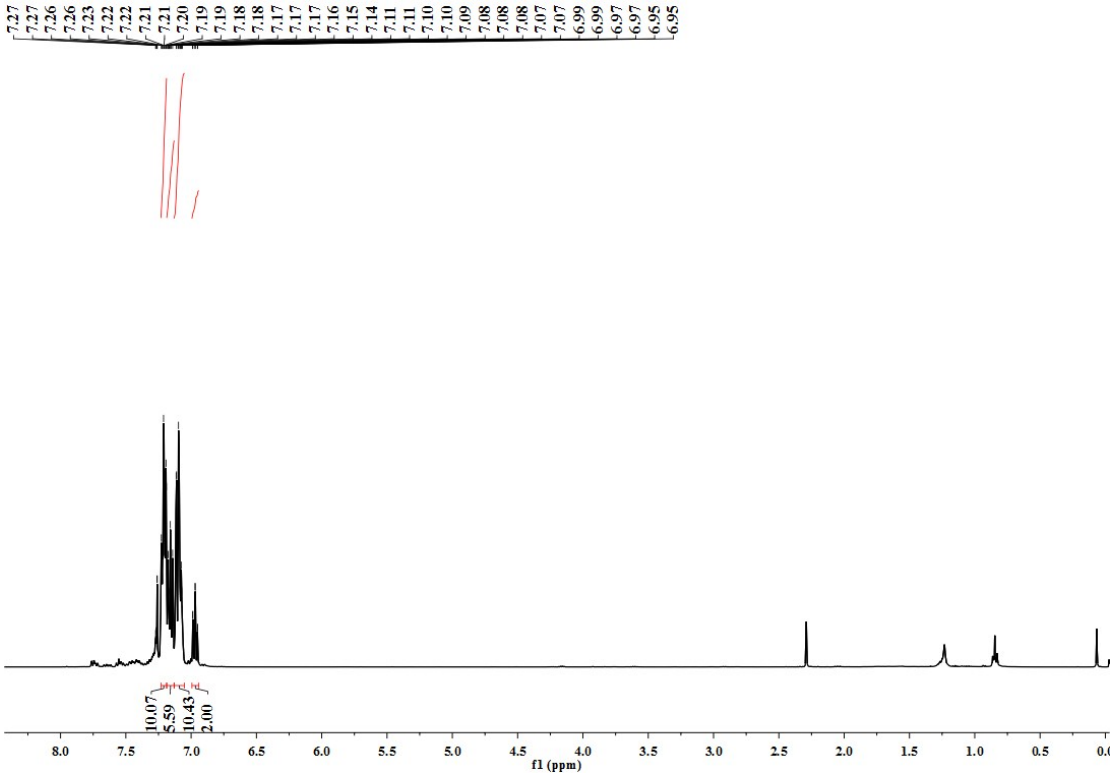


Figure S13:^{1}H NMR spectrum of ligand **L4** in $CDCl_3$.

