Electronic versus steric control in palladium complexes of carboranyl phosphine-iminophosphorane ligands.

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Table S1. Summary of crystal and refinement data for the palladium complexes **Pd1**-**Pd6**.

	Pd1·1.1MeCN	**Pd2·4CH_2Cl_2**	**Pd3·2CH_2Cl_2**	**Pd4.½CH_2Cl_2**	**Pd5**	**Pd6·2$CHCl_3$**
Empirical Formula	$C_{29.2}H_{36.3}B_{10}Cl_2N_{2.1}P_2Pd$	$C_{60}H_{78}B_{20}Cl_{12}N_2P_4Pd_2$	$C_{68}H_{78}B_{20}Cl_8N_2P_4Pd_2$	$C_{27.5}H_{34}B_{10}Cl_3NP_2Pd$	$C_{28}H_{35}B_{10}Cl_2NP_2Pd$	$C_{39}H_{33}Cl_8NP_2Pd$
Formula weight	764.04	1805.52	1759.80	761.34	732.91	967.60
Temperature (K)	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystalline system	Triclinic	Triclinic	Monoclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	P -1	P -1	$P2_1/n$	Pbcn	$P2_1/c$	$P2_1/c$
Cell Constants (Å, °)	a = 14.3478(5)	a = 10.0348(9)	a = 9.6471(8)	a = 16.5388(16)	a = 12.4520(8)	a = 15.7503(16)
	b = 15.2150(6)	b = 12.5745(13)	b = 20.3872(16)	b = 15.5576(14)	b = 16.2137(8)	b = 15.9367(16)
	c = 17.8257(6)	c = 17.0634(17)	c = 20.3717(15)	c = 26.972(2)	c = 17.6328(11)	c = 17.0977(16)
	α = 90.742(2)	α = 108.249(6)	α = 90	α = 90	α = 90	α = 90
	β = 100.401(2)	β = 95.507(6)	β = 100.521(3)	β = 90	β = 109.186(4)	β = 107.832(5)
	γ = 109.907(2)	γ = 98.630(6)	γ = 90	γ = 90	γ = 90	γ = 90
Volume ($Å^3$)	3587.1(2)	1998.1(3)	3939.3(5)	6940.0(11)	2695.2(9)	4085.5(7)
Z	4	1	2	8	4	4
Absorption coefficient (mm^{-1})	0.781	0.971	0.852	0.880	0.829	1.086
F(000)	1545	908	1776	3064	1480	1944
Theta range for data collection (°)	1.428-26.371	2.077-27.103	1.998-26.021	1.510-25.688	1.732-30.508	1.788-26.372
Index ranges	-17 ≤ h ≤ 17	-12 ≤ h ≤ 12	-11 ≤ h ≤ 11	-20 ≤ h ≤ 19	-17 ≤ h ≤ 17	-19 ≤ h ≤ 19
	-19≤ k ≤ 19	-16 ≤ k ≤ 16	-25 ≤ k ≤ 25	-18 ≤ k ≤ 18	-23 ≤ k ≤ 23	-19 ≤ k ≤ 19
	-22 ≤ l ≤ 22	-21 ≤ l ≤ 21	-25 ≤ l ≤ 24	-32 ≤ l ≤ 32	-25 ≤ l ≤ 25	-21 ≤ l ≤ 19
Size (mm)	0.45 x 0.12 x 0.06	0.22 x 0.05 x 0.04	0.45 x 0.10 x 0.06	0.62 x 0.04 x 0.03	0.42 x 0.23 x 0.11	0.60 x 0.09 x 0.03
Collected reflections	56187	63178	36811	47928	77182	60588
Independent reflections	14618 [R(int) = 0. 0.0726]	8784 [R(int) = 0.0707]	7760 [R(int) = 0.0527]	6592 [R(int) = 0.1230]	10260 [R(int) = 0.0785]	8352 [R(int) = 0.0864]
Data/ restraints/ parameters	14618 / 62 / 926	8784 / 0 / 452	7760 / 0 / 470	6592 / 668 / 502	10260 / 0 / 402	8352 / 0 / 460
Goodness-on-fit (F^2)	1.010	1.037	1.026	1.056	1.048	1.013
Final R indices [I>2s(I)][a]	R_1 = 0.0423	R_1 = 0.0371	R_1 = 0.0402	R_1 = 0.0621	R_1 = 0.0362	R_1 = 0.0422
	wR_2 = 0.0766	wR_2 = 0.0783	wR_2 = 0.0882	wR_2 = 0.0976	wR_2 = 0.0708	wR_2 = 0.0766
R indices (all data)	R_1 = 0.0705	R_1 = 0.0603	R_1 = 0.0576	R_1 = 0.1124	R_1 = 0.0564	R_1 = 0.0787
	wR_2 = 0.0867	wR_2 = 0.0866	wR_2 = 0.0958	wR_2 = 0.1125	wR_2 = 0.0764	wR_2 = 0.0885
Largest diff. peak and hole ($e \cdot Å^{-3}$)	0.553 and -0.637	0.648 and -0.861	0.901 and -1.060	0.698 and -1.054	0.505 and -0.881	1.728 and -1.195

[a] $R_1 = \sum[|F_o|- |F_c|/\Sigma|F_o|]$; $wR_2 = [|\Sigma(F_o^2-F_c^2)/\Sigma(F_o^2)]^{1/2}$

Table S2. Mulliken charges and natural charges (NPA) of the iminophosphorane N atoms of ligands **L1-L5** and stretching frequencies calculated with DFT (TPSSh/6-31+G(d,p)) compared with the experimental values.

	Mulliken	**NPA**	**υ(PN)$_{calcd}$**	**υ(PN)$_{exp}$**
L1	-0.052	-1.06505	1349	1369
L2	-0.240	-1.06930	1357	1304
L3	+0.156	-1.04612	1376	1375
L4	-0.829	-1.30039	1409	1433
L5	-0.903	-1.30544	1393	1374

Table S3. Distances, electron densities at the bond critical points (ρ_{BCP}, au), Laplacian of the electron density ($\nabla^2\rho_{BCP}$), total electron energy density (H(r)) and Laplacian bond orders (LBO) of the Pd-N bonds calculated with DFT (TPSSh/6-31+G(d,p)) for the mononuclear complexes [PdLCl$_2$] (L = **L1-L5**) with chelating (P,N) coordination.

	Pd-N / Å	ρ_{BCP}	$\nabla\rho_{BCP}$	H(r)	LBO
Pd1	2.156	0.0810	0.3284	-0.0113	0.175
Pd2	2.160	0.0804	0.3254	-0.0110	0.179
Pd3	2.189	0.0751	0.3056	-0.0089	0.157
Pd4	2.125	0.0874	0.3370	-0.0148	0.173
Pd5	2.142	0.0841	0.3250	-0.0132	0.161