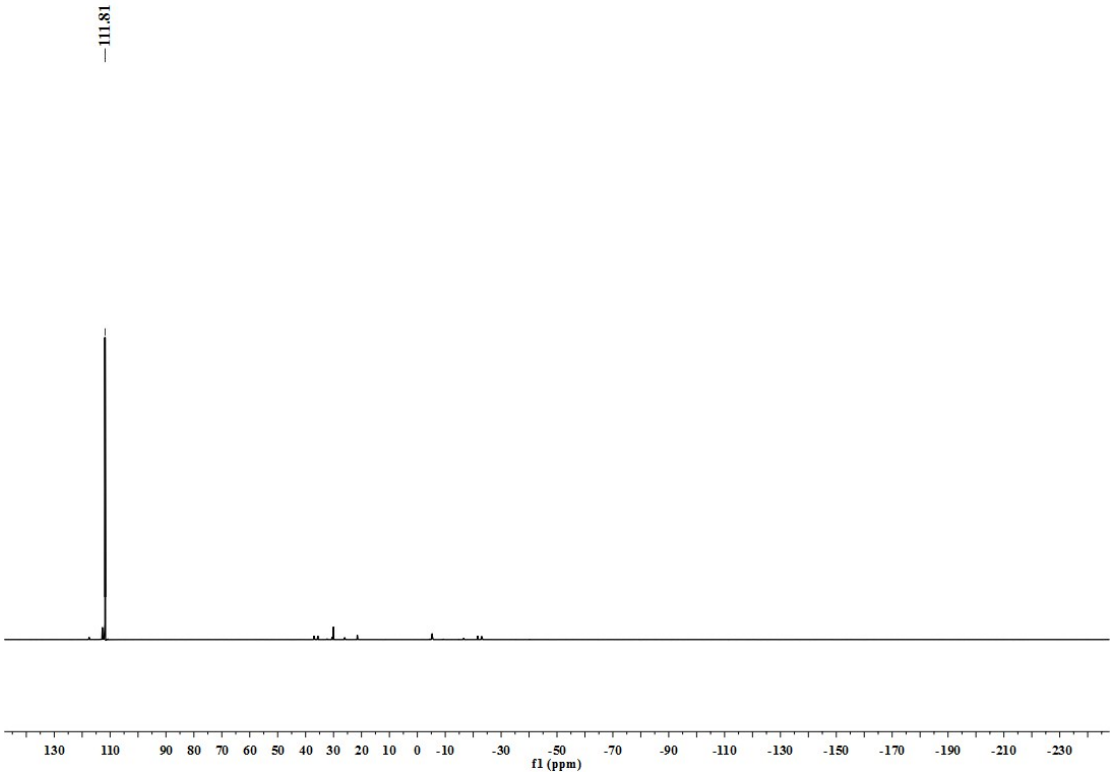


Figure S14: ^{31}P NMR spectrum of ligand **L4** in $CDCl_3$

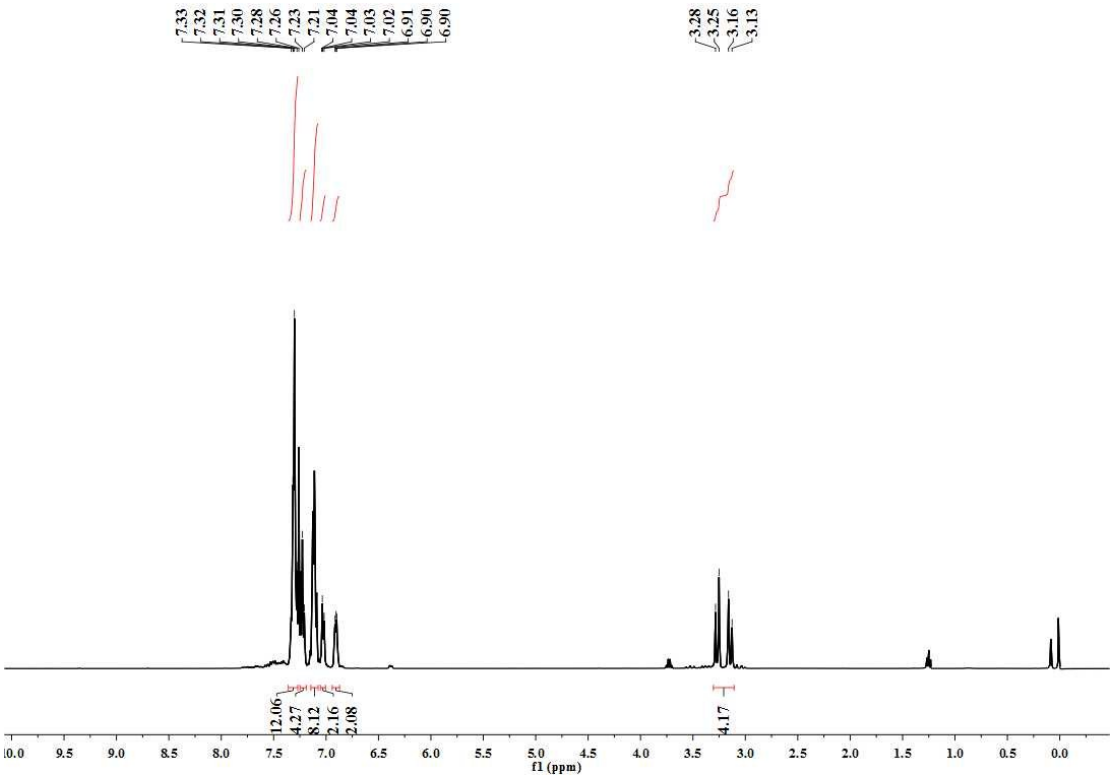


Figure S15: ^{1}H NMR spectrum of ligand **L5** in $CDCl_3$

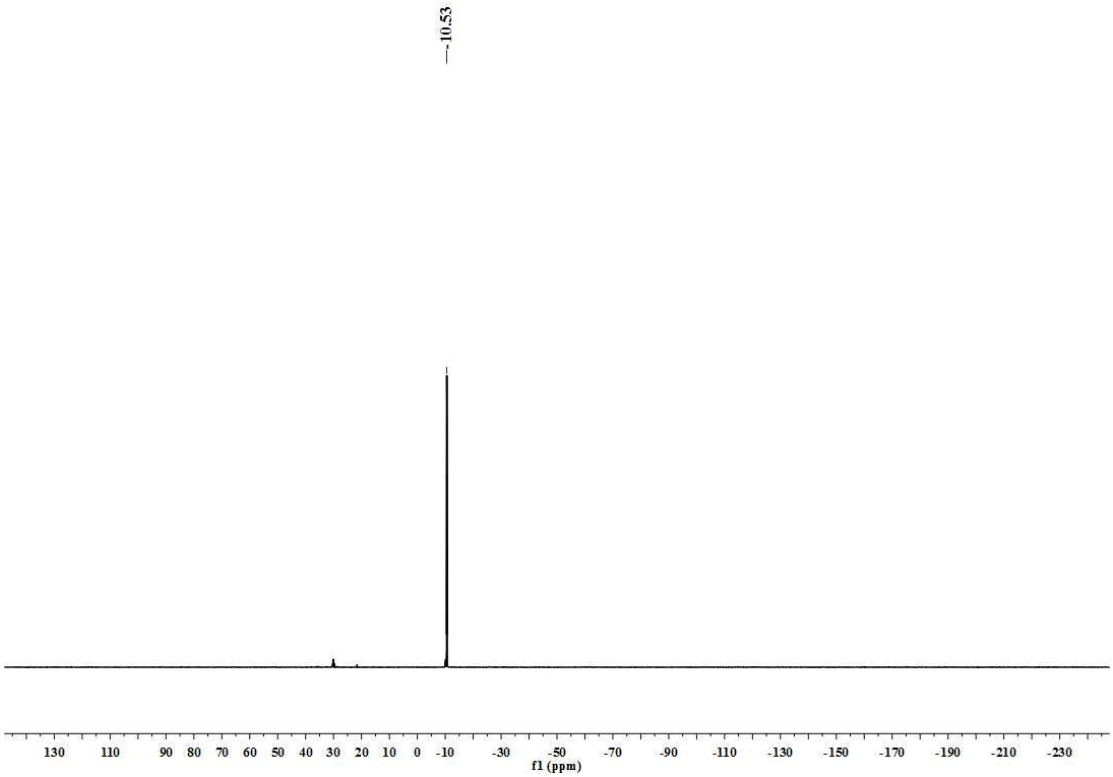


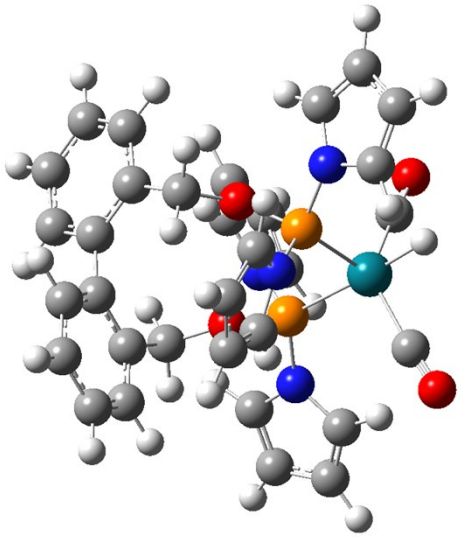
Figure S16: ^{31}P NMR spectrum of ligand **L5** in $CDCl_3$

5. The calculated bite angle of the major intermediates

The DFT calculation was performed using Gaussain 09 program[3]
M06-optimized coordinates of various species

L1 system

Complex I

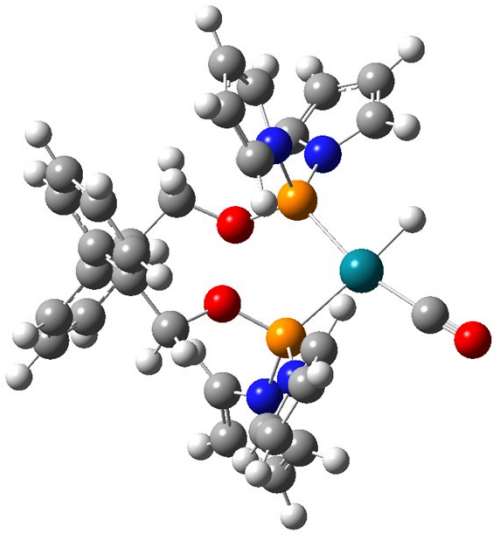


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.400161	-2.313691	3.843543
2	6	0	2.105957	-3.546436	3.267626
3	6	0	2.064212	-3.672252	1.884423

4	6	0	2.297272	-2.573342	1.051283
5	6	0	2.583818	-1.329036	1.634449
6	6	0	2.636095	-1.217280	3.025476
7	6	0	2.281332	-2.767237	-0.425402
8	6	0	3.500882	-2.885895	-1.098329
9	6	0	3.547817	-3.102930	-2.469995
10	6	0	2.365635	-3.206174	-3.195231
11	6	0	1.148909	-3.084041	-2.537885
12	6	0	1.089458	-2.869994	-1.160076
13	8	0	1.385009	0.541080	0.894888
14	8	0	-0.508725	-1.240953	-0.583404
15	15	0	-1.844623	-0.471875	-0.086388
16	7	0	-3.163564	-1.282715	-0.851410
17	7	0	-2.066070	-1.135709	1.496483
18	15	0	0.843596	1.697606	-0.113404
19	7	0	1.721130	3.071411	0.497263
20	6	0	1.981538	3.265567	1.846474
21	6	0	2.286261	4.585261	2.042436
22	6	0	2.177255	5.240484	0.783503
23	6	0	1.810266	4.299108	-0.139559
24	7	0	1.783698	1.464663	-1.551863
25	6	0	1.379236	0.572130	-2.538707
26	6	0	2.425794	0.364016	-3.391305
27	6	0	3.522847	1.142832	-2.921201
28	6	0	3.115374	1.796368	-1.792431
29	6	0	-3.279862	-1.201766	2.176041
30	6	0	-3.018347	-1.318038	3.512105
31	6	0	-1.603673	-1.287848	3.678698
32	6	0	-1.043492	-1.153274	2.439712
33	6	0	-3.563155	-2.610428	-0.692674
34	6	0	-4.554575	-2.871977	-1.594765
35	6	0	-4.782706	-1.682091	-2.344537
36	6	0	-3.924558	-0.730232	-1.875917
37	1	0	2.440729	-2.207739	4.926032
38	1	0	1.914604	-4.414077	3.896444
39	1	0	1.850132	-4.639150	1.427892
40	1	0	2.845308	-0.240044	3.464140
41	1	0	4.424271	-2.811774	-0.523367
42	1	0	4.510017	-3.196253	-2.970648
43	1	0	2.391689	-3.378495	-4.269866
44	1	0	0.214975	-3.147860	-3.098145
45	1	0	1.919300	2.433750	2.538262
46	1	0	2.568376	5.035731	2.986993
47	1	0	2.361646	6.288722	0.578576
48	1	0	1.611995	4.381731	-1.202496
49	1	0	0.382491	0.145636	-2.508233
50	1	0	2.408811	-0.271101	-4.269260
51	1	0	4.502732	1.227083	-3.377807
52	1	0	3.633728	2.484582	-1.136601
53	1	0	-4.216756	-1.176707	1.632902
54	1	0	-3.763002	-1.427582	4.291900
55	1	0	-1.058530	-1.368272	4.612217
56	1	0	-0.010789	-1.049269	2.125379
57	1	0	-3.127069	-3.225556	0.084917
58	1	0	-5.074715	-3.817075	-1.702011
59	1	0	-5.511434	-1.540630	-3.133758
60	1	0	-3.787294	0.305073	-2.161242
61	45	0	-1.525472	1.866306	-0.246596
62	6	0	-2.168587	2.240245	-2.048278
63	8	0	-2.524737	2.542150	-3.102070
64	6	0	-2.291876	2.257319	1.520123
65	8	0	-2.721293	2.555932	2.543145
66	6	0	2.681681	-0.079809	0.814930
67	1	0	2.921346	-0.288434	-0.236357
68	1	0	3.434241	0.616061	1.217385
69	6	0	-0.252015	-2.657282	-0.530169

70	1	0	-1.035977	-3.180694	-1.095949
71	1	0	-0.288430	-2.988768	0.516931
72	1	0	-1.282880	3.458525	-0.260468