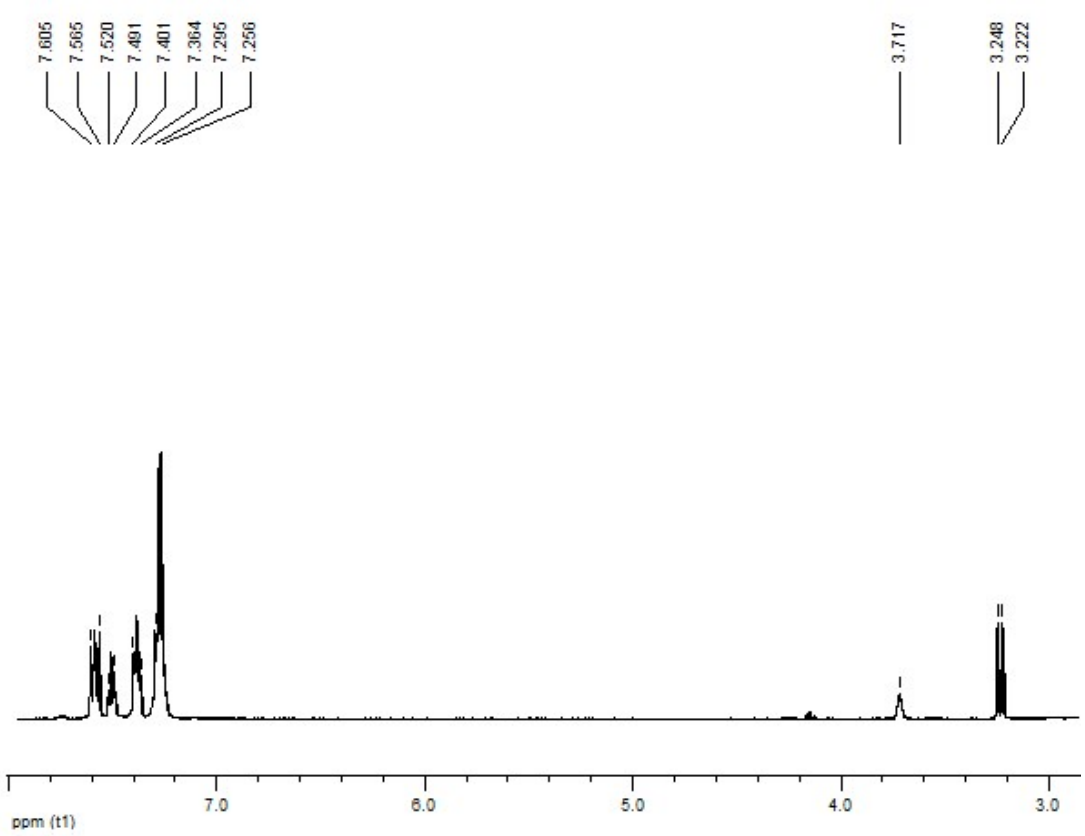

Figure S.1. ^{1}H NMR spectrum ($CDCl_3$) of **L1.**

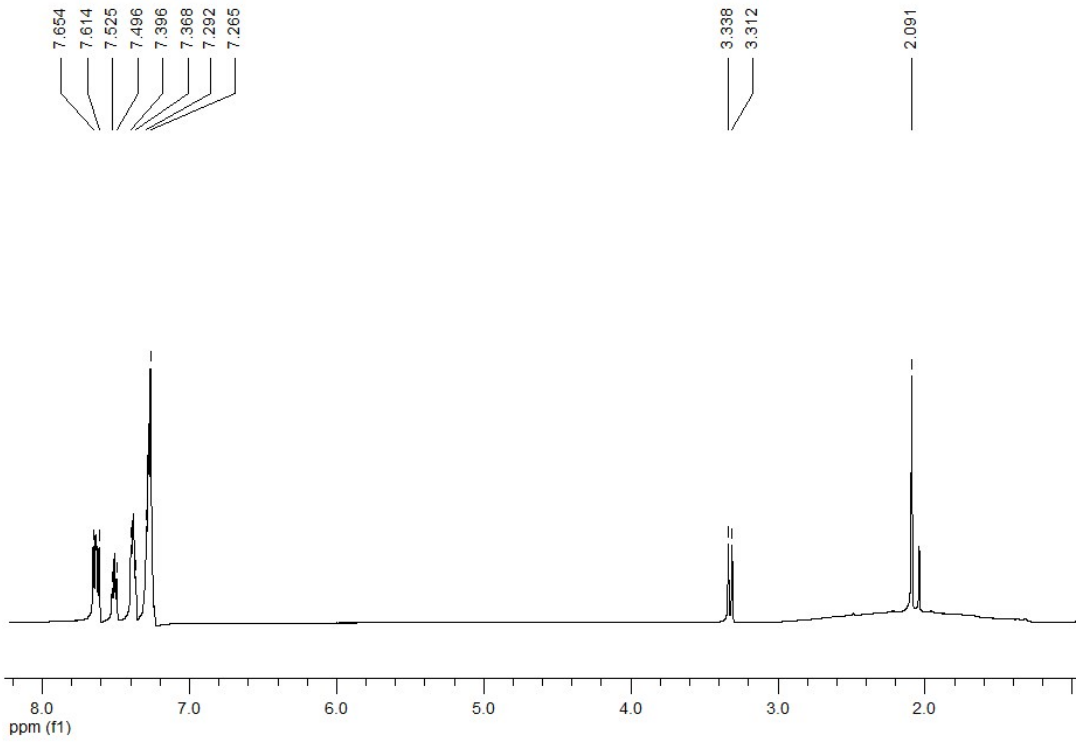

Figure S.2. ^{1}H NMR spectrum ($CDCl_3$) of **L2.**

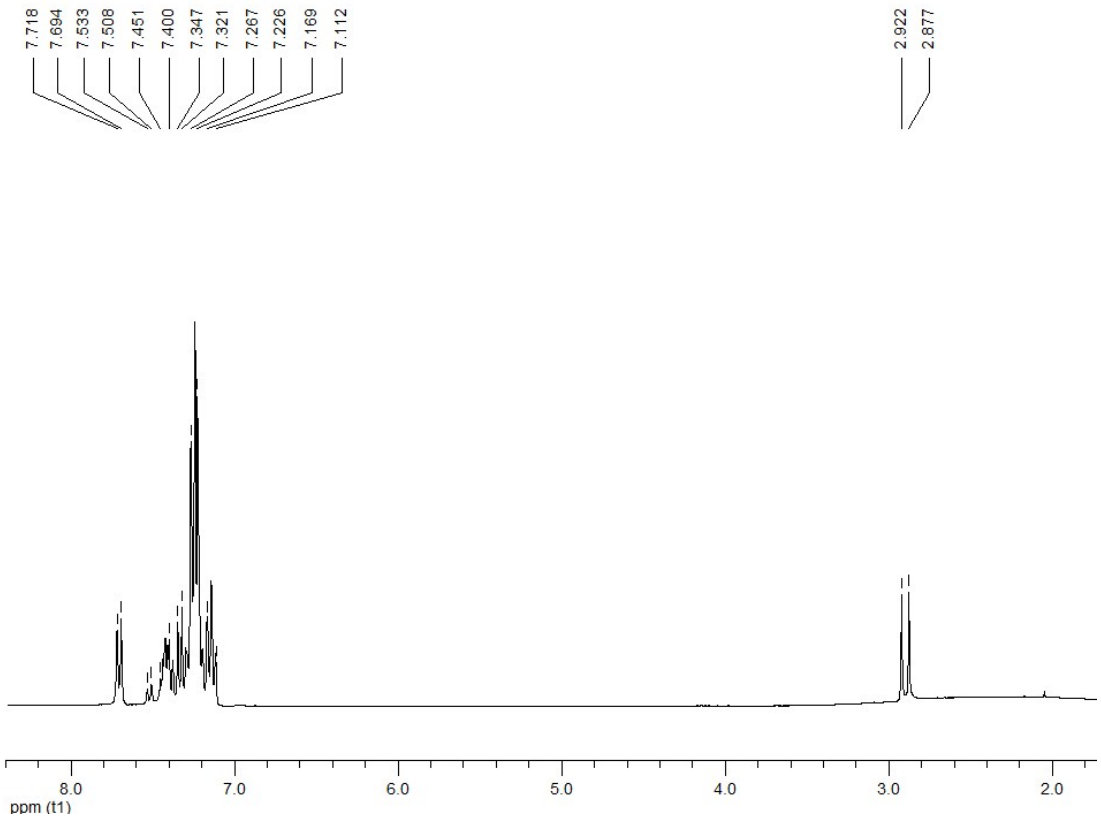

Figure S.3. ^{1}H NMR spectrum ($CDCl_3$) of **L3.**

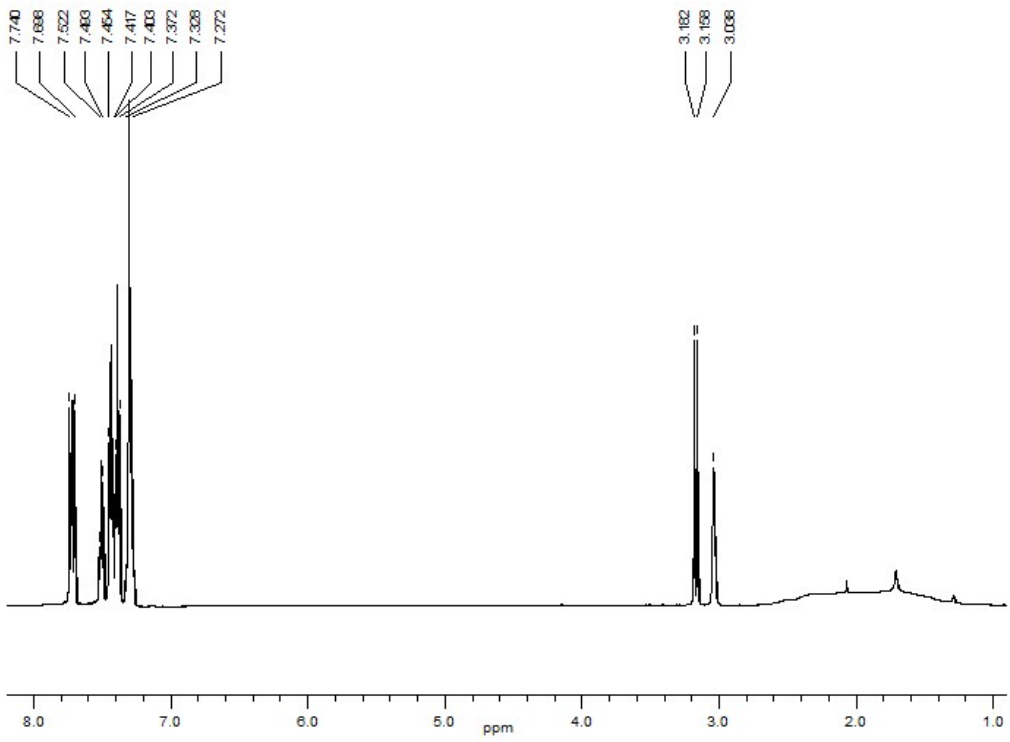

Figure S.4. ^{1}H NMR spectrum ($CDCl_3$) of **L4.**

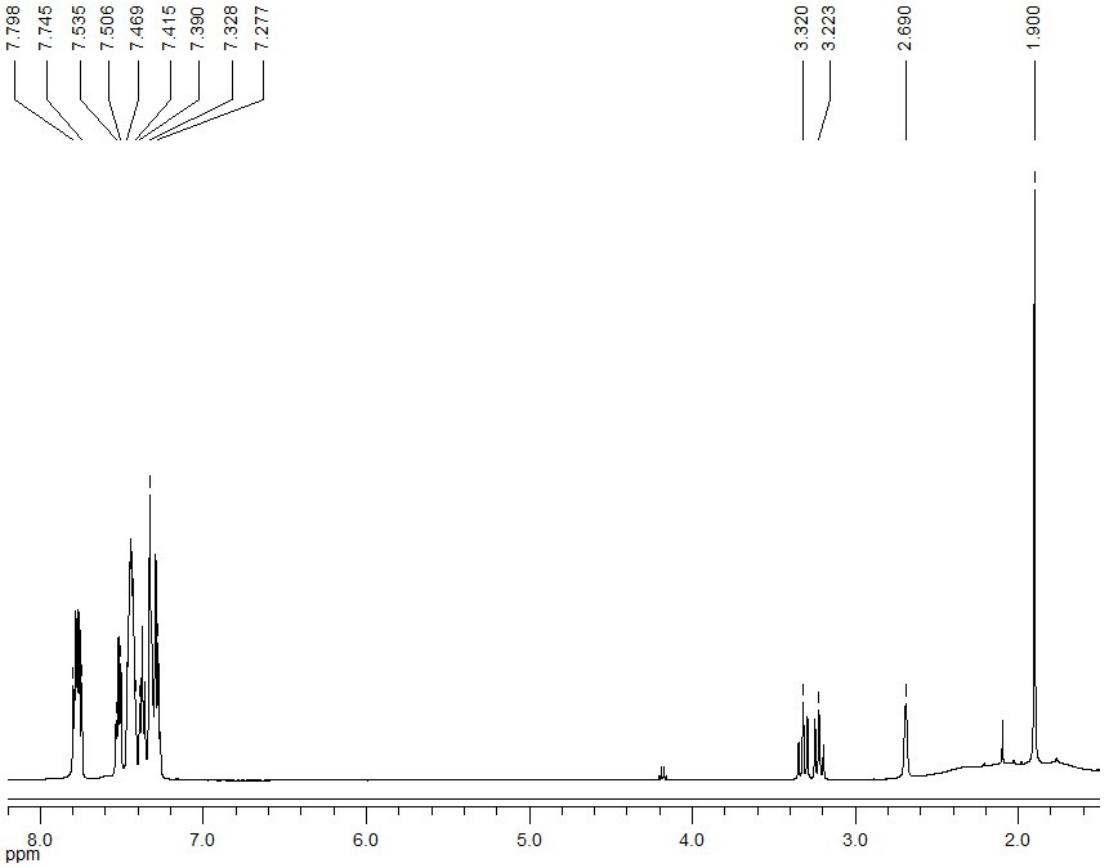

Figure S.5. ^{1}H NMR spectrum ($CDCl_3$) of **L5.**

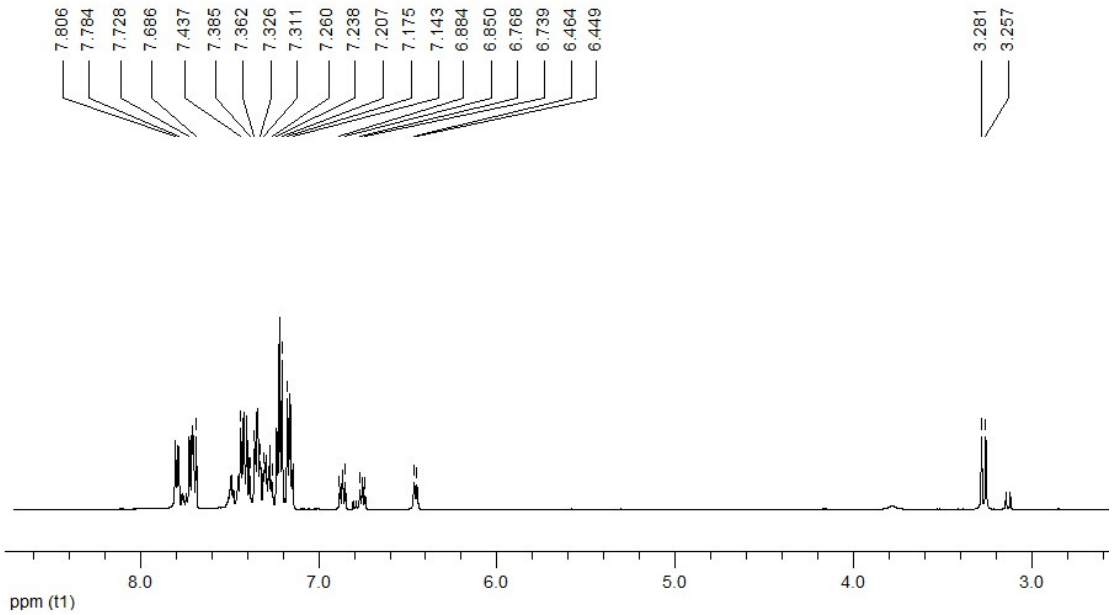

Figure S.6. ^{1}H NMR spectrum ($CDCl_3$) of **L6.**

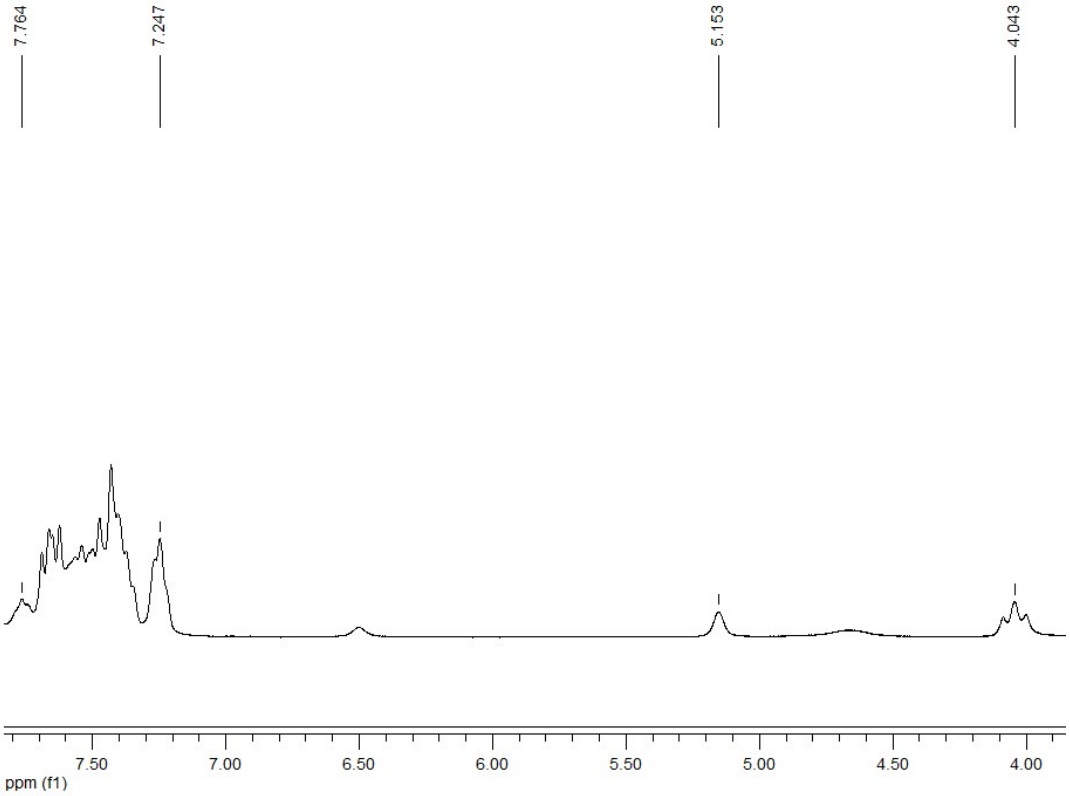

Figure S.7. ^{1}H NMR spectrum ($CDCl_3$) of **Pd1.**

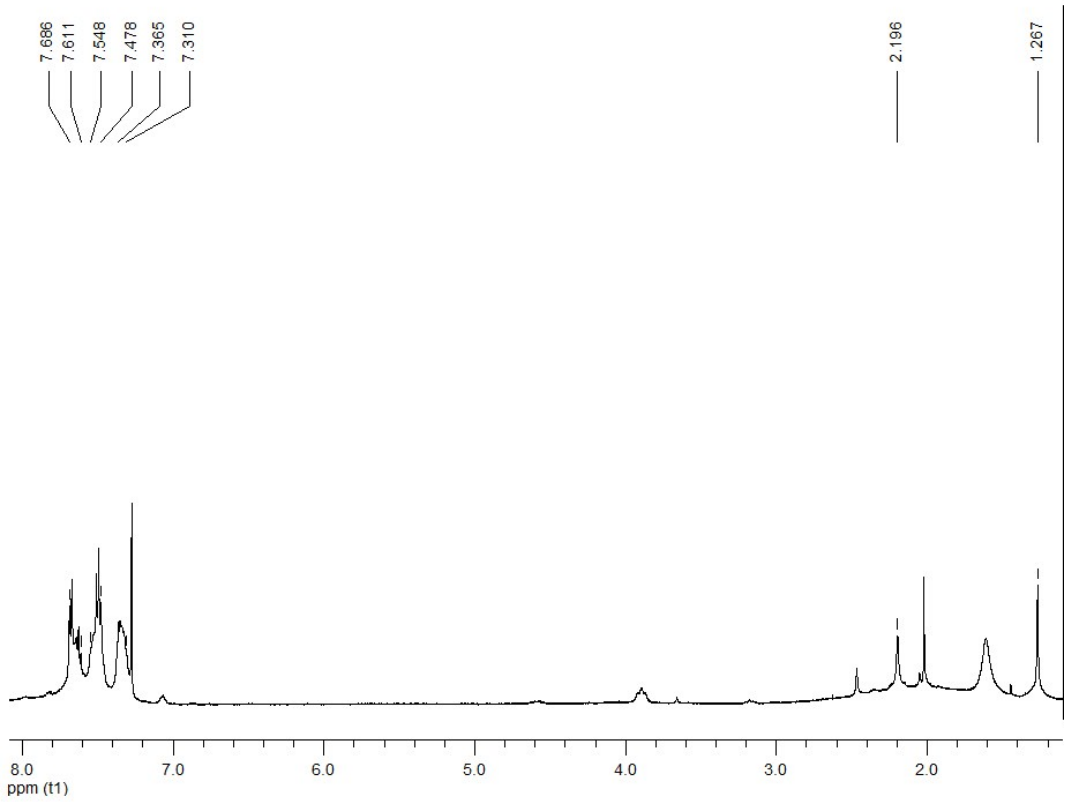

Figure S.8. ^{1}H NMR spectrum ($CDCl_3$) of **Pd2.**

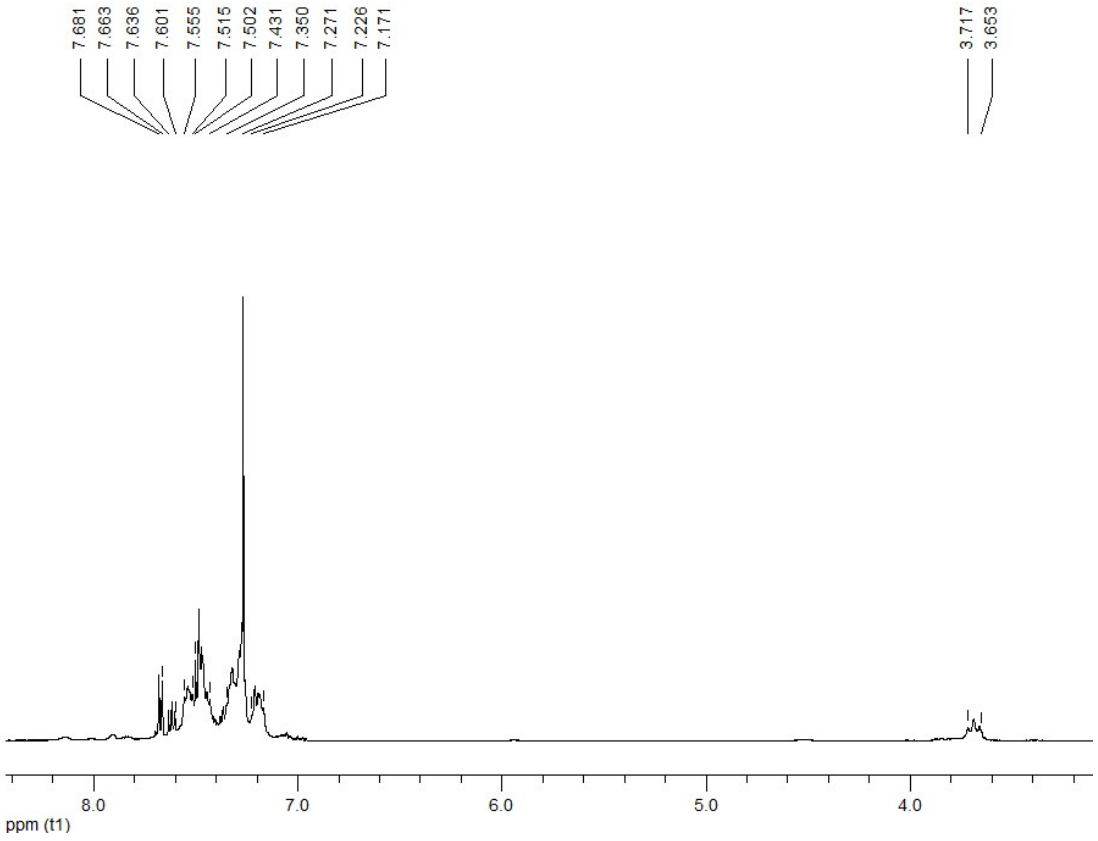

Figure S.9. ^{1}H NMR spectrum ($CDCl_3$) of **Pd3.**

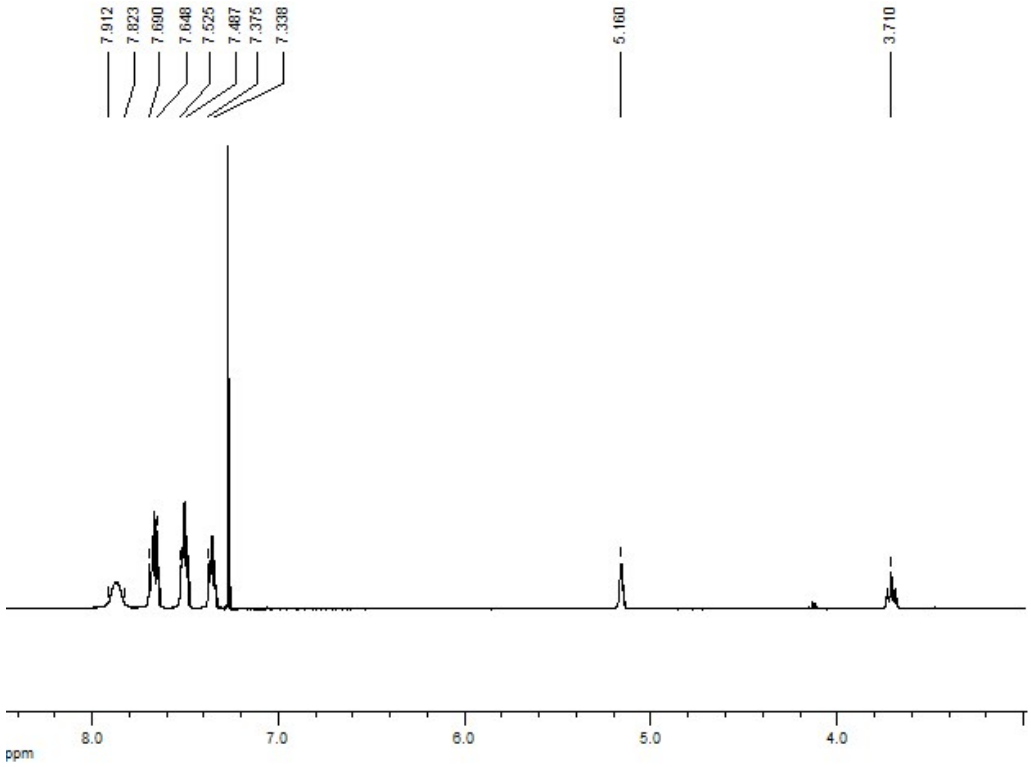

Figure S.10. ^{1}H NMR spectrum ($CDCl_3$) of **Pd4.**

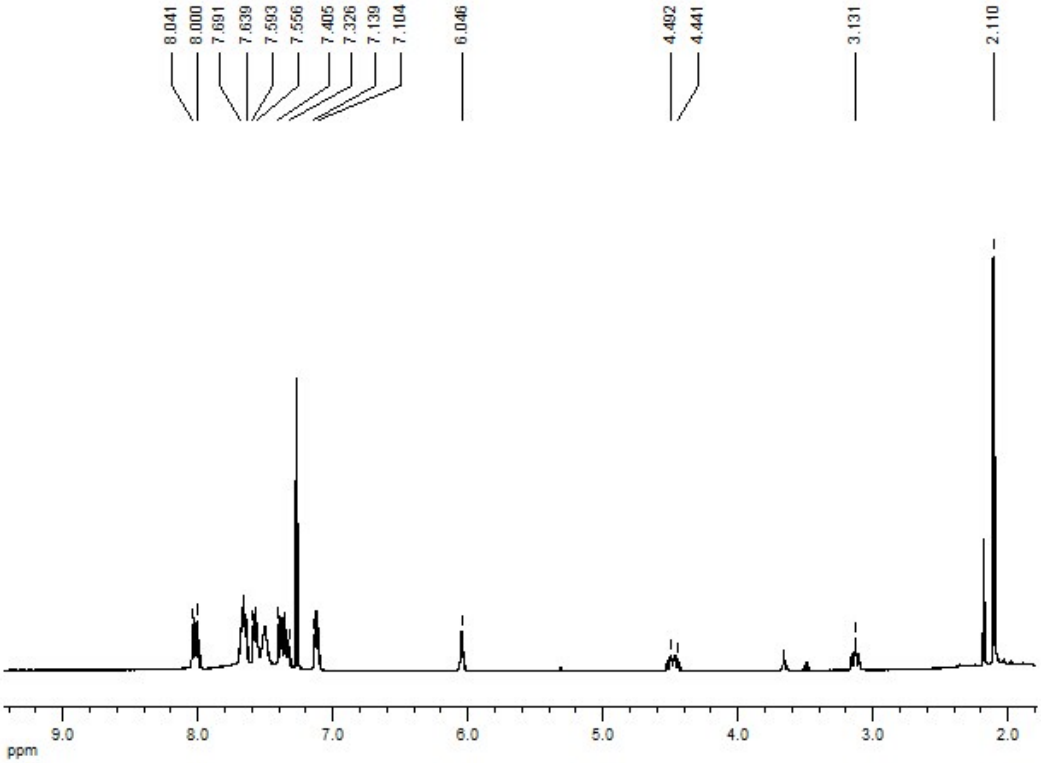

Figure S.11. ^{1}H NMR spectrum ($CDCl_3$) of **Pd5.**

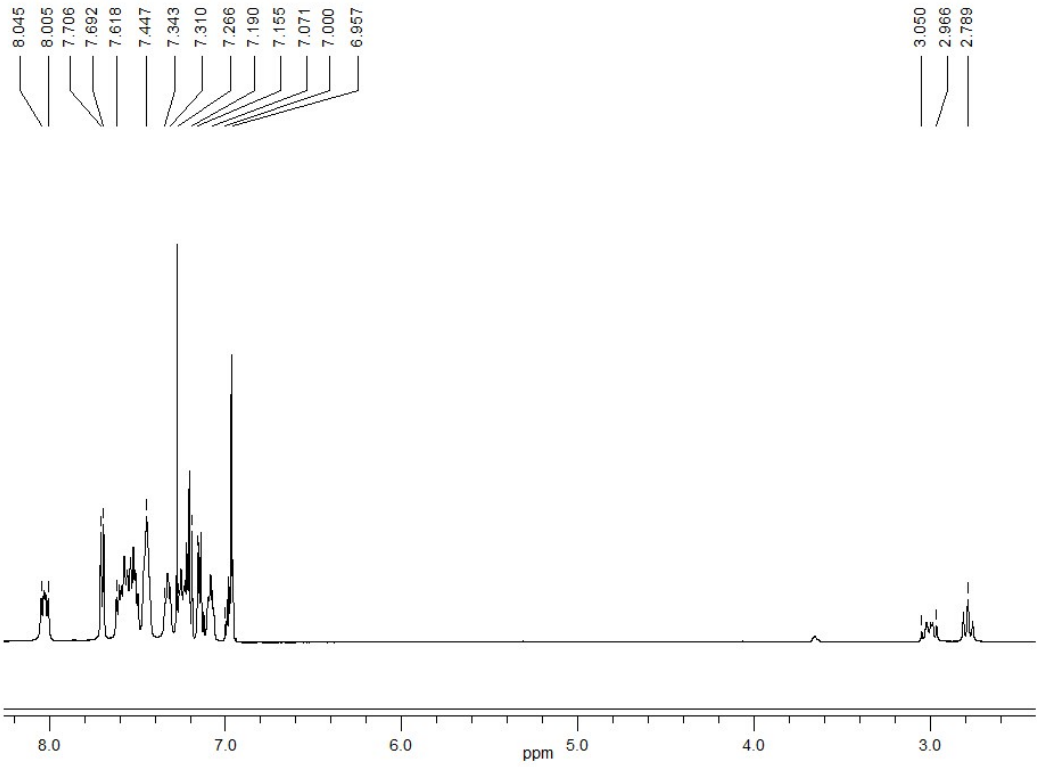

Figure S.12. ^{1}H NMR spectrum ($CDCl_3$) of **Pd6.**

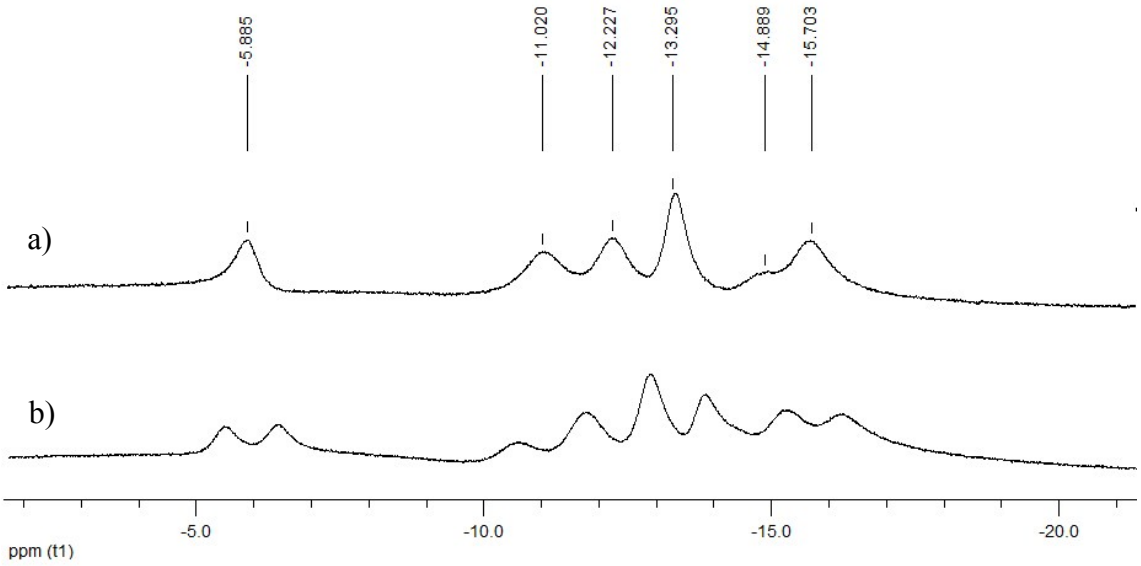

Figure S.13. (a) $^{11}B\{^{1}H\}$ NMR and (b) ^{11}B NMR spectra ($CDCl_3$) of **L1.**

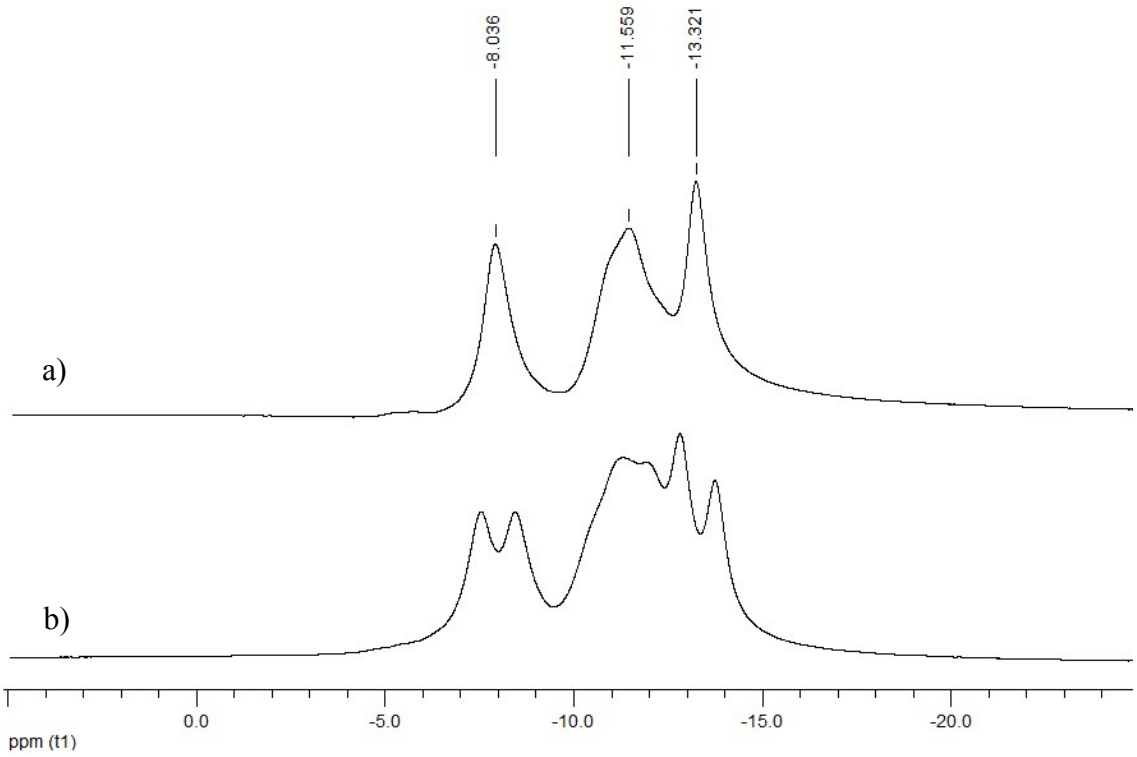

Figure S.14. (a) $^{11}B\{^{1}H\}$ NMR and (b) ^{11}B NMR spectra ($CDCl_3$) of **L2.**

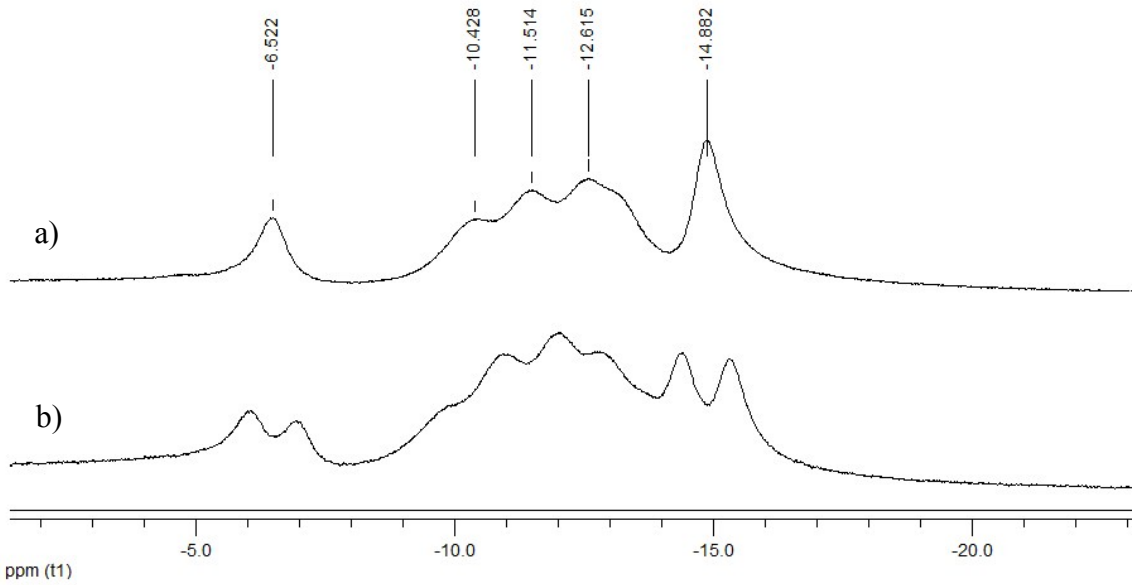

Figure S.15. (a) $^{11}B\{^{1}H\}$ NMR and (b) ^{11}B NMR spectra ($CDCl_3$) of **L3.**