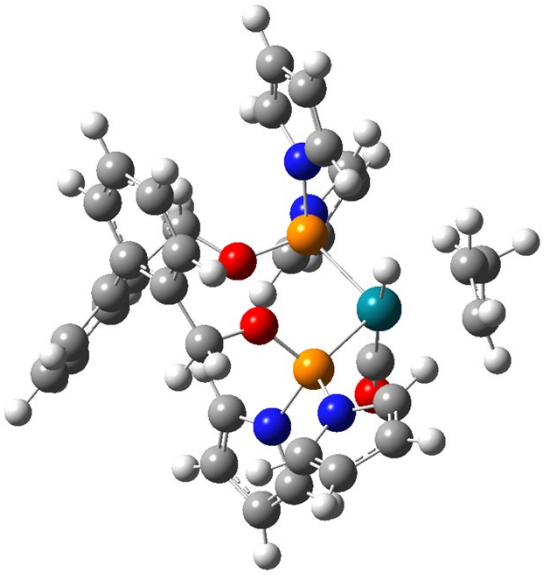
Complex II



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.242009	3.293242	3.703698
2	6	0	0.705845	4.118270	3.103209
3	6	0	0.804461	4.163028	1.718439
4	6	0	-0.027216	3.382052	0.908464
5	6	0	-0.980748	2.550951	1.515478
6	6	0	-1.077906	2.521024	2.908944
7	6	0	0.124784	3.468697	-0.571448
8	6	0	-0.709440	4.312771	-1.306065
9	6	0	-0.582147	4.419188	-2.687496

10	6	0	0.386861	3.678330	-3.355057
11	6	0	1.217979	2.830020	-2.632811
12	6	0	1.103495	2.723170	-1.247957
13	8	0	-1.505129	0.288608	1.037059
14	8	0	1.104255	0.584558	-0.286441
15	15	0	1.619509	-0.903157	0.102834
16	7	0	3.061319	-1.088670	-0.839814
17	7	0	2.364063	-0.606957	1.638958
18	15	0	-1.765275	-0.989359	0.068840
19	7	0	-3.261736	-1.553762	0.716058
20	6	0	-4.081654	-0.880286	1.613748
21	6	0	-5.274386	-1.544327	1.684827
22	6	0	-5.200936	-2.656893	0.797544
23	6	0	-3.962382	-2.642344	0.219818
24	7	0	-2.339959	-0.296784	-1.401475
25	6	0	-1.488462	0.167144	-2.399129
26	6	0	-2.220245	0.925698	-3.268800
27	6	0	-3.566629	0.938587	-2.799696
28	6	0	-3.616473	0.195751	-1.653839
29	6	0	3.224378	-1.476690	2.295913
30	6	0	3.284223	-1.109947	3.612602
31	6	0	2.407634	-0.001457	3.789028
32	6	0	1.839734	0.274640	2.576351
33	6	0	4.323421	-0.534143	-0.651308
34	6	0	5.005998	-0.607320	-1.833921
35	6	0	4.139481	-1.197411	-2.799251
36	6	0	2.958440	-1.477893	-2.171015
37	1	0	-0.328045	3.251820	4.787968
38	1	0	1.365283	4.731497	3.714895
39	1	0	1.540751	4.810189	1.241153
40	1	0	-1.812858	1.858130	3.368223
41	1	0	-1.469683	4.890305	-0.779687
42	1	0	-1.242337	5.083624	-3.242330
43	1	0	0.491096	3.755931	-4.435868
44	1	0	1.968944	2.225820	-3.145105
45	1	0	-3.710497	-0.018118	2.152829
46	1	0	-6.108177	-1.277453	2.324054
47	1	0	-5.971648	-3.397590	0.619309
48	1	0	-3.498835	-3.301362	-0.505637
49	1	0	-0.431940	-0.079176	-2.375981
50	1	0	-1.834724	1.414927	-4.156228
51	1	0	-4.411547	1.428028	-3.270766
52	1	0	-4.440771	-0.057923	-0.996176
53	1	0	3.725988	-2.269483	1.751891
54	1	0	3.900304	-1.579477	4.370671
55	1	0	2.218290	0.540086	4.709021
56	1	0	1.089703	1.003701	2.289148
57	1	0	4.612117	-0.149005	0.319206
58	1	0	6.028358	-0.283307	-1.992827
59	1	0	4.372433	-1.412733	-3.835576
60	1	0	2.040053	-1.930886	-2.532554
61	45	0	-0.034635	-2.480334	-0.197397
62	6	0	1.044561	-4.036853	-0.471836
63	8	0	1.648235	-5.001067	-0.634980
64	6	0	-1.867538	1.644347	0.716180
65	1	0	-1.757738	1.821301	-0.361334
66	1	0	-2.927232	1.793324	0.977086
67	6	0	1.947596	1.725693	-0.520855
68	1	0	2.812287	1.426517	-1.130725
69	1	0	2.314337	2.098457	0.446632
70	1	0	-1.257842	-3.530183	-0.487273

Complex III

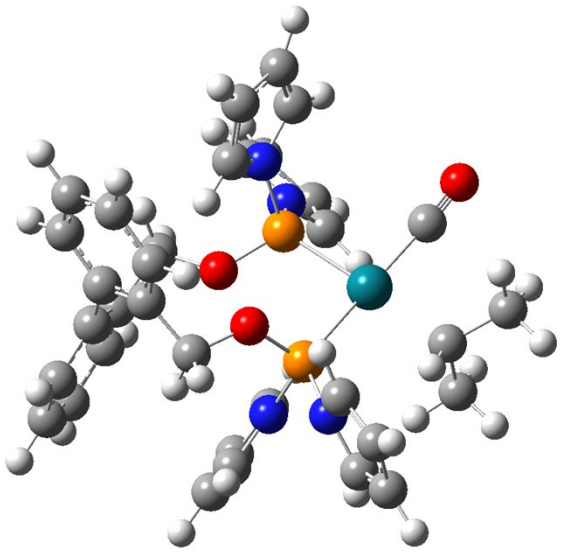


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.834828	-1.818639	3.845292
2	6	0	-3.978761	-1.265434	3.279589
3	6	0	-4.115507	-1.220414	1.896825
4	6	0	-3.115595	-1.711506	1.052448
5	6	0	-1.959136	-2.265963	1.627461
6	6	0	-1.833836	-2.310947	3.016801
7	6	0	-3.336009	-1.677576	-0.420025

8	6	0	-3.652586	-2.874343	-1.070713
9	6	0	-3.924316	-2.905871	-2.432886
10	6	0	-3.896534	-1.727360	-3.170174
11	6	0	-3.579156	-0.533953	-2.535636
12	6	0	-3.293959	-0.490285	-1.170118
13	8	0	-0.059641	-1.413855	0.588942
14	15	0	-0.339684	1.927677	-0.231776
15	7	0	-0.910353	3.405758	-0.935813
16	7	0	-0.883919	2.241077	1.395778
17	15	0	1.316774	-1.194889	-0.242672
18	7	0	2.390436	-2.136534	0.770548
19	6	0	2.428309	-1.926783	2.141314
20	6	0	3.612868	-2.415684	2.624231
21	6	0	4.347372	-2.923002	1.515901
22	6	0	3.589838	-2.719664	0.392267
23	7	0	1.225463	-2.305330	-1.565979
24	6	0	0.934202	-1.894066	-2.861522
25	6	0	0.769690	-3.000915	-3.643880
26	6	0	0.953981	-4.143819	-2.812840
27	6	0	1.222970	-3.699265	-1.549345
28	6	0	-0.649885	3.419377	2.095711
29	6	0	-0.744720	3.155127	3.434648
30	6	0	-1.015533	1.764758	3.578530
31	6	0	-1.073694	1.224013	2.323438
32	6	0	-2.102708	4.086535	-0.709633
33	6	0	-2.191256	5.108540	-1.613635
34	6	0	-1.027849	5.060964	-2.435096
35	6	0	-0.264487	4.013147	-2.002723
36	1	0	-2.720635	-1.862288	4.926907
37	1	0	-4.770124	-0.872712	3.915498
38	1	0	-5.017470	-0.800588	1.450262
39	1	0	-0.920374	-2.725850	3.446638
40	1	0	-3.691798	-3.792575	-0.483586
41	1	0	-4.165948	-3.851314	-2.915490
42	1	0	-4.114707	-1.738797	-4.236388
43	1	0	-3.531625	0.392832	-3.108435
44	1	0	1.601272	-1.425220	2.636409
45	1	0	3.917373	-2.423941	3.664314
46	1	0	5.321054	-3.398527	1.545031
47	1	0	3.781554	-2.953183	-0.648959
48	1	0	0.875141	-0.835313	-3.086293
49	1	0	0.544427	-2.997601	-4.703816
50	1	0	0.905018	-5.183383	-3.117004
51	1	0	1.438609	-4.237085	-0.634393
52	1	0	-0.453064	4.342756	1.563693
53	1	0	-0.645411	3.885417	4.229456
54	1	0	-1.168837	1.221384	4.504339
55	1	0	-1.228611	0.202309	1.994967
56	1	0	-2.752702	3.798252	0.107842
57	1	0	-3.000768	5.827221	-1.676435
58	1	0	-0.779652	5.732390	-3.248766
59	1	0	0.687340	3.620254	-2.341773
60	45	0	1.800209	1.090365	-0.508788
61	6	0	2.370286	1.435799	1.348954
62	8	0	2.688921	1.678528	2.425574
63	1	0	1.344594	0.972774	-2.060018
64	6	0	-0.775437	-2.640234	0.789027
65	6	0	-2.824213	0.811271	-0.591492
66	8	0	-1.397077	0.808395	-0.729120
67	1	0	-1.060802	-3.053493	-0.188119
68	1	0	-0.130972	-3.363930	1.311081
69	1	0	-3.092905	0.930036	0.467335
70	1	0	-3.239077	1.659665	-1.155977
71	6	0	3.399626	2.367329	-1.406402
72	6	0	3.889434	1.058510	-1.322006
73	6	0	4.931106	0.646307	-0.321438