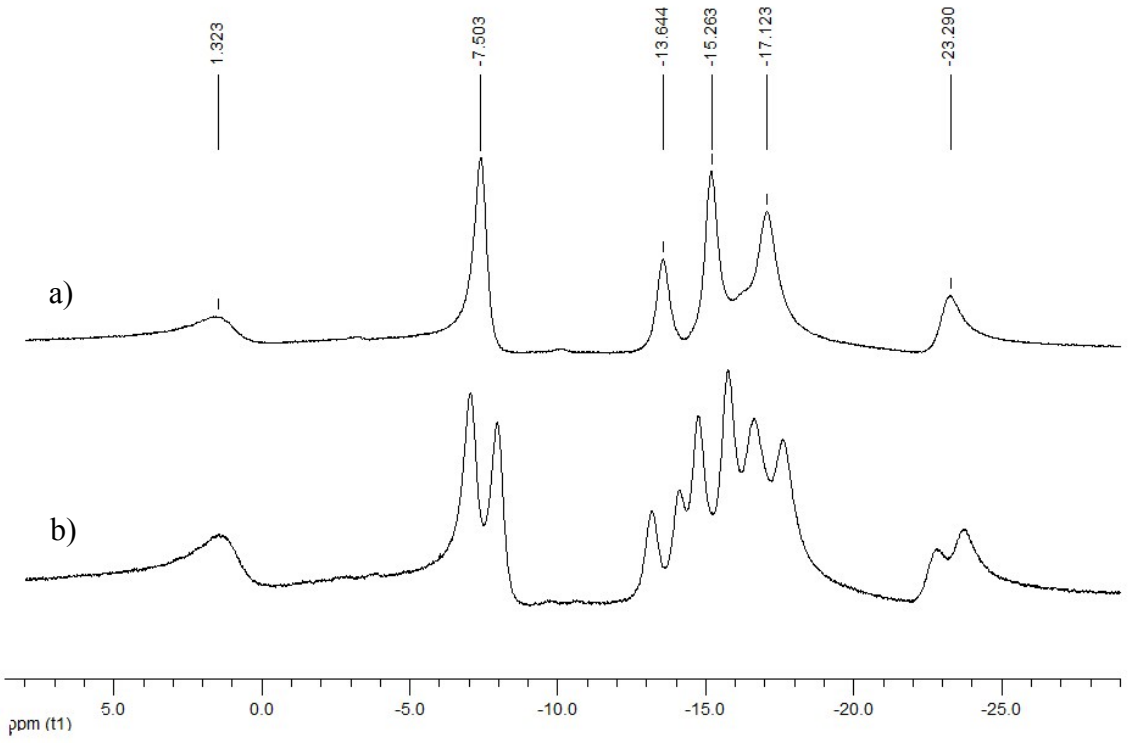

Figure S.16. (a) $^{11}B\{^{1}H\}$ NMR and (b) ^{11}B NMR spectra ($CDCl_3$) of **L4.**

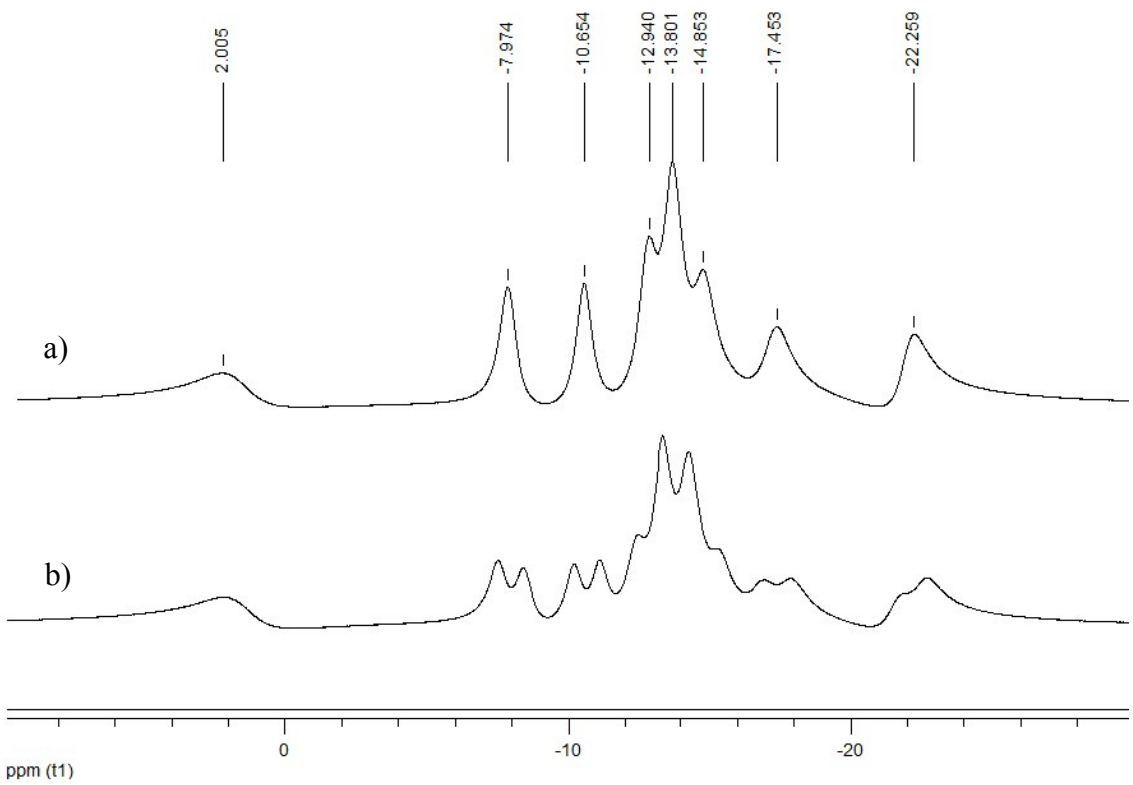

Figure S.17. (a) $^{11}B\{^{1}H\}$ NMR and (b) ^{11}B NMR spectra ($CDCl_3$) of **L5.**

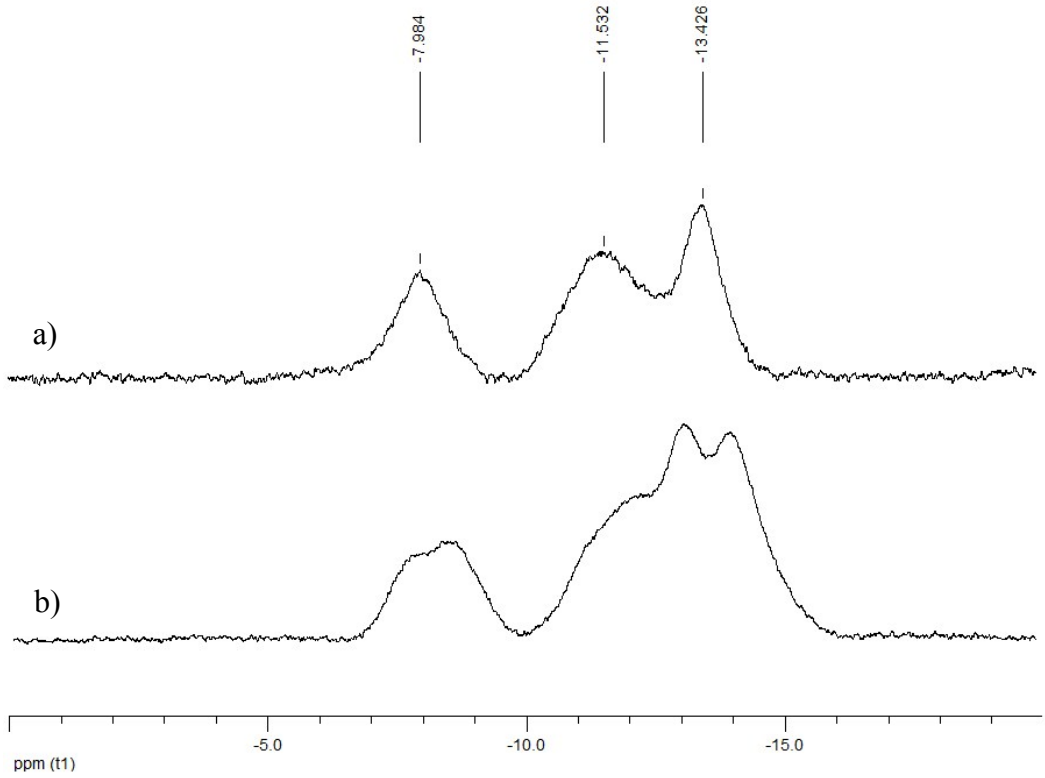

Figure S.18. (a) $^{11}B\{^{1}H\}$ NMR and (b) ^{11}B NMR spectra ($CDCl_3$) of **Pd1.**

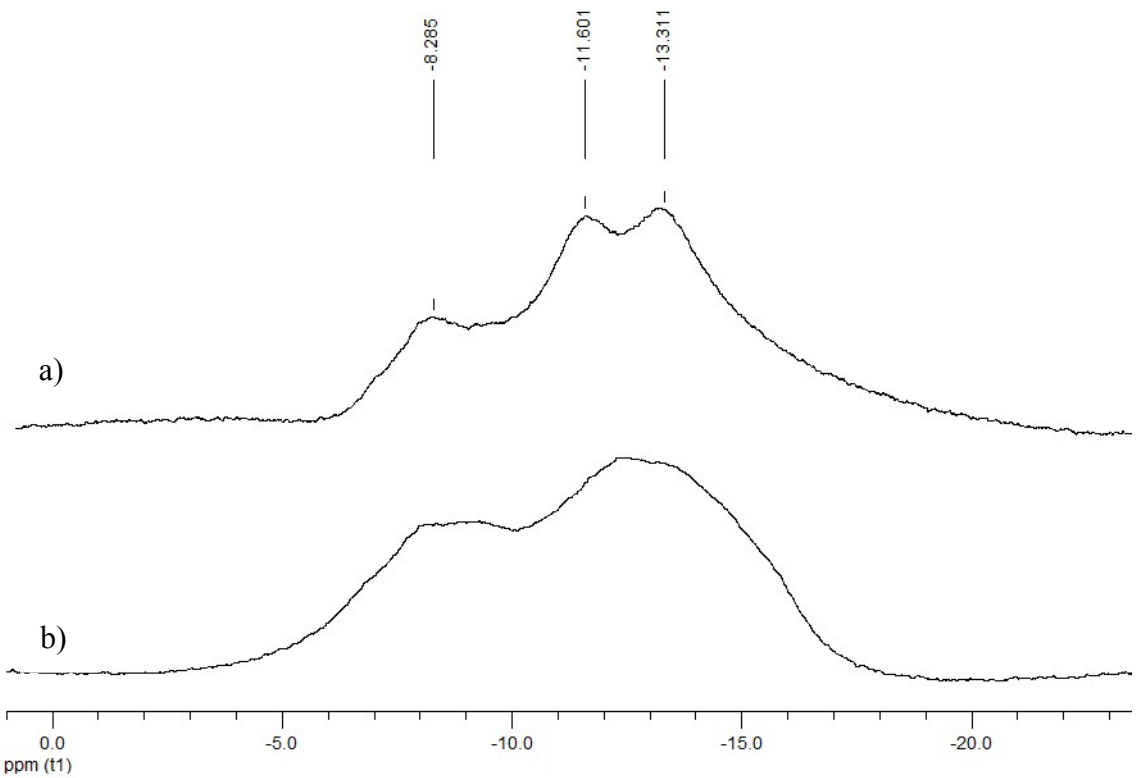

Figure S.19. (a) $^{11}B\{^{1}H\}$ NMR and (b) ^{11}B NMR spectra ($CDCl_3$) of **Pd2.**

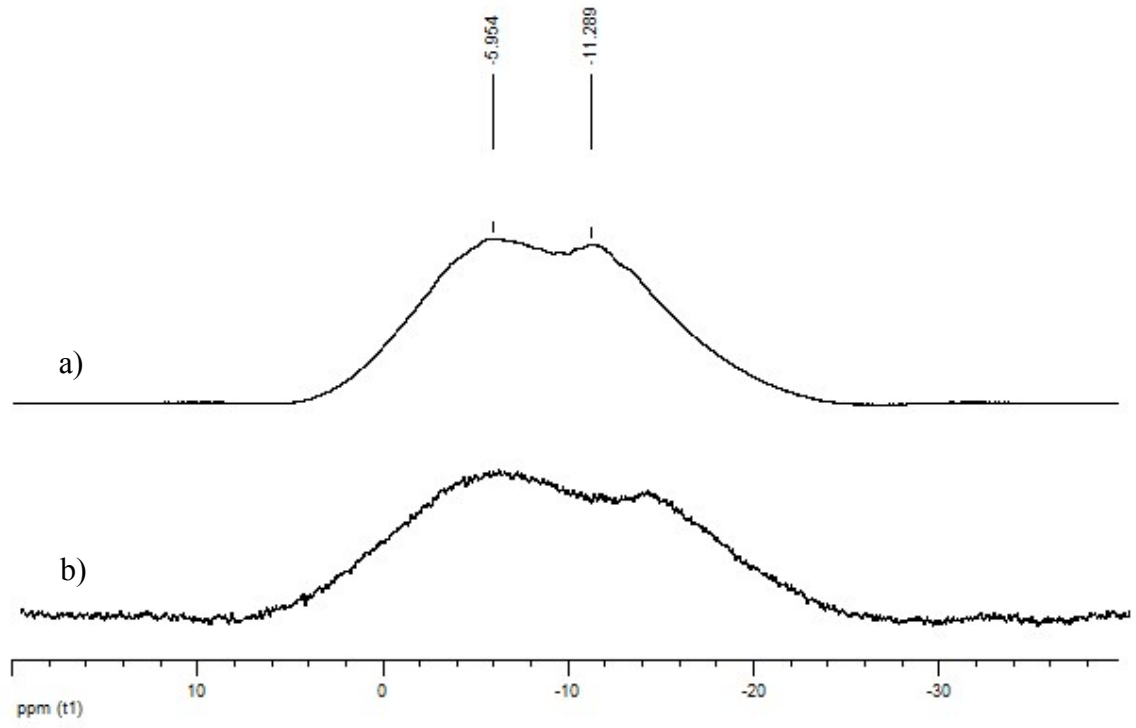

Figure S.20. (a) $^{11}B\{^{1}H\}$ NMR and (b) ^{11}B NMR spectra ($CDCl_3$) of **Pd3.**

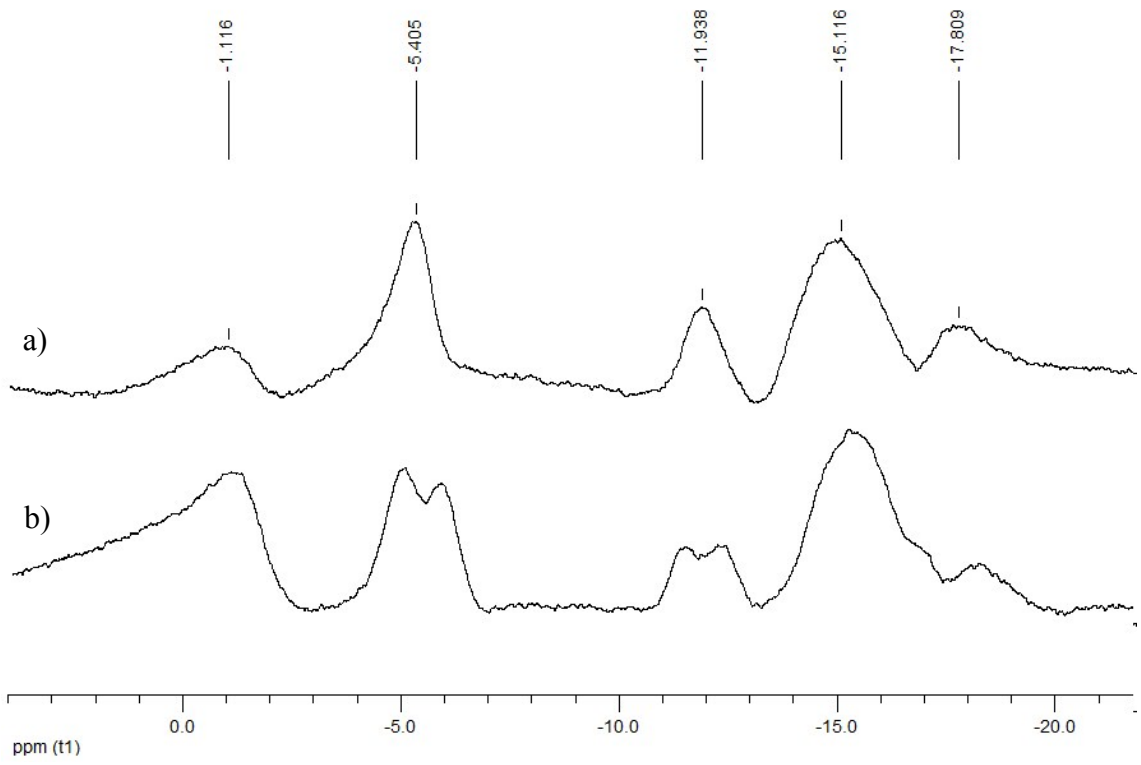

Figure S.21. (a) $^{11}B\{^{1}H\}$ NMR and (b) ^{11}B NMR spectra ($CDCl_3$) of **Pd4.**

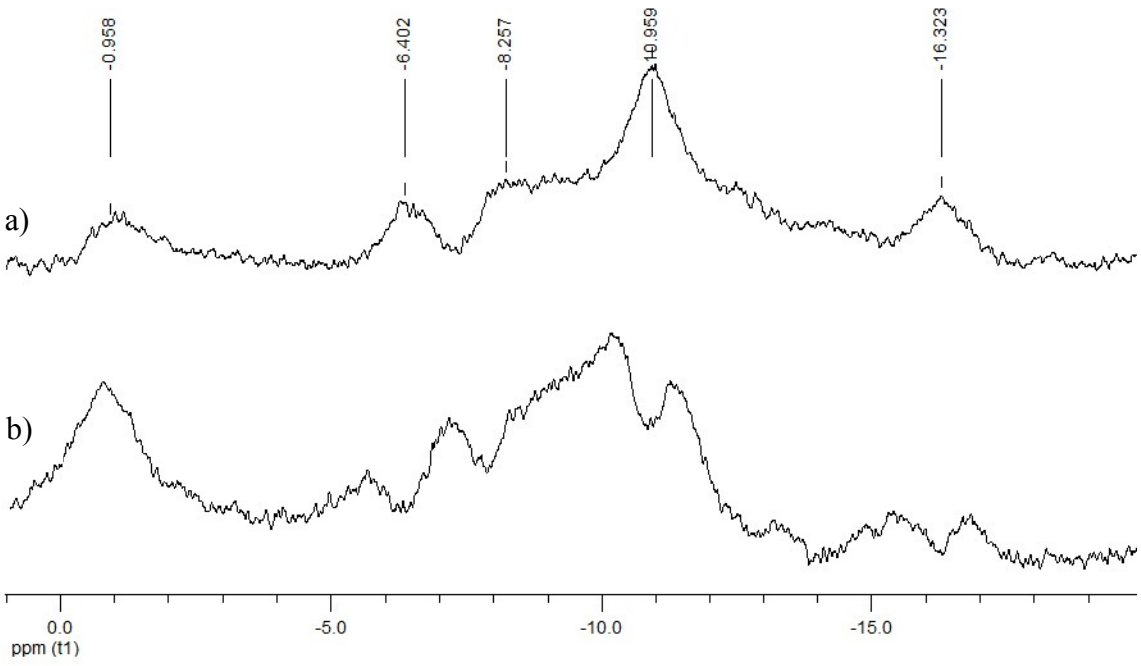

Figure S.22. (a) $^{11}B\{^{1}H\}$ NMR and (b) ^{11}B NMR spectra ($CDCl_3$) of **Pd5.**