74	1	0	3.022043	2.756605	-2.349975
75	1	0	3.737419	3.118746	-0.690890
76	1	0	4.974961	1.352623	0.519209
77	1	0	4.745876	-0.355774	0.091238
78	1	0	5.928049	0.628686	-0.788607
79	1	0	3.827928	0.436339	-2.219241

Complex IV

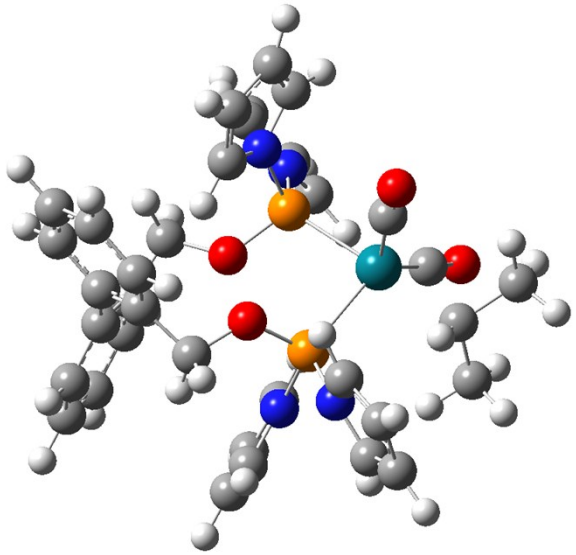


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.510285	-0.303303	3.830363
2	6	0	-4.449474	0.383169	3.065720
3	6	0	-4.475057	0.215409	1.686572
4	6	0	-3.560966	-0.625016	1.043186
5	6	0	-2.609437	-1.310176	1.816112
6	6	0	-2.598995	-1.141952	3.202131
7	6	0	-3.660204	-0.807478	-0.431785
8	6	0	-4.286256	-1.955511	-0.923289
9	6	0	-4.422164	-2.170660	-2.290101
10	6	0	-3.931166	-1.230828	-3.188380

11	6	0	-3.306832	-0.085587	-2.709596
12	6	0	-3.166499	0.142633	-1.341219
13	8	0	-0.345970	-1.314506	1.156803
14	8	0	-1.078078	0.864231	-0.552807
15	15	0	0.221487	1.746590	-0.151256
16	7	0	0.252159	3.054505	-1.287753
17	7	0	-0.395989	2.647255	1.200965
18	15	0	0.899805	-1.489332	0.139814
19	7	0	1.512332	-3.017385	0.694554
20	6	0	1.708716	-3.281791	2.044725
21	6	0	2.554465	-4.350504	2.158564
22	6	0	2.924207	-4.746139	0.841936
23	6	0	2.294025	-3.905271	-0.033550
24	7	0	0.277074	-2.034805	-1.372809
25	6	0	0.310118	-1.249908	-2.521625
26	6	0	-0.325418	-1.918862	-3.526108
27	6	0	-0.773862	-3.163841	-2.995423
28	6	0	-0.395190	-3.217083	-1.684855
29	6	0	0.142422	3.835734	1.679080
30	6	0	-0.243346	3.990310	2.982234
31	6	0	-1.014060	2.847265	3.340050
32	6	0	-1.072110	2.029738	2.245382
33	6	0	-0.644029	4.106163	-1.451294
34	6	0	-0.301139	4.791702	-2.583421
35	6	0	0.835575	4.147379	-3.152032
36	6	0	1.152470	3.090593	-2.346037
37	1	0	-3.486262	-0.182161	4.911757
38	1	0	-5.168336	1.045719	3.544383
39	1	0	-5.218159	0.738708	1.084232
40	1	0	-1.843726	-1.668947	3.787198
41	1	0	-4.673874	-2.685125	-0.211395
42	1	0	-4.912604	-3.073091	-2.651314
43	1	0	-4.026533	-1.391108	-4.260973
44	1	0	-2.901645	0.646756	-3.408984
45	1	0	1.219301	-2.673619	2.796894
46	1	0	2.869250	-4.811450	3.087638
47	1	0	3.574084	-5.569449	0.569333
48	1	0	2.309517	-3.861353	-1.116051
49	1	0	0.796776	-0.279902	-2.500421
50	1	0	-0.454183	-1.560716	-4.541007
51	1	0	-1.313288	-3.940167	-3.526391
52	1	0	-0.497738	-4.001603	-0.944950
53	1	0	0.737565	4.469306	1.031370
54	1	0	-0.010495	4.841640	3.611450
55	1	0	-1.482572	2.654245	4.298676
56	1	0	-1.518539	1.051006	2.105204
57	1	0	-1.420308	4.283172	-0.716725
58	1	0	-0.803010	5.674833	-2.962530
59	1	0	1.368553	4.441344	-4.048608
60	1	0	1.943993	2.350004	-2.405094
61	45	0	2.159155	0.484193	0.082881
62	6	0	3.259187	2.024490	0.339069
63	8	0	3.864600	2.987905	0.516825
64	6	0	-1.528718	-2.132257	1.184809
65	1	0	-1.797373	-2.427088	0.163078
66	1	0	-1.311358	-3.038202	1.770937
67	6	0	-2.392181	1.338473	-0.876523
68	1	0	-2.319633	2.091167	-1.675120
69	1	0	-2.829485	1.813136	0.014227
70	6	0	4.266090	-1.107339	-1.231387
71	6	0	3.923561	-0.746947	0.205014
72	6	0	5.133059	-0.172379	0.921456
73	1	0	5.112763	-1.818311	-1.267086
74	1	0	4.568879	-0.218084	-1.805554
75	1	0	3.428860	-1.573764	-1.772749
76	1	0	5.551744	0.697065	0.392580

77	1	0	4.899706	0.141432	1.947375
78	1	0	5.938775	-0.925878	0.982714
79	1	0	3.625553	-1.656426	0.747984

Complex V

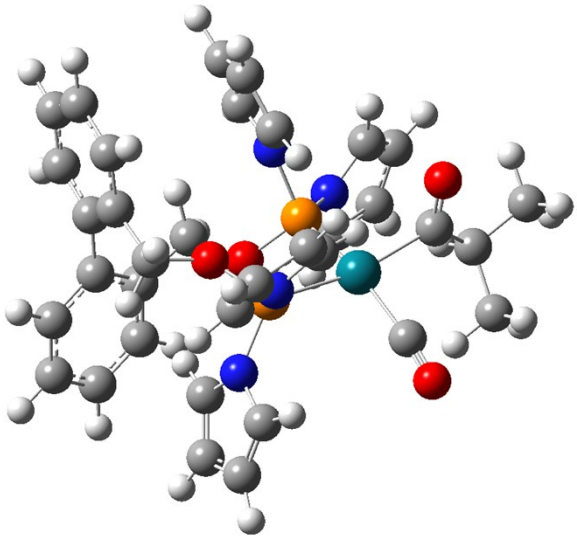


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.535203	-0.935212	3.833872
2	6	0	-4.532664	-0.319552	3.083986
3	6	0	-4.514323	-0.413444	1.697337
4	6	0	-3.500915	-1.110239	1.031988
5	6	0	-2.493517	-1.728128	1.791733
6	6	0	-2.524163	-1.631847	3.183911
7	6	0	-3.557390	-1.215843	-0.453140
8	6	0	-4.027732	-2.403133	-1.020252
9	6	0	-4.154489	-2.542692	-2.397777