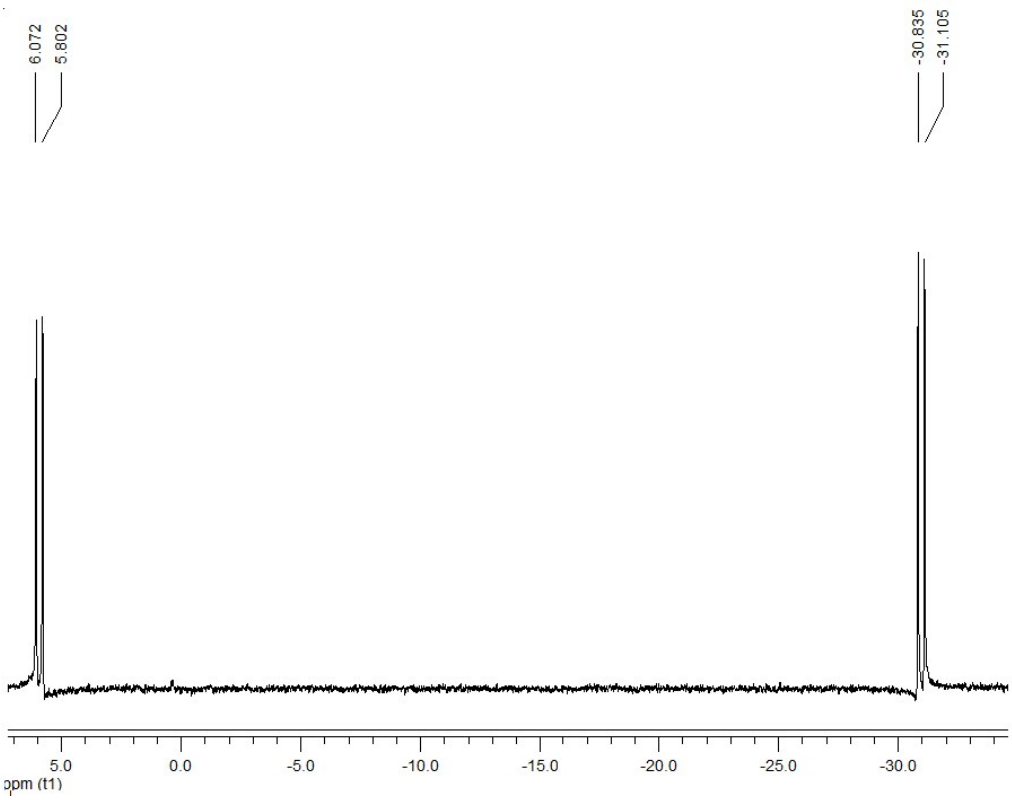

Figure S.23. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **L1.**

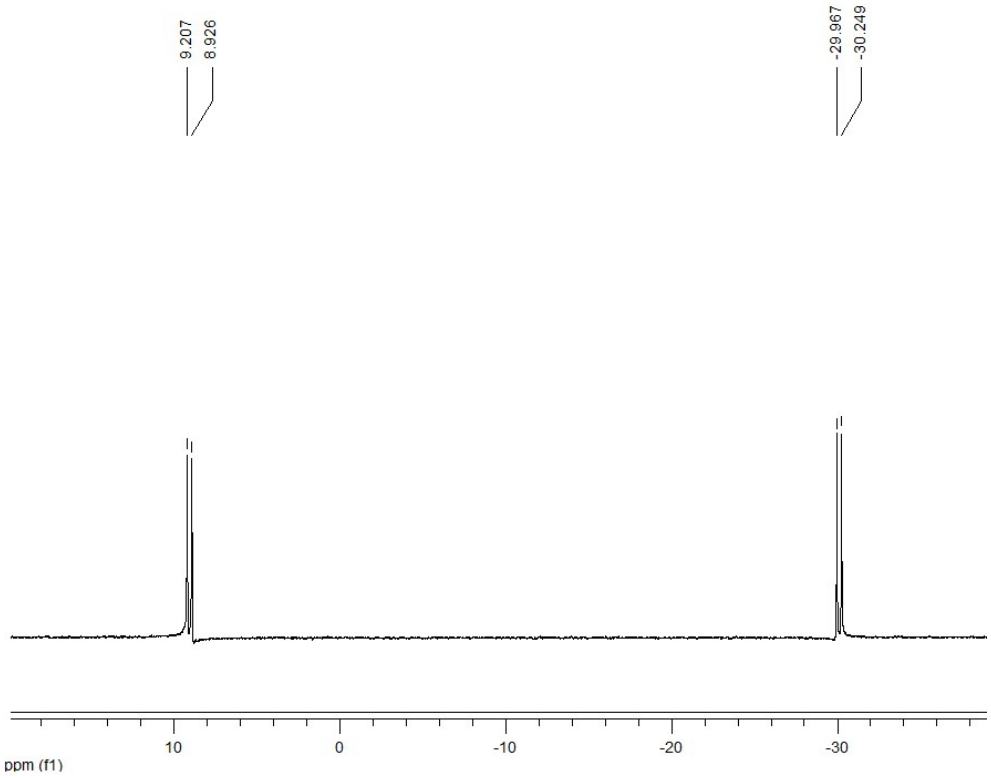

Figure S.24. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **L2.**

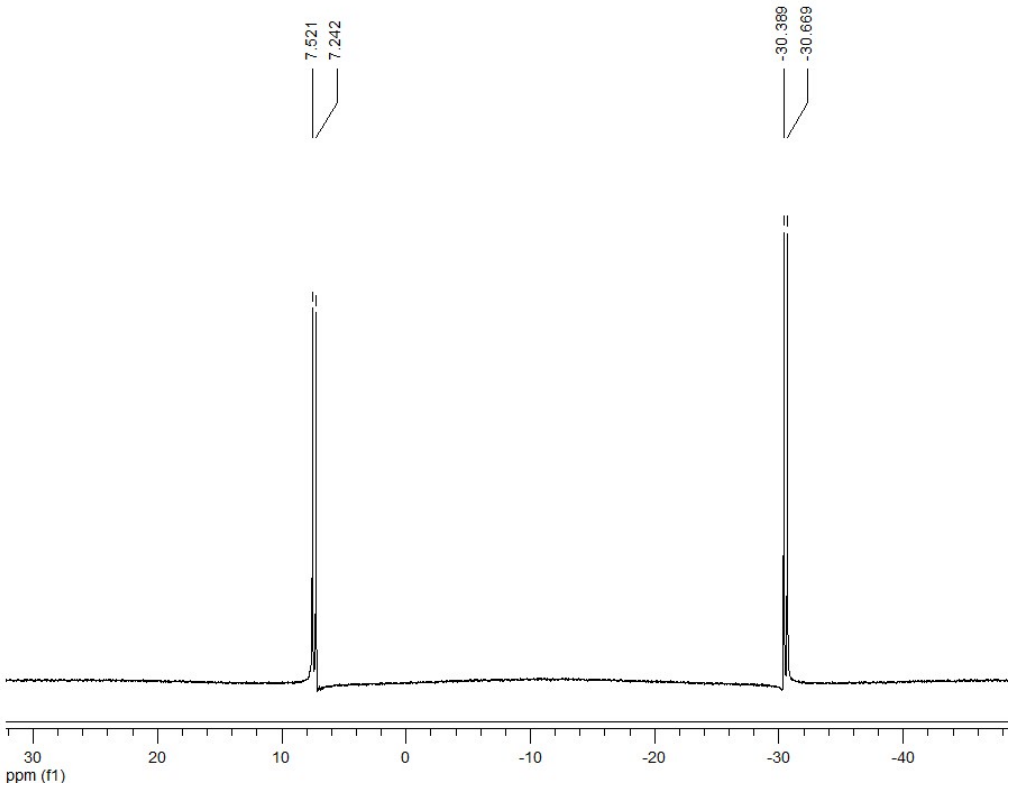

Figure S.25. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **L3.**

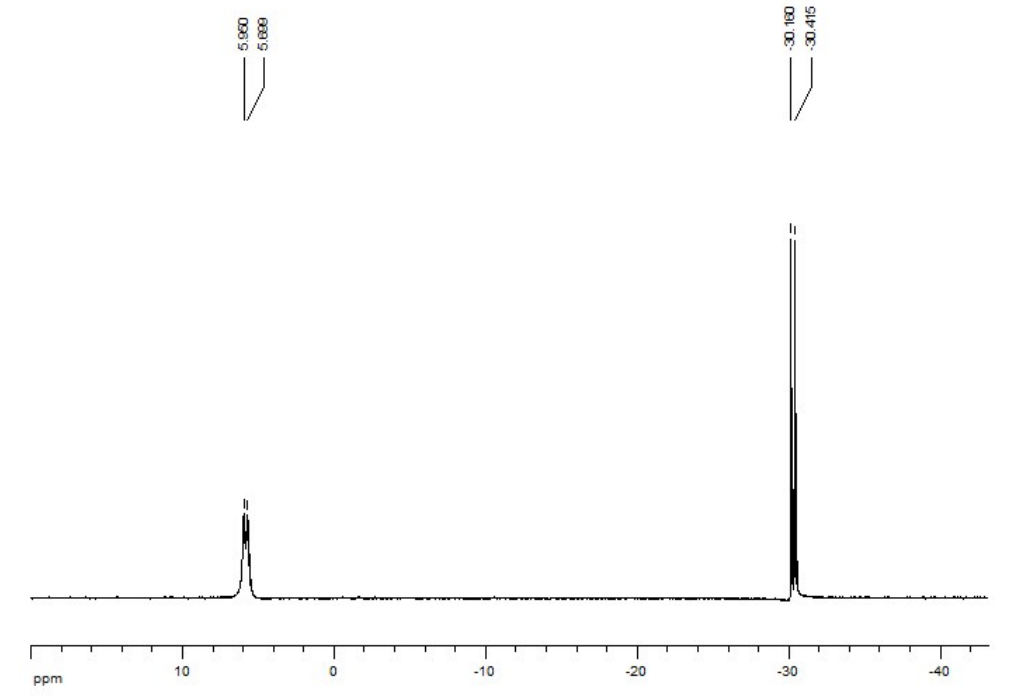

Figure S.26. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **L4.**

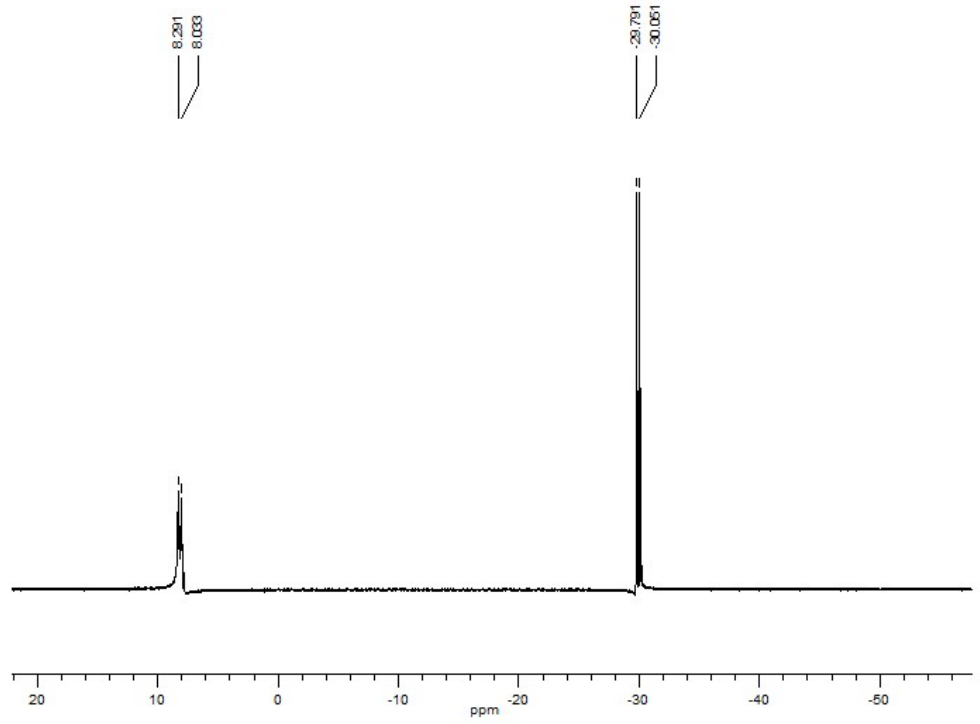

Figure S.27. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **L5.**

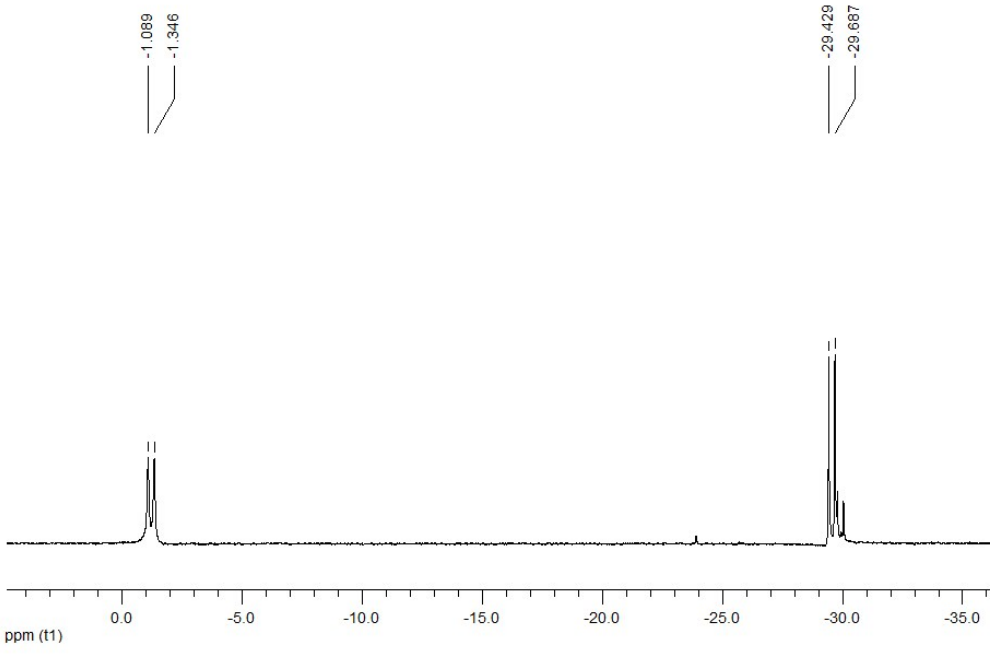

Figure S.28. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **L6.**

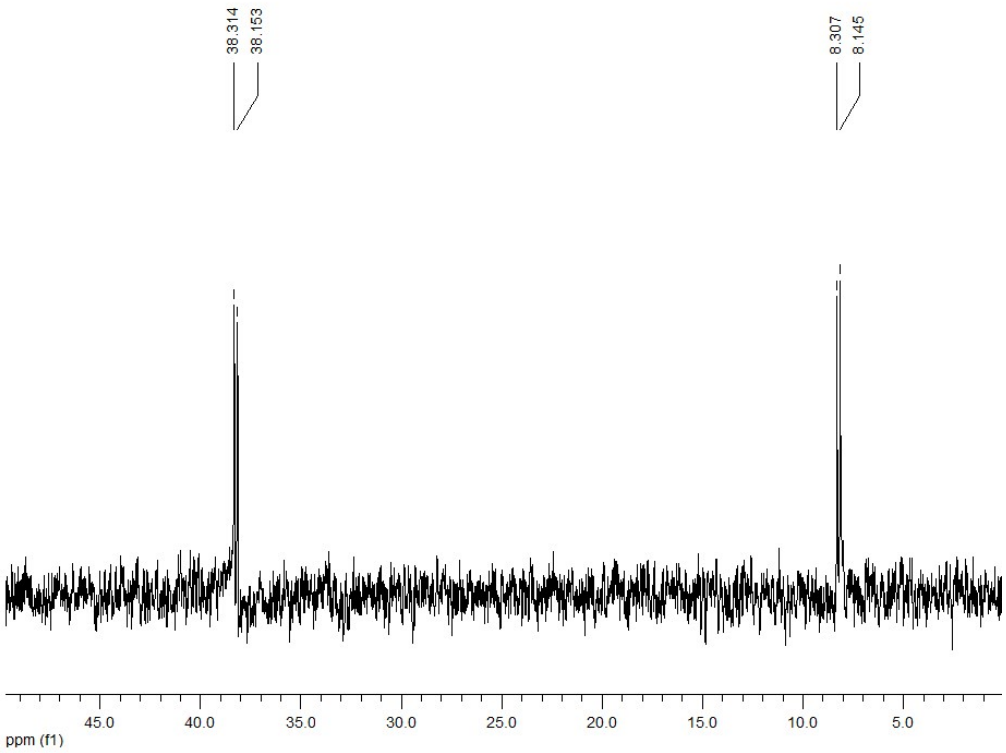

Figure S.29. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **Pd1.**

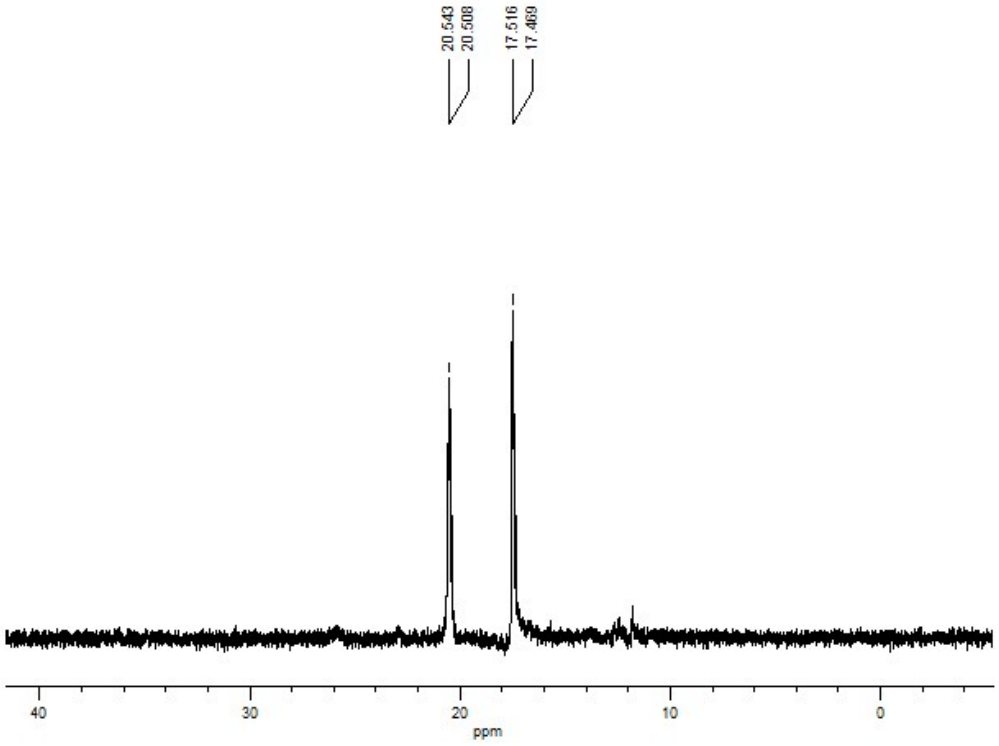

Figure S.30. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **Pd2.**

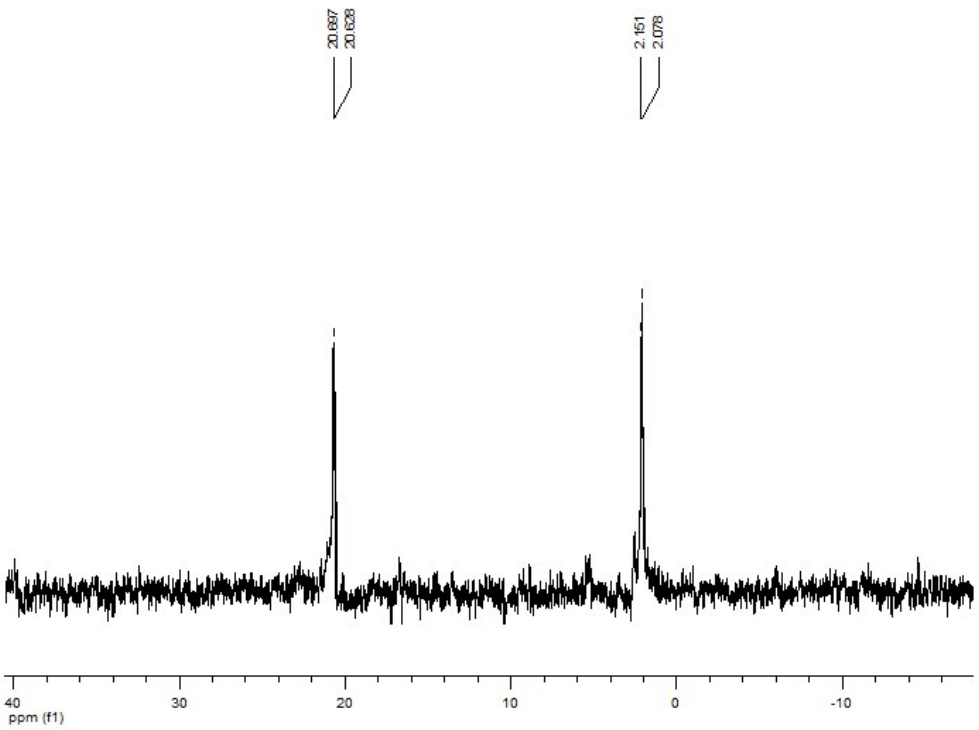

Figure S.31. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **Pd3.**

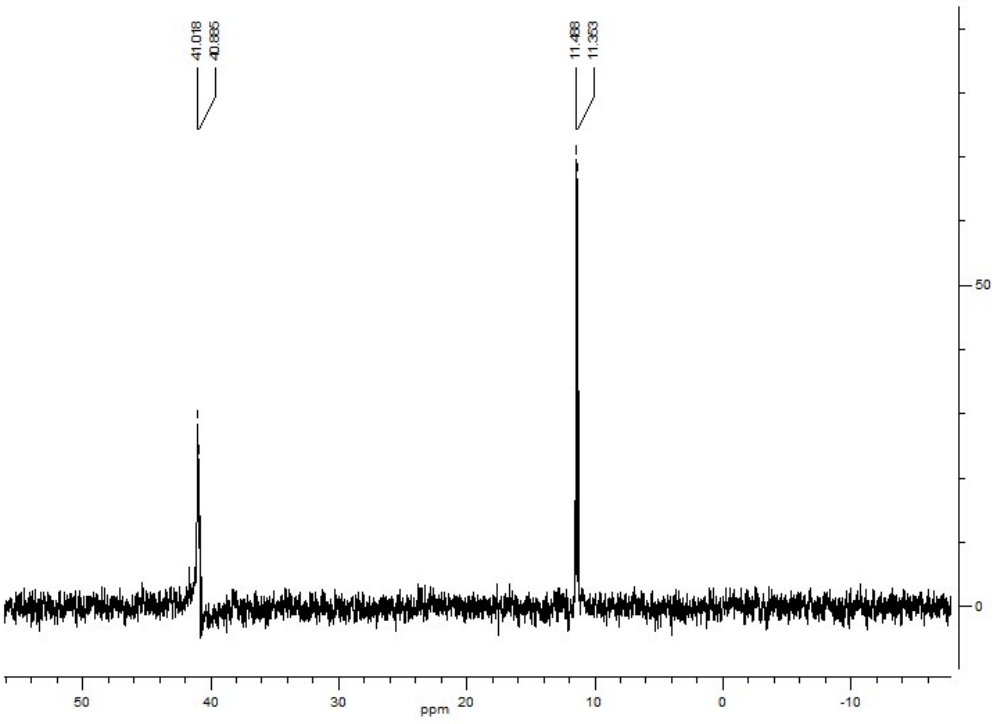

Figure S.32. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **Pd4.**

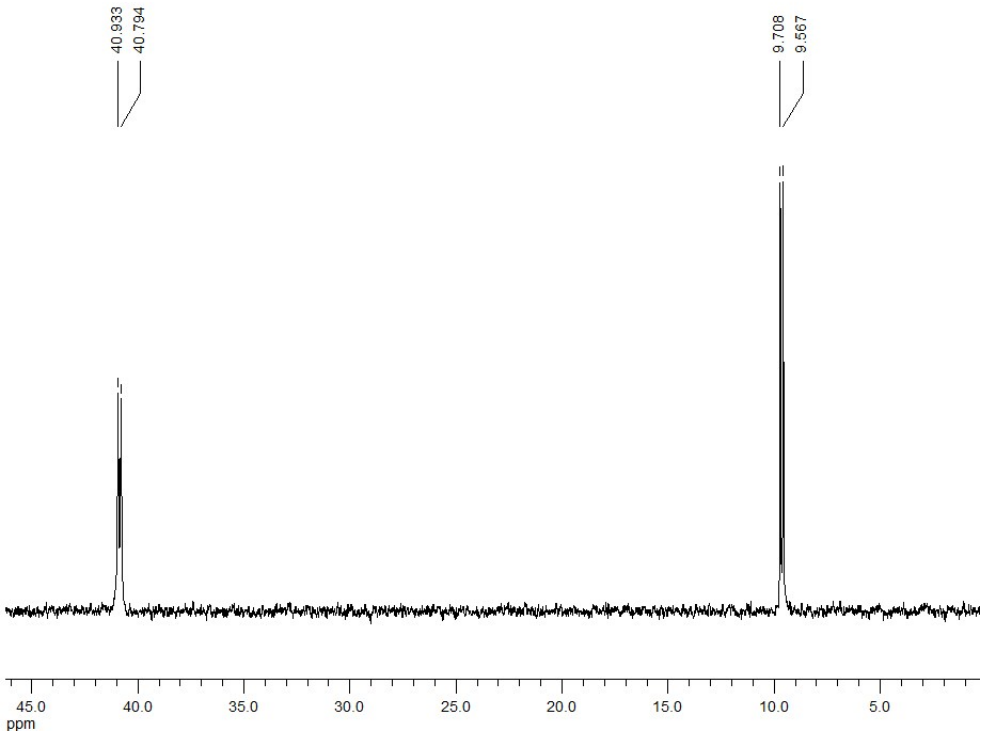

Figure S.33. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **Pd5.**

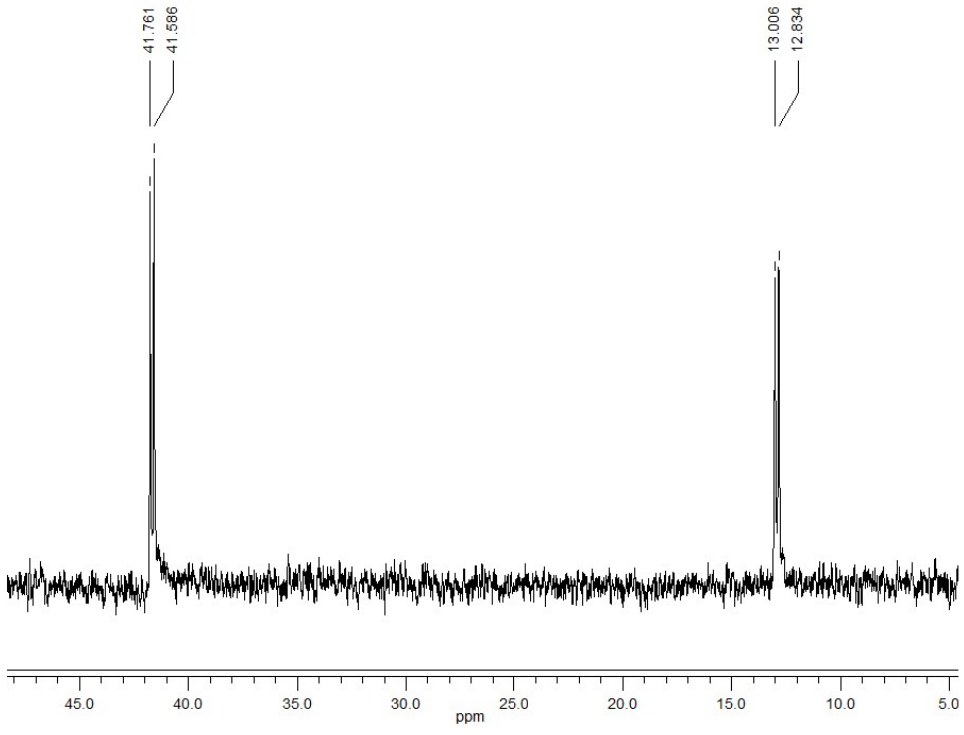

Figure S.34. $^{31}P\{^{1}H\}$ NMR spectrum ($CDCl_3$) of **Pd6.**