10	6	0	-3.806094	-1.488749	-3.233746
11	6	0	-3.330571	-0.306401	-2.681412
12	6	0	-3.209362	-0.150745	-1.300879
13	8	0	-0.306932	-1.351885	1.012784
14	8	0	-1.202863	0.824965	-0.571379
15	15	0	-0.054763	1.875348	-0.131784
16	7	0	-0.391595	3.265208	-1.113414
17	7	0	-0.674069	2.499651	1.361848
18	15	0	0.958267	-1.366991	-0.009970
19	7	0	1.816621	-2.743798	0.646696
20	6	0	2.090024	-2.830917	2.006482
21	6	0	3.068703	-3.769158	2.195184
22	6	0	3.437793	-4.263595	0.912741
23	6	0	2.672496	-3.611059	-0.015739
24	7	0	0.391937	-2.125770	-1.460506
25	6	0	0.195105	-1.402996	-2.631628
26	6	0	-0.349385	-2.231165	-3.569917
27	6	0	-0.505563	-3.514462	-2.969478
28	6	0	-0.051563	-3.429012	-1.684092
29	6	0	-0.227978	3.659787	1.986784
30	6	0	-0.542146	3.580031	3.315429
31	6	0	-1.169494	2.320134	3.534414
32	6	0	-1.218479	1.668938	2.333703
33	6	0	-1.425587	4.187540	-0.966559
34	6	0	-1.569252	4.865964	-2.144314
35	6	0	-0.619528	4.338858	-3.065749
36	6	0	0.080131	3.360751	-2.417846
37	1	0	-3.544599	-0.871301	4.920421
38	1	0	-5.331744	0.228754	3.579775
39	1	0	-5.301275	0.056438	1.106624
40	1	0	-1.724857	-2.103187	3.757915
41	1	0	-4.306075	-3.224337	-0.358856
42	1	0	-4.525844	-3.477017	-2.815459
43	1	0	-3.894997	-1.589801	-4.314017
44	1	0	-3.031774	0.519636	-3.328445
45	1	0	1.545992	-2.213228	2.713032
46	1	0	3.470478	-4.081121	3.152288
47	1	0	4.176300	-5.027496	0.698696
48	1	0	2.644011	-3.693860	-1.095513
49	1	0	0.465248	-0.352411	-2.666312
50	1	0	-0.609237	-1.953202	-4.584947
51	1	0	-0.899764	-4.408501	-3.439871
52	1	0	0.045488	-4.180269	-0.909495
53	1	0	0.261793	4.440197	1.415701
54	1	0	-0.355693	4.350175	4.054902
55	1	0	-1.553971	1.936800	4.472738
56	1	0	-1.563894	0.676663	2.068219
57	1	0	-1.948696	4.274126	-0.022409
58	1	0	-2.276122	5.667441	-2.326645
59	1	0	-0.456525	4.660623	-4.087641
60	1	0	0.888153	2.724977	-2.758954
61	45	0	2.065630	0.803621	-0.051020
62	6	0	2.887456	1.681076	-1.559858
63	8	0	3.448157	2.226488	-2.412086
64	6	0	-1.309156	-2.373173	1.140808
65	1	0	-1.558389	-2.772126	0.150096
66	1	0	-0.907425	-3.189601	1.759712
67	6	0	-2.598296	1.110144	-0.772346
68	1	0	-2.695555	1.930128	-1.499351
69	1	0	-3.036748	1.432439	0.182764
70	6	0	2.309573	1.133240	1.891857
71	8	0	2.525354	1.280950	3.011700
72	6	0	4.329356	-0.938245	-1.247986
73	6	0	3.982610	-0.250384	0.059437
74	6	0	5.121430	0.640444	0.514478
75	1	0	5.144873	-1.664000	-1.084543

76	1	0	4.678719	-0.219951	-2.003272
77	1	0	3.487081	-1.488336	-1.687247
78	1	0	5.296560	1.468113	-0.187284
79	1	0	4.954710	1.077735	1.506315
80	1	0	6.056445	0.055329	0.564628
81	1	0	3.780445	-1.009823	0.829565

Complex VI



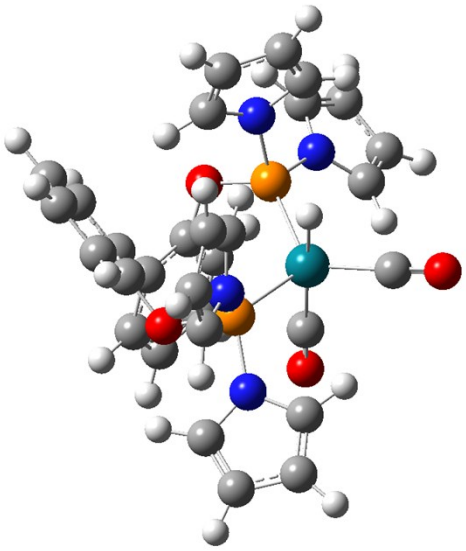
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.292836	-0.851546	4.022290
2	6	0	-4.423671	-0.466534	3.307166
3	6	0	-4.498221	-0.719654	1.942902
4	6	0	-3.448983	-1.348488	1.264539
5	6	0	-2.308023	-1.732371	1.987350
6	6	0	-2.246866	-1.479752	3.359415
7	6	0	-3.598567	-1.627564	-0.191488
8	6	0	-3.991321	-2.903720	-0.599597
9	6	0	-4.170091	-3.203337	-1.946035

10	6	0	-3.952118	-2.223466	-2.907024
11	6	0	-3.559082	-0.951143	-2.510779
12	6	0	-3.383879	-0.636930	-1.164371
13	8	0	-0.114546	-1.296822	1.215265
14	8	0	-1.492795	0.588537	-0.486743
15	15	0	-0.429054	1.782676	-0.219533
16	7	0	-0.693480	2.940096	-1.475462
17	7	0	-1.215117	2.642382	1.064930
18	15	0	1.047179	-1.207893	0.093567
19	7	0	2.046712	-2.541360	0.606605
20	6	0	2.359829	-2.780098	1.937204
21	6	0	3.435242	-3.626718	1.983074
22	6	0	3.823228	-3.897684	0.640555
23	6	0	2.972655	-3.208525	-0.181854
24	7	0	0.450675	-1.939926	-1.348281
25	6	0	0.228685	-1.213701	-2.513824
26	6	0	-0.314270	-2.044289	-3.449185
27	6	0	-0.439963	-3.334646	-2.854835
28	6	0	0.038191	-3.253000	-1.579053
29	6	0	-0.975264	3.965319	1.415836
30	6	0	-1.378454	4.146369	2.710440
31	6	0	-1.849641	2.892027	3.193657
32	6	0	-1.717311	1.984013	2.180348
33	6	0	-1.799172	3.745001	-1.734989
34	6	0	-1.606530	4.361965	-2.939548
35	6	0	-0.351081	3.926447	-3.454809
36	6	0	0.186231	3.059672	-2.546173
37	1	0	-3.226152	-0.660725	5.091805
38	1	0	-5.251307	0.027366	3.813301
39	1	0	-5.385899	-0.431013	1.379192
40	1	0	-1.348912	-1.772211	3.905870
41	1	0	-4.162051	-3.667108	0.160220
42	1	0	-4.478619	-4.204681	-2.241974
43	1	0	-4.081798	-2.449371	-3.964064
44	1	0	-3.367510	-0.181922	-3.259806
45	1	0	1.776279	-2.319092	2.725868
46	1	0	3.888905	-4.024110	2.883783
47	1	0	4.634622	-4.538626	0.315462
48	1	0	2.931368	-3.128496	-1.262224
49	1	0	0.498277	-0.164034	-2.555108
50	1	0	-0.586824	-1.766092	-4.460669
51	1	0	-0.831706	-4.230346	-3.323983
52	1	0	0.170988	-4.010993	-0.816446
53	1	0	-0.548870	4.654554	0.695849
54	1	0	-1.352981	5.084156	3.253307
55	1	0	-2.252989	2.683106	4.178233
56	1	0	-1.917412	0.919160	2.140067
57	1	0	-2.599387	3.826363	-1.009037
58	1	0	-2.288054	5.066921	-3.402195
59	1	0	0.109510	4.232151	-4.386789
60	1	0	1.124583	2.511743	-2.536267
61	45	0	1.777430	0.990456	-0.085777
62	6	0	3.639719	0.197958	-0.489839
63	8	0	3.773864	0.033214	-1.682103
64	6	0	-1.110310	-2.329570	1.313965
65	1	0	-1.361677	-2.701132	0.313507
66	1	0	-0.687698	-3.158864	1.902091
67	6	0	-2.888915	0.726066	-0.789479
68	1	0	-3.010802	1.429226	-1.626129
69	1	0	-3.404668	1.135658	0.091510
70	6	0	2.515225	2.674871	0.488280
71	8	0	2.849904	3.700208	0.894341
72	6	0	5.961617	-0.707770	-0.160157
73	6	0	4.695269	-0.219363	0.527185
74	6	0	4.983329	0.880059	1.540304
75	1	0	6.668331	-1.106048	0.579324

76	1	0	6.454312	0.116304	-0.694204
77	1	0	5.743327	-1.492575	-0.893040
78	1	0	5.387093	1.777760	1.049419
79	1	0	4.083170	1.168443	2.096840
80	1	0	5.731714	0.532507	2.263979
81	1	0	4.225757	-1.059041	1.072299

II. L3 system

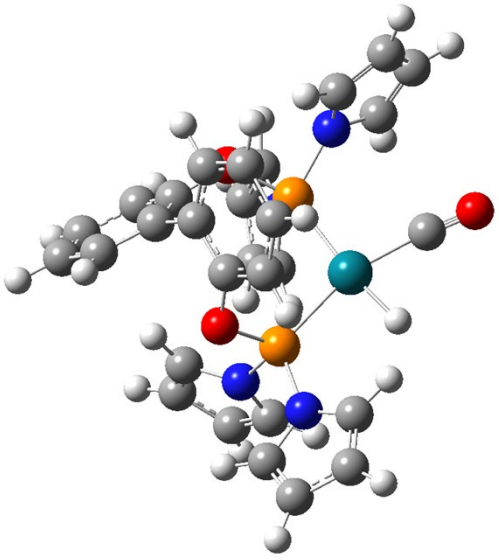
Complex I



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.924754	-2.354603	3.299496
2	6	0	-0.668352	-2.190670	3.875925
3	6	0	0.073824	-1.043221	3.617027
4	6	0	-0.419794	-0.040638	2.779616
5	6	0	-1.671911	-0.242280	2.191219
6	6	0	-2.428339	-1.381777	2.443280
7	6	0	0.313896	1.225429	2.547776
8	6	0	-0.208532	2.429738	3.032359
9	6	0	0.450637	3.636086	2.833099