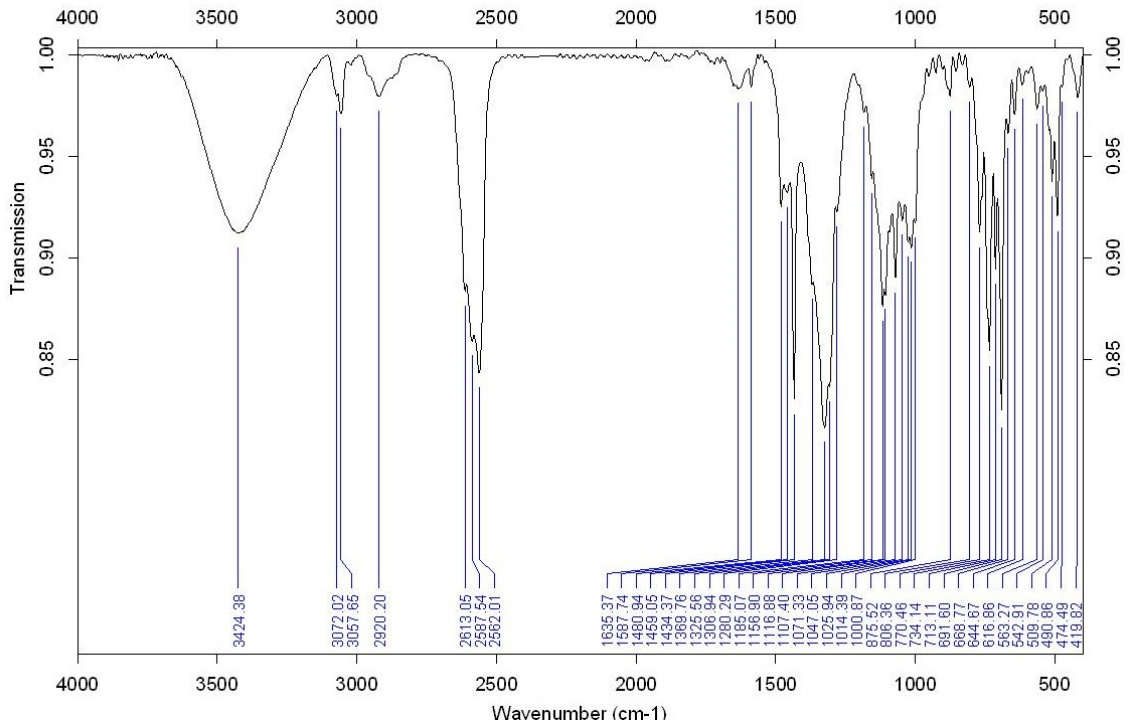

Figure S.35. IR spectrum of **L1.**

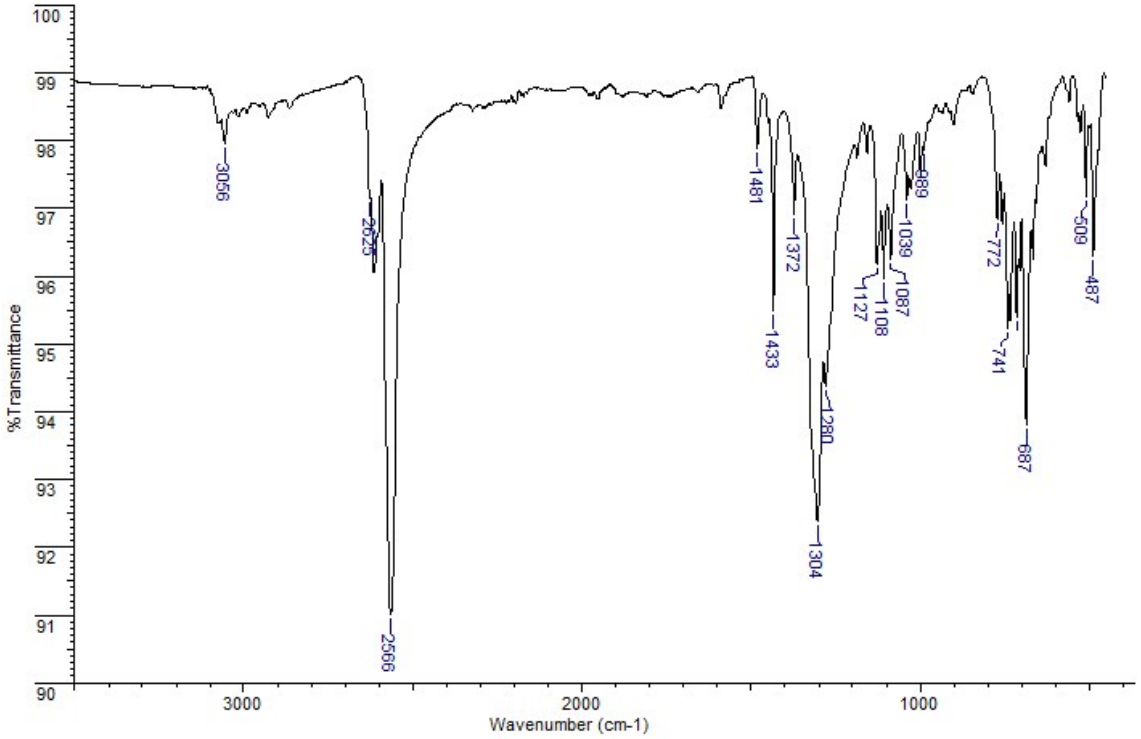

Figure S.36. IR spectrum of **L2.**

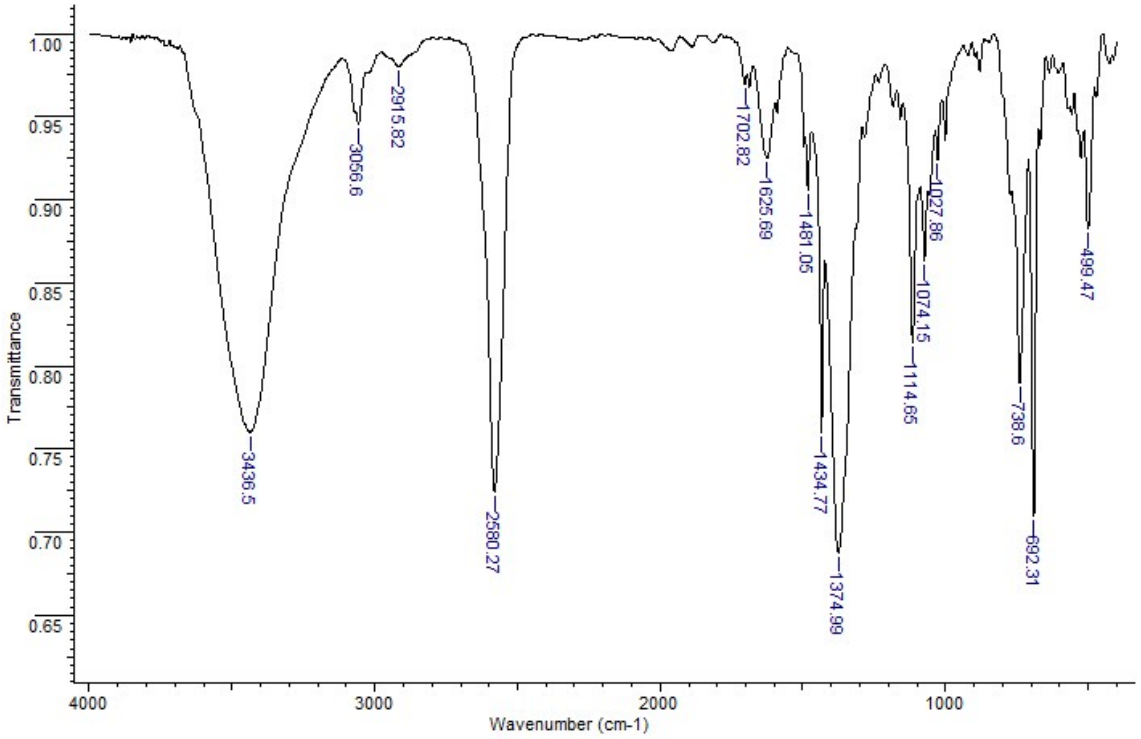

Figure S.37. IR spectrum of **L3.**

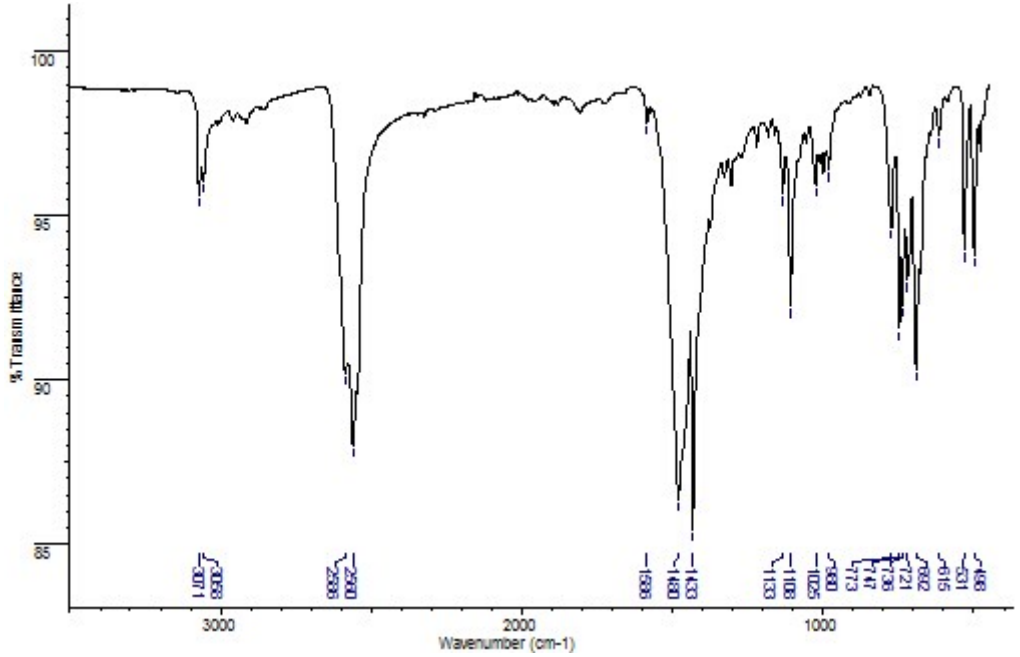

Figure S.38. IR spectrum of **L4.**

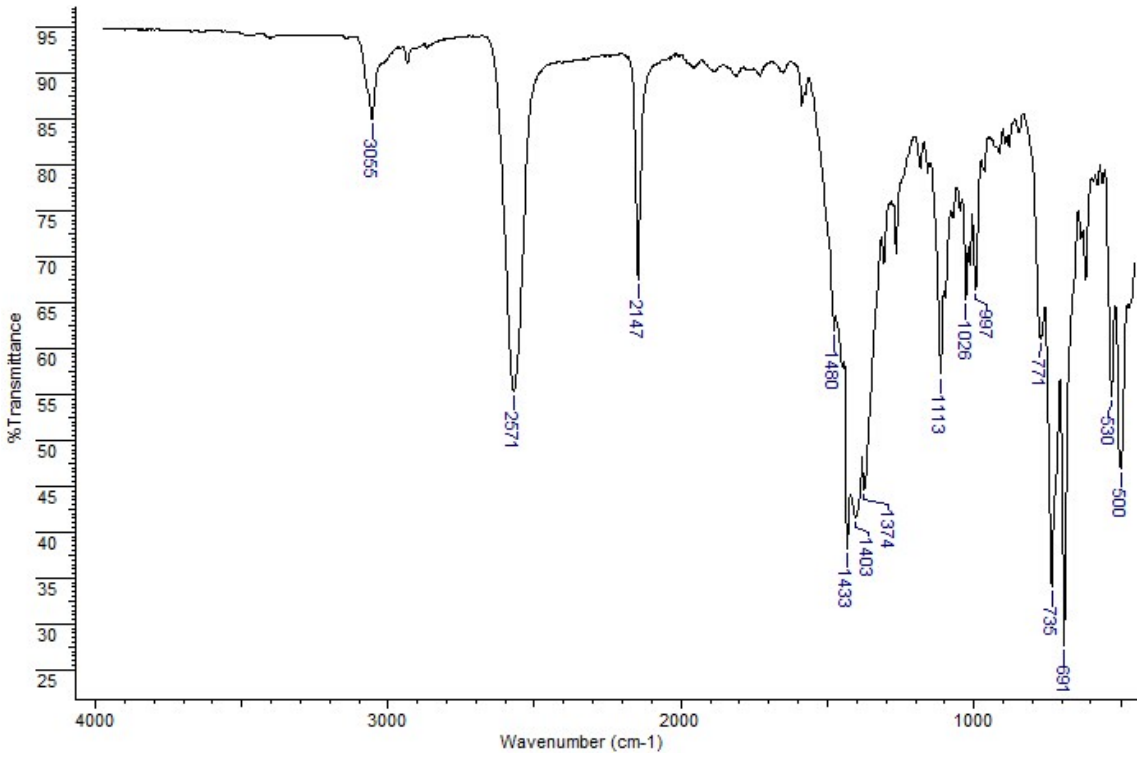

Figure S.39. IR spectrum of **L5.**

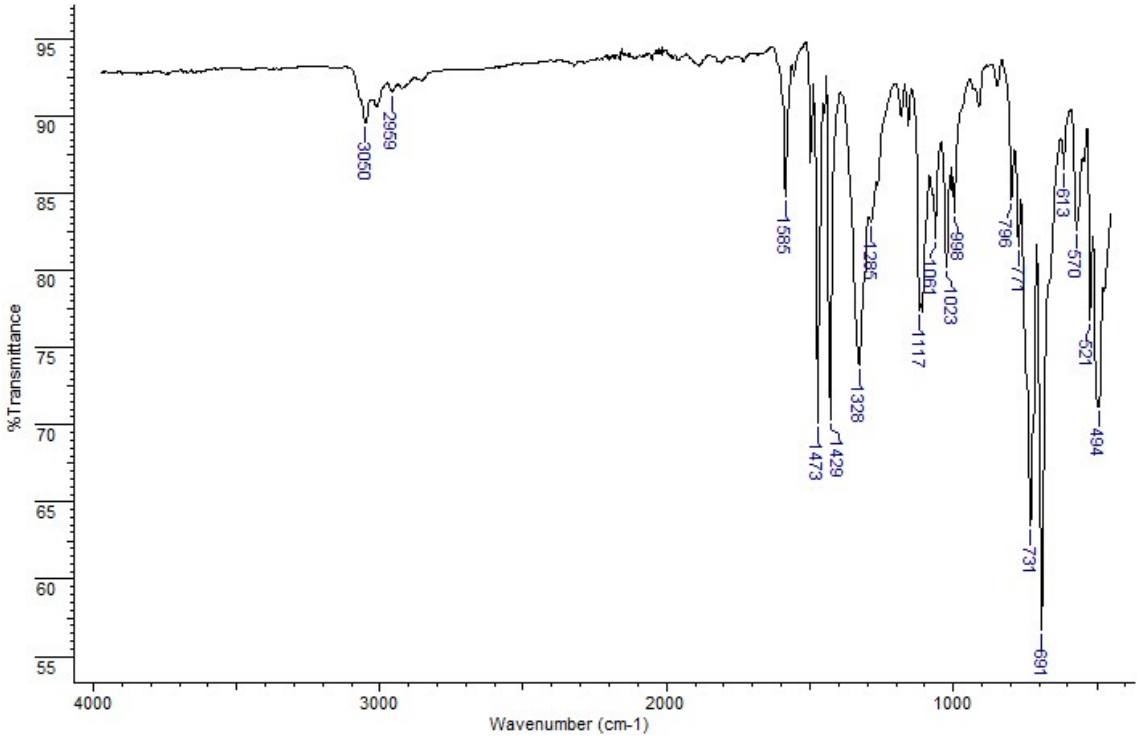

Figure S.40. IR spectrum of **L6.**

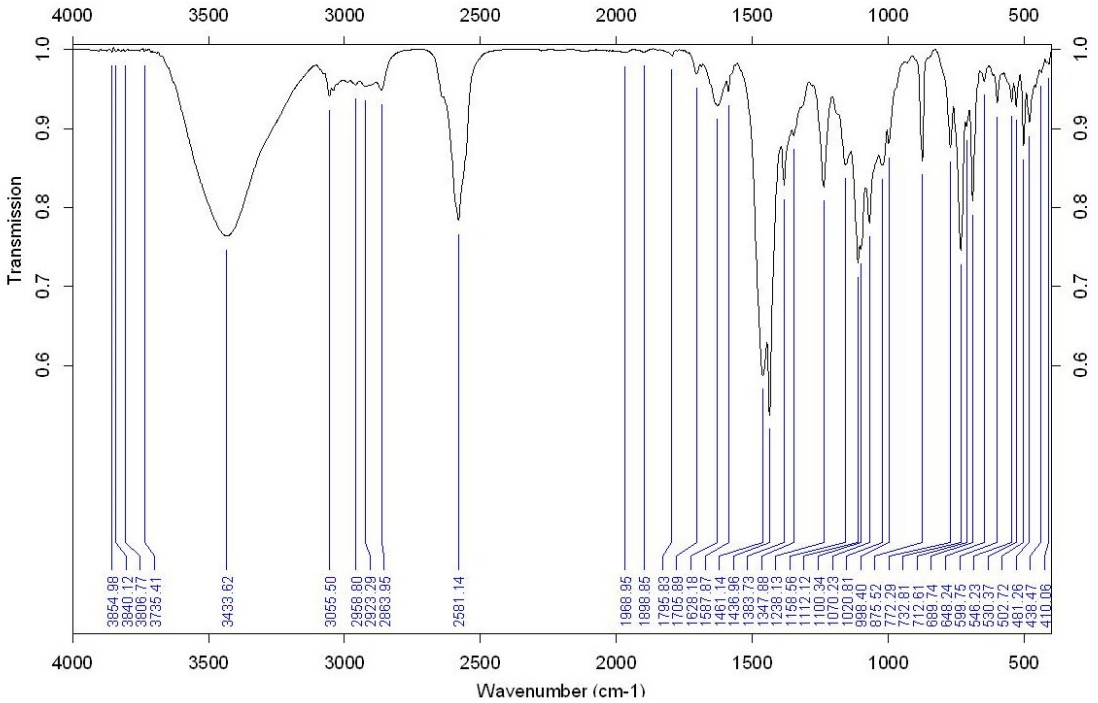

Figure S.41. IR spectrum of **Pd1.**

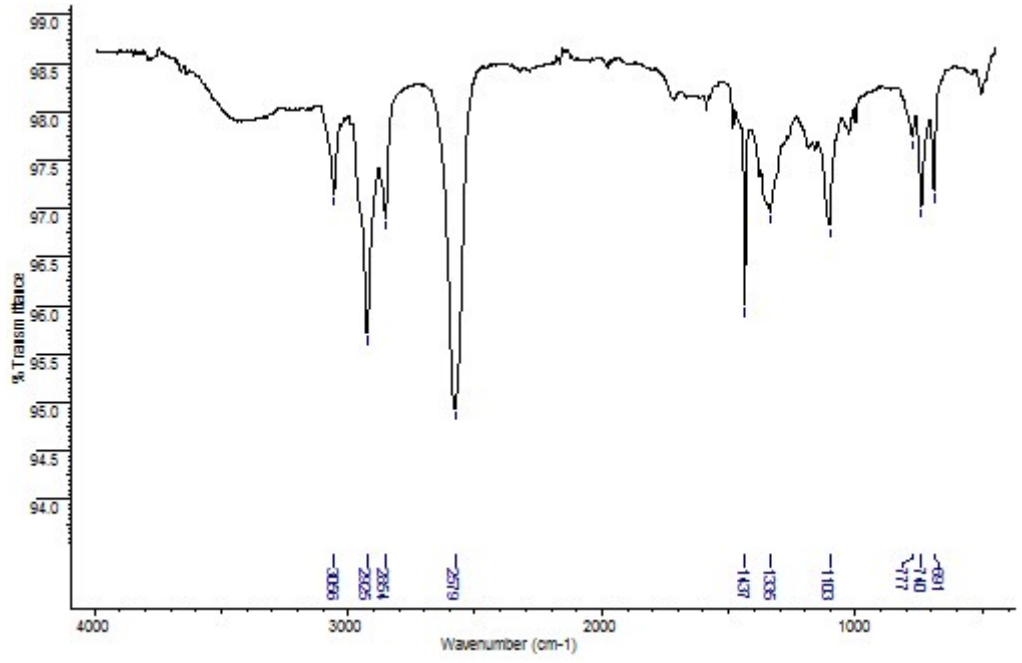

Figure S.42. IR spectrum of **Pd2.**

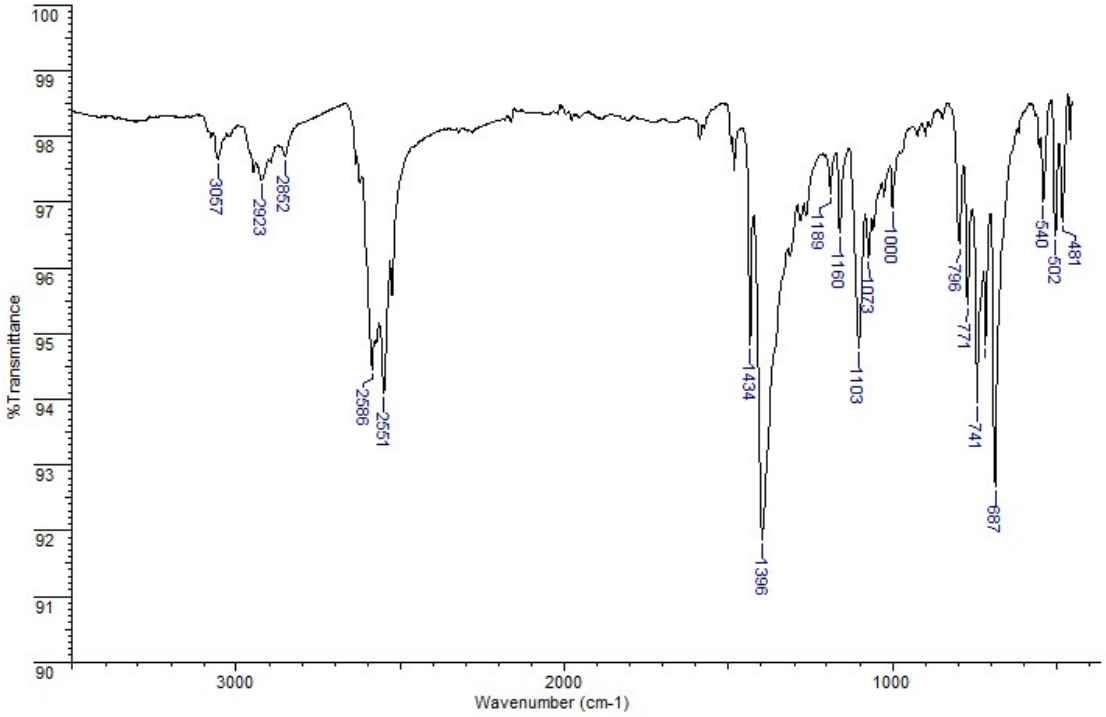

Figure S.43. IR spectrum of **Pd3.**

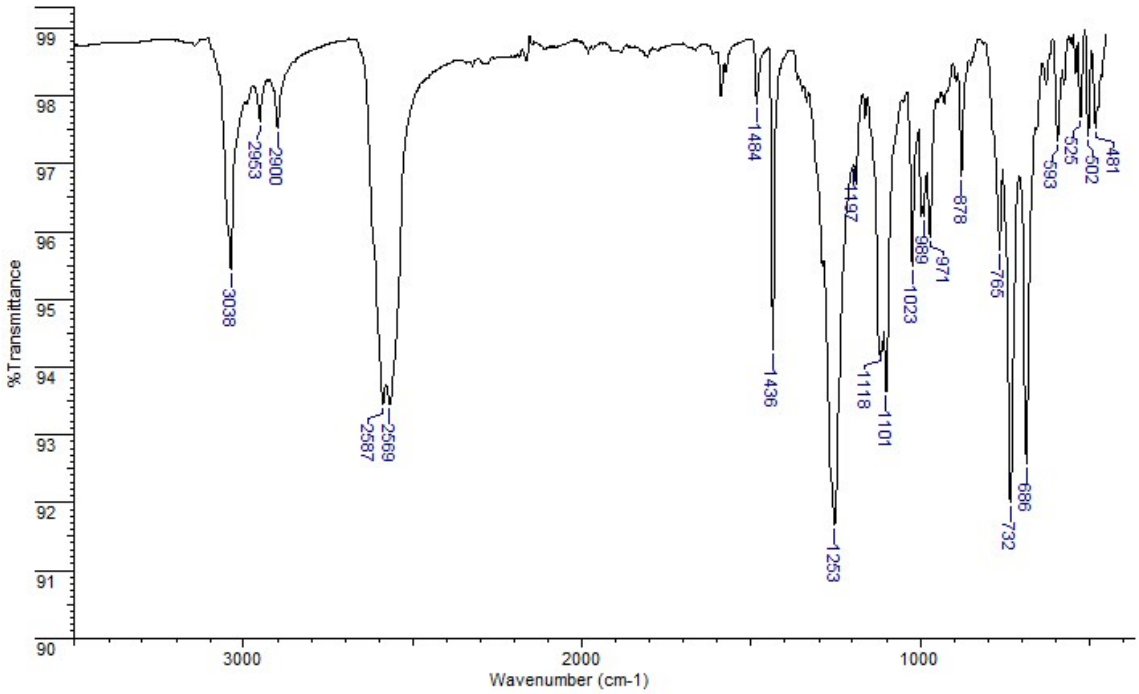

Figure S.44. IR spectrum of **Pd4.**

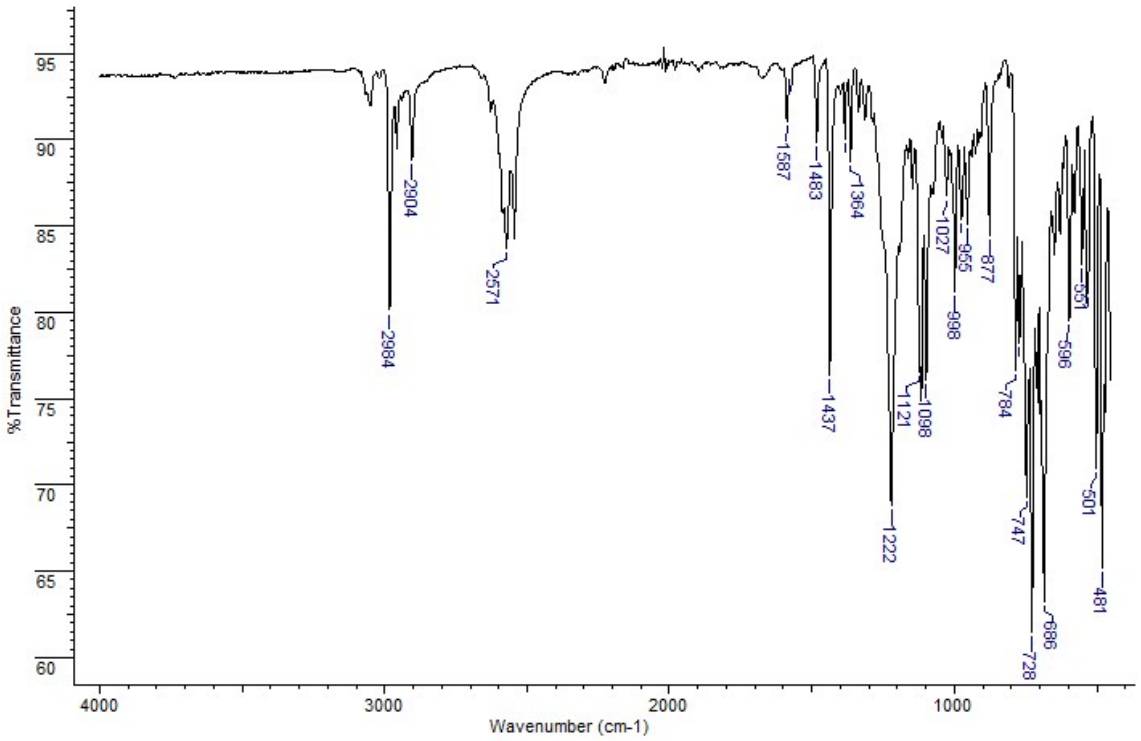

Figure S.45. IR spectrum of **Pd5.**

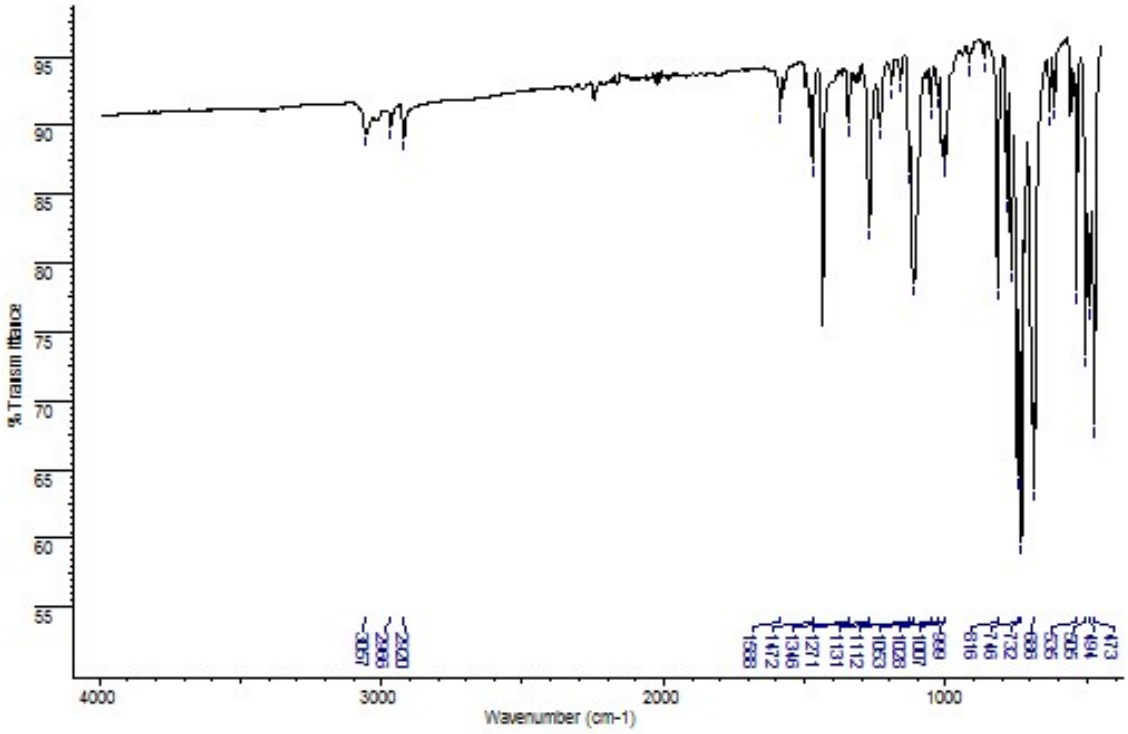

Figure S.46. IR spectrum of **Pd6.**

Table S4. Optimized Cartesian coordinates (Å) obtained for **L1** with DFT calculations TPSSh/6-31+G(d,p) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-2.468168	1.858399	-1.028366
2	5	-3.005646	1.153034	0.503065
3	1	-2.253970	1.129176	1.420733
4	5	-4.009822	-0.276999	0.148389
5	1	-3.919055	-1.246883	0.818640
6	5	-4.083913	-0.457658	-1.608008
7	1	-3.978791	-1.487684	-2.174017
8	5	-3.896964	2.401361	-1.923665
9	1	-3.744235	3.240060	-2.744638