10	6	0	1.655039	3.660404	2.133947
11	6	0	2.196069	2.479419	1.642878
12	6	0	1.526771	1.276136	1.854361
13	8	0	-2.153489	0.709410	1.309952
14	15	0	1.890317	-0.312940	-0.206187
15	7	0	2.813941	0.896092	-1.026276
16	7	0	3.037856	-1.593910	-0.126664
17	15	0	-2.018490	0.325544	-0.297105
18	7	0	-3.598876	-0.273010	-0.633406
19	6	0	-3.868854	-1.558777	-1.089002
20	6	0	-5.214358	-1.772172	-1.000910
21	6	0	-5.802653	-0.588456	-0.461792
22	6	0	-4.798345	0.309801	-0.239151
23	7	0	-2.226915	1.940300	-0.864792
24	6	0	-2.654304	2.209651	-2.160405
25	6	0	-2.123800	3.406548	-2.550831
26	6	0	-1.311871	3.885403	-1.480302
27	6	0	-1.370410	2.963735	-0.472057
28	6	0	3.239678	-2.479137	-1.178597
29	6	0	4.362821	-3.211283	-0.918253
30	6	0	4.882628	-2.767290	0.331815
31	6	0	4.066010	-1.773903	0.793730
32	6	0	4.197857	1.042271	-0.997441
33	6	0	4.511583	2.242814	-1.570267
34	6	0	3.291051	2.873521	-1.952679
35	6	0	2.268711	2.036525	-1.606911
36	1	0	-2.509860	-3.248817	3.504932
37	1	0	-0.266038	-2.956577	4.535840
38	1	0	1.054151	-0.906200	4.072267
39	1	0	-3.402925	-1.486468	1.964800
40	1	0	-1.155116	2.403256	3.571177
41	1	0	0.023536	4.558259	3.222551
42	1	0	2.177190	4.600885	1.969083
43	1	0	3.135770	2.469240	1.090859
44	1	0	-3.058937	-2.187134	-1.441878
45	1	0	-5.733008	-2.675681	-1.299443
46	1	0	-6.856024	-0.418654	-0.269287
47	1	0	-4.804881	1.315351	0.163539
48	1	0	-3.314263	1.518713	-2.671962
49	1	0	-2.315916	3.906002	-3.493344
50	1	0	-0.768906	4.823189	-1.447336
51	1	0	-0.909095	2.944379	0.509986
52	1	0	2.552070	-2.494395	-2.016690
53	1	0	4.766069	-3.994462	-1.549231
54	1	0	5.756642	-3.152389	0.844715
55	1	0	4.099824	-1.179615	1.696133
56	1	0	4.825136	0.247416	-0.609357
57	1	0	5.514824	2.622994	-1.726988
58	1	0	3.180416	3.836192	-2.438117
59	1	0	1.193112	2.151398	-1.691303
60	45	0	-0.182846	-0.909258	-1.117093
61	6	0	-0.285533	-2.546800	0.008189
62	8	0	-0.271563	-3.515088	0.620986
63	6	0	-0.286300	-1.748613	-2.879752
64	8	0	-0.318387	-2.178861	-3.945682
65	8	0	2.095886	0.106527	1.386275
66	1	0	-0.025501	0.401288	-2.044842

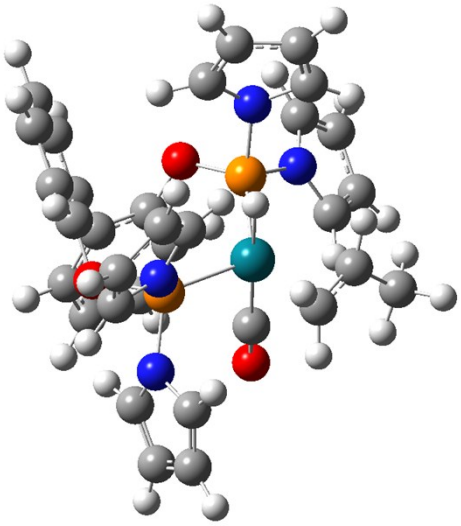
Complex II



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.238305	-2.904806	2.990659
2	6	0	-0.125800	-2.458736	3.699202
3	6	0	0.279481	-1.132584	3.595025
4	6	0	-0.408850	-0.234367	2.777349
5	6	0	-1.506083	-0.712080	2.058400
6	6	0	-1.935871	-2.029626	2.166298
7	6	0	0.002002	1.180323	2.631575
8	6	0	-0.757491	2.210195	3.192963

9	6	0	-0.409784	3.542648	3.004395
10	6	0	0.699577	3.864728	2.226076
11	6	0	1.470083	2.857384	1.658673
12	6	0	1.126567	1.525797	1.877980
13	8	0	-2.158735	0.154788	1.190180
14	15	0	1.770431	-0.067695	-0.142823
15	7	0	2.336515	1.237565	-1.103449
16	7	0	3.221438	-1.003470	-0.058301
17	15	0	-1.907188	-0.131504	-0.414350
18	7	0	-3.451998	-0.692564	-0.917564
19	6	0	-3.782238	-2.018951	-1.187986
20	6	0	-5.142113	-2.126732	-1.212719
21	6	0	-5.683894	-0.836867	-0.931925
22	6	0	-4.638047	0.017901	-0.742573
23	7	0	-2.061200	1.493454	-0.970750
24	6	0	-2.180825	1.802991	-2.321690
25	6	0	-1.909317	3.134958	-2.479774
26	6	0	-1.589014	3.662375	-1.196199
27	6	0	-1.672413	2.639220	-0.292843
28	6	0	4.067730	-1.278112	-1.124750
29	6	0	4.787607	-2.401447	-0.821262
30	6	0	4.349547	-2.863872	0.452031
31	6	0	3.379513	-2.004267	0.889867
32	6	0	3.529952	1.940379	-0.954410
33	6	0	3.445688	3.081644	-1.700868
34	6	0	2.157770	3.106225	-2.316174
35	6	0	1.496535	1.976174	-1.932761
36	1	0	-1.563475	-3.939831	3.074213
37	1	0	0.424488	-3.144449	4.340505
38	1	0	1.148145	-0.774504	4.147482
39	1	0	-2.805785	-2.354079	1.594771
40	1	0	-1.639682	1.945845	3.775559
41	1	0	-1.011026	4.329552	3.455716
42	1	0	0.969694	4.905800	2.059177
43	1	0	2.341823	3.085186	1.045873
44	1	0	-2.998851	-2.749227	-1.351860
45	1	0	-5.698229	-3.031501	-1.429078
46	1	0	-6.733458	-0.569121	-0.889926
47	1	0	-4.609965	1.074155	-0.504797
48	1	0	-2.474997	1.040223	-3.034152
49	1	0	-1.952543	3.680408	-3.415512
50	1	0	-1.332595	4.688259	-0.957452
51	1	0	-1.513525	2.615003	0.778015
52	1	0	4.084462	-0.631853	-1.994539
53	1	0	5.560209	-2.841048	-1.441103
54	1	0	4.723369	-3.725141	0.993312
55	1	0	2.784097	-1.991470	1.795835
56	1	0	4.320137	1.543278	-0.328406
57	1	0	4.228891	3.823787	-1.808824
58	1	0	1.763123	3.871803	-2.974187
59	1	0	0.498112	1.616958	-2.167574
60	45	0	-0.023549	-1.296084	-1.046258
61	6	0	1.107806	-2.590018	-1.895879
62	8	0	1.689497	-3.421010	-2.432866
63	8	0	1.953094	0.531015	1.392091
64	1	0	-1.104386	-2.222343	-1.820738

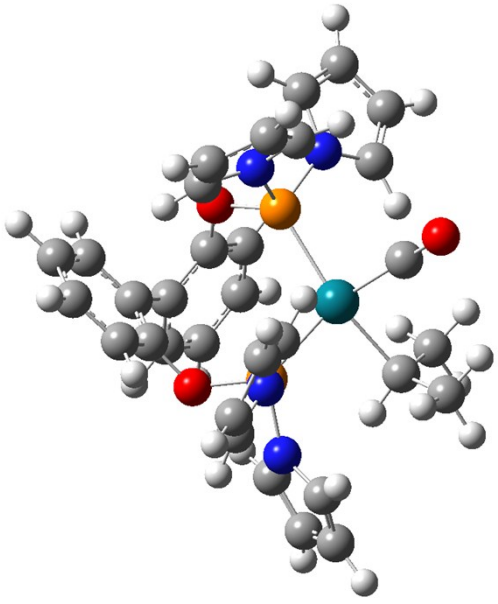
Complex III



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.612788	-1.874436	3.590340
2	6	0	-0.345197	-1.624204	4.109250
3	6	0	0.347498	-0.479660	3.729422
4	6	0	-0.203564	0.427128	2.820972
5	6	0	-1.467434	0.142351	2.296420
6	6	0	-2.178838	-0.990407	2.679013
7	6	0	0.506933	1.660747	2.416397
8	6	0	-0.016824	2.920897	2.721470
9	6	0	0.633748	4.084617	2.329525
10	6	0	1.822270	4.005926	1.607591

11	6	0	2.361390	2.765528	1.289038
12	6	0	1.707491	1.608174	1.703524
13	8	0	-2.000585	0.998541	1.351625
14	15	0	1.972764	-0.276314	-0.079439
15	7	0	3.117920	0.587874	-1.045477
16	7	0	2.928999	-1.690730	0.227504
17	15	0	-1.959677	0.450952	-0.217819
18	7	0	-3.559360	-0.199069	-0.354176
19	6	0	-3.841074	-1.552069	-0.502446
20	6	0	-5.171196	-1.747534	-0.258923
21	6	0	-5.736217	-0.479334	0.068423
22	6	0	-4.733103	0.446677	0.015302
23	7	0	-2.264419	1.990234	-0.936687
24	6	0	-2.751396	2.084603	-2.237514
25	6	0	-2.258592	3.226314	-2.803256
26	6	0	-1.406077	3.846857	-1.842118
27	6	0	-1.407247	3.063326	-0.722526
28	6	0	3.498708	-2.455673	-0.781850
29	6	0	3.677179	-3.728139	-0.312926
30	6	0	3.171933	-3.768297	1.018402
31	6	0	2.704845	-2.518587	1.319907
32	6	0	4.473553	0.727763	-0.762040
33	6	0	4.988025	1.687967	-1.586826
34	6	0	3.921414	2.177989	-2.397630
35	6	0	2.790137	1.500552	-2.043032
36	1	0	-2.162693	-2.764814	3.888989
37	1	0	0.100859	-2.317637	4.819757
38	1	0	1.336985	-0.272704	4.137155
39	1	0	-3.168657	-1.164842	2.256018
40	1	0	-0.957657	2.972792	3.268652
41	1	0	0.209192	5.054090	2.583454
42	1	0	2.334867	4.912471	1.291634
43	1	0	3.292966	2.674244	0.730561
44	1	0	-3.051397	-2.247117	-0.760442
45	1	0	-5.692316	-2.696130	-0.315997
46	1	0	-6.773744	-0.274048	0.306852
47	1	0	-4.727969	1.513344	0.202981
48	1	0	-3.427442	1.328919	-2.622039
49	1	0	-2.505550	3.601939	-3.789675
50	1	0	-0.877546	4.786476	-1.955452
51	1	0	-0.891967	3.172583	0.225691
52	1	0	3.753036	-2.002288	-1.733087
53	1	0	4.149882	-4.540684	-0.852572
54	1	0	3.174920	-4.620994	1.687374
55	1	0	2.230528	-2.128467	2.213497
56	1	0	4.933619	0.115333	0.003816
57	1	0	6.024936	2.003250	-1.617657
58	1	0	3.985998	2.943995	-3.161513
59	1	0	1.764647	1.583554	-2.385211
60	45	0	-0.133030	-0.729576	-0.996464
61	8	0	2.273951	0.380387	1.416995
62	6	0	-0.676348	-1.472329	-3.113400
63	6	0	-1.679535	-2.583214	-3.185480
64	6	0	0.676607	-1.688785	-2.870680
65	1	0	-0.955285	-0.555157	-3.637402
66	1	0	-2.686314	-2.251696	-2.902746
67	1	0	-1.397757	-3.429850	-2.543215
68	1	0	-1.747003	-2.962509	-4.217157
69	1	0	1.428034	-0.996822	-3.249930
70	1	0	1.034481	-2.691636	-2.629243
71	6	0	-0.415095	-2.415074	0.000292
72	8	0	-0.628108	-3.378119	0.590810
73	1	0	0.047111	0.643063	-1.824788

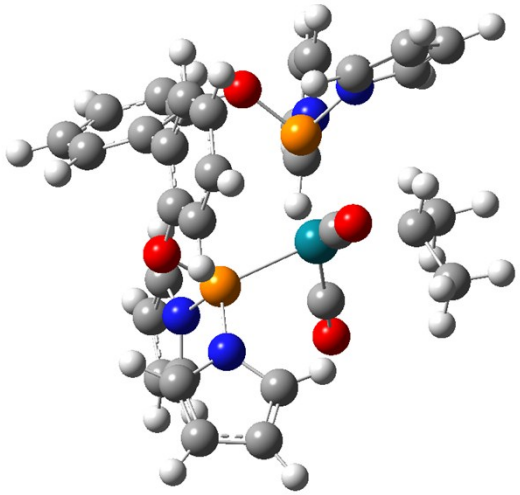
Complex IV



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z-
1	6	0	-1.055628	-1.518160	3.897220
2	6	0	0.092593	-0.872091	4.349181
3	6	0	0.460855	0.355990	3.809367
4	6	0	-0.303747	0.953512	2.805954
5	6	0	-1.440800	0.279109	2.358404
6	6	0	-1.831593	-0.943034	2.896342
7	6	0	0.071781	2.234505	2.167796
8	6	0	-0.689613	3.391263	2.350964

9	6	0	-0.367563	4.571386	1.691087
10	6	0	0.713652	4.601708	0.813013
11	6	0	1.483362	3.462260	0.612902
12	6	0	1.167031	2.293841	1.302174
13	8	0	-2.159112	0.835195	1.312601
14	15	0	1.808119	0.046304	-0.002135
15	7	0	2.388299	0.910812	-1.375799
16	7	0	3.278670	-0.751231	0.460726
17	15	0	-1.951847	0.067706	-0.140013
18	7	0	-3.401620	-0.867313	-0.223713
19	6	0	-3.440390	-2.255549	-0.116749
20	6	0	-4.723043	-2.631829	0.160812
21	6	0	-5.509146	-1.444046	0.249389
22	6	0	-4.681443	-0.382237	0.024217
23	7	0	-2.455330	1.378361	-1.142300
24	6	0	-2.893877	1.178996	-2.449161
25	6	0	-2.646319	2.318151	-3.163198
26	6	0	-2.004176	3.242980	-2.289132
27	6	0	-1.876753	2.639869	-1.069158
28	6	0	4.220222	-1.325613	-0.379820
29	6	0	4.991151	-2.183265	0.357682
30	6	0	4.494823	-2.167779	1.691129
31	6	0	3.438457	-1.297905	1.726679
32	6	0	3.570650	1.642680	-1.454241
33	6	0	3.528739	2.400832	-2.590189
34	6	0	2.276601	2.156448	-3.229595
35	6	0	1.595331	1.251637	-2.467869
36	1	0	-1.350543	-2.474833	4.324134
37	1	0	0.699763	-1.323835	5.131448
38	1	0	1.359602	0.866387	4.155682
39	1	0	-2.736394	-1.425587	2.523899
40	1	0	-1.551951	3.348309	3.015599
41	1	0	-0.968296	5.464298	1.852594
42	1	0	0.962608	5.517776	0.280533
43	1	0	2.334709	3.461033	-0.067221
44	1	0	-2.534397	-2.835830	-0.249962
45	1	0	-5.072913	-3.651317	0.274220
46	1	0	-6.574146	-1.385350	0.442972
47	1	0	-4.868151	0.684590	0.011613
48	1	0	-3.361820	0.242787	-2.732441
49	1	0	-2.918468	2.485186	-4.198988
50	1	0	-1.691344	4.252889	-2.528280
51	1	0	-1.460300	2.996146	-0.134002
52	1	0	4.261394	-1.052481	-1.427119
53	1	0	5.834806	-2.752186	-0.015273
54	1	0	4.885604	-2.722388	2.536420
55	1	0	2.787201	-0.993401	2.539337
56	1	0	4.326602	1.539467	-0.685061
57	1	0	4.317347	3.058360	-2.938896
58	1	0	1.921141	2.595881	-4.153986
59	1	0	0.611310	0.807015	-2.582714
60	45	0	-0.044254	-1.235611	-0.605298
61	6	0	-0.818308	-1.888040	-2.225218
62	8	0	-1.199630	-2.135861	-3.286431
63	8	0	1.992086	1.197239	1.185775
64	6	0	1.274047	-2.915581	-0.721639
65	6	0	1.894952	-3.278977	-2.052351
66	6	0	0.404291	-4.016882	-0.148048
67	1	0	2.069960	-2.694768	0.000211
68	1	0	2.409843	-2.426221	-2.516157
69	1	0	1.143347	-3.637863	-2.770321
70	1	0	2.639677	-4.083772	-1.925766
71	1	0	-0.121646	-3.700497	0.768406
72	1	0	1.025375	-4.886045	0.133463
73	1	0	-0.346292	-4.373468	-0.869332

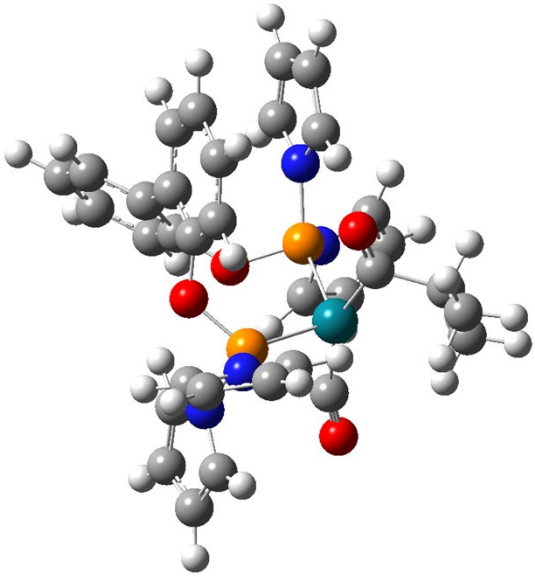
Complex V



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.212574	-1.333867	4.163431
2	6	0	-0.010539	-0.744101	4.545747
3	6	0	0.433588	0.410966	3.910693
4	6	0	-0.306208	0.993659	2.878793
5	6	0	-1.499634	0.372732	2.504784
6	6	0	-1.964535	-0.773676	3.137120
7	6	0	0.144748	2.216593	2.177833
8	6	0	-0.594814	3.401401	2.237949
9	6	0	-0.174605	4.544440	1.570073
10	6	0	0.996392	4.517081	0.816234
11	6	0	1.742550	3.347709	0.729686

12	6	0	1.313799	2.210721	1.411611
13	8	0	-2.214124	0.908677	1.445094
14	15	0	1.920561	0.065128	0.027034
15	7	0	2.904822	0.909808	-1.117462
16	7	0	3.098766	-1.063216	0.617150
17	15	0	-2.001208	0.179239	-0.022269
18	7	0	-3.452621	-0.747167	-0.070072
19	6	0	-3.655809	-1.892965	-0.832231
20	6	0	-4.982878	-2.212268	-0.778800
21	6	0	-5.630400	-1.234966	0.033503
22	6	0	-4.680200	-0.346271	0.449630
23	7	0	-2.469361	1.499653	-1.024129
24	6	0	-3.445564	1.475030	-2.016853
25	6	0	-3.224560	2.528745	-2.856839
26	6	0	-2.065277	3.217745	-2.394384
27	6	0	-1.612175	2.562970	-1.284247
28	6	0	4.103707	-1.708091	-0.092499
29	6	0	4.534059	-2.776663	0.645913
30	6	0	3.756766	-2.817780	1.837987
31	6	0	2.879583	-1.769479	1.792279
32	6	0	4.176866	1.434281	-0.910429
33	6	0	4.465572	2.277759	-1.946425
34	6	0	3.335318	2.298430	-2.817505
35	6	0	2.392142	1.467568	-2.285012
36	1	0	-1.561775	-2.239331	4.655410
37	1	0	0.582203	-1.182826	5.346180
38	1	0	1.375080	0.874340	4.204037
39	1	0	-2.901313	-1.219565	2.804767
40	1	0	-1.517774	3.408559	2.816557
41	1	0	-0.765271	5.456143	1.632035
42	1	0	1.330342	5.408103	0.287944
43	1	0	2.664003	3.302496	0.149359
44	1	0	-2.817814	-2.371342	-1.327919
45	1	0	-5.446080	-3.065947	-1.259584
46	1	0	-6.682704	-1.200861	0.291658
47	1	0	-4.742652	0.542770	1.064891
48	1	0	-4.209731	0.706516	-2.018776
49	1	0	-3.834567	2.788751	-3.713989
50	1	0	-1.625386	4.109964	-2.824818
51	1	0	-0.766147	2.758095	-0.633147
52	1	0	4.429713	-1.329596	-1.053714
53	1	0	5.334682	-3.452216	0.367962
54	1	0	3.848093	-3.531588	2.648305
55	1	0	2.120114	-1.439866	2.494665
56	1	0	4.745064	1.150372	-0.032589
57	1	0	5.395146	2.820305	-2.077663
58	1	0	3.235017	2.861225	-3.737979
59	1	0	1.392990	1.207632	-2.618638
60	45	0	-0.123074	-1.075824	-0.731041
61	6	0	-0.653984	-0.680185	-2.556062
62	8	0	-0.981058	-0.453607	-3.638026
63	8	0	2.073406	1.059882	1.357399
64	6	0	-0.334676	-2.452680	0.654852
65	8	0	-0.415539	-3.307305	1.420964
66	6	0	1.148435	-2.624011	-1.665885
67	6	0	2.002375	-2.126322	-2.816695
68	6	0	0.305707	-3.805087	-2.110675
69	1	0	1.807800	-2.930014	-0.839990
70	1	0	2.603092	-1.241239	-2.574360
71	1	0	1.398024	-1.880529	-3.701761
72	1	0	2.705406	-2.921685	-3.120093
73	1	0	-0.267641	-4.260030	-1.293644
74	1	0	0.955988	-4.590997	-2.533894
75	1	0	-0.407660	-3.522284	-2.89916

Complex VI



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.001384	1.571652	2.997958
2	6	0	-3.742369	2.911196	2.729403
3	6	0	-2.738057	3.254846	1.833445
4	6	0	-1.955765	2.289080	1.188017
5	6	0	-2.233713	0.949357	1.489043
6	6	0	-3.241857	0.588120	2.376169

7	6	0	-0.991268	2.725814	0.149722
8	6	0	-1.470887	3.612676	-0.823837
9	6	0	-0.660426	4.111335	-1.832869
10	6	0	0.674111	3.732253	-1.886758
11	6	0	1.186945	2.868420	-0.929313
12	6	0	0.364259	2.363105	0.074697
13	8	0	-1.433985	-0.044711	0.971269
14	8	0	0.909166	1.576099	1.074134
15	15	0	1.834912	0.244321	0.756585
16	7	0	3.402145	0.923813	0.520969
17	7	0	1.996703	-0.174242	2.427466
18	15	0	-1.476168	-0.813771	-0.481700
19	7	0	-2.715868	-1.986125	-0.104902
20	6	0	-2.689702	-2.754799	1.050502
21	6	0	-3.430975	-3.885836	0.837646
22	6	0	-3.906526	-3.838775	-0.503283
23	6	0	-3.438288	-2.681487	-1.064229
24	7	0	-2.424378	0.191196	-1.500877
25	6	0	-1.911405	0.841734	-2.622404
26	6	0	-2.917655	1.562073	-3.194632
27	6	0	-4.092085	1.370195	-2.406486
28	6	0	-3.771026	0.536684	-1.374810
29	6	0	3.065370	-0.915130	2.916291
30	6	0	2.685901	-1.489385	4.097978
31	6	0	1.330504	-1.122007	4.337783
32	6	0	0.924043	-0.336244	3.294427
33	6	0	3.995573	1.941066	1.260025
34	6	0	5.134229	2.328010	0.612970
35	6	0	5.252999	1.536498	-0.569221
36	6	0	4.181285	0.691908	-0.605792
37	1	0	-4.789455	1.288114	3.692895
38	1	0	-4.320662	3.692476	3.218792
39	1	0	-2.532559	4.304227	1.624724
40	1	0	-3.420929	-0.469724	2.562067
41	1	0	-2.525039	3.885207	-0.792363
42	1	0	-1.076813	4.784500	-2.580029
43	1	0	1.328063	4.106608	-2.671661
44	1	0	2.238385	2.589857	-0.957895
45	1	0	-2.132710	-2.420721	1.919249
46	1	0	-3.627436	-4.659690	1.570671
47	1	0	-4.543254	-4.566600	-0.992762
48	1	0	-3.576154	-2.262771	-2.054427
49	1	0	-0.856699	0.770062	-2.863861
50	1	0	-2.823658	2.179608	-4.080456
51	1	0	-5.071909	1.798563	-2.585448
52	1	0	-4.367737	0.134417	-0.565449
53	1	0	4.008873	-0.932666	2.382998
54	1	0	3.318814	-2.091080	4.739896
55	1	0	0.729568	-1.388172	5.199789
56	1	0	-0.021720	0.147655	3.085108
57	1	0	3.536813	2.283097	2.179856
58	1	0	5.822456	3.094677	0.950637
59	1	0	6.045971	1.586539	-1.306103
60	1	0	3.873552	-0.052911	-1.330822
61	45	0	0.804986	-1.328690	-0.537450
62	6	0	0.721033	-2.736669	0.937075
63	8	0	0.823690	-3.686409	1.571246
64	6	0	1.322931	-0.602102	-2.317682
65	8	0	1.377363	0.491512	-2.824460
66	6	0	3.193424	-1.616518	-3.637679
67	6	0	1.763297	-1.843106	-3.159198
68	6	0	1.625826	-3.224066	-2.522195
69	1	0	3.465327	-2.368683	-4.390182
70	1	0	3.901960	-1.721922	-2.801957
71	1	0	3.314653	-0.620644	-4.077472
72	1	0	2.279912	-3.326980	-1.642449

73	1	0	0.592193	-3.461867	-2.234704
74	1	0	1.944617	-3.995017	-3.238043
75	1	0	1.089931	-1.787152	-4.031299