10	5	-3.813836	2.592692	-0.160374
11	1	-3.683222	3.658187	0.345393
12	5	-4.773710	1.271118	0.571300
13	1	-5.330771	1.403438	1.610750
14	5	-5.444596	0.271596	-0.748404
15	1	-6.474801	-0.310293	-0.667900
16	5	-4.890919	0.970393	-2.283848
17	1	-5.402841	0.859433	-3.345323
18	5	-5.331740	2.047137	-0.936057
19	1	-6.295065	2.736116	-0.990956
20	6	-2.637339	0.123324	-0.817347
21	6	-3.197896	0.874017	-2.206483
22	1	-2.588307	0.669884	-3.077866
23	7	-1.512001	-0.668182	-1.002253
24	15	-0.408622	-1.057303	0.080857
25	6	0.692224	-2.221598	-0.776979
26	6	1.658145	-2.945125	-0.058392
27	6	0.575216	-2.395482	-2.163300
28	6	2.499833	-3.837932	-0.724434
29	1	1.747365	-2.823385	1.018160
30	6	1.421459	-3.289852	-2.825136
31	1	-0.185639	-1.835093	-2.696673
32	6	2.381477	-4.010965	-2.107953
33	1	3.243868	-4.397033	-0.165071
34	1	1.326414	-3.426886	-3.898390
35	1	3.034737	-4.708888	-2.623882
36	6	-1.008979	-1.951259	1.566028
37	6	-1.546004	-3.238312	1.380828
38	6	-1.031782	-1.376595	2.846729
39	6	-2.086816	-3.938761	2.459412
40	1	-1.543299	-3.687409	0.391323
41	6	-1.578632	-2.079287	3.925140
42	1	-0.635793	-0.379353	3.011949
43	6	-2.104601	-3.359530	3.733563
44	1	-2.497832	-4.932049	2.305534
45	1	-1.596617	-1.623028	4.910403
46	1	-2.530626	-3.902850	4.571823
47	1	-1.370233	2.238739	-1.236968
48	6	0.662693	0.293502	0.751834
49	1	-0.002380	1.017522	1.233136

50	1	1.323537	-0.122079	1.521217
51	15	1.651909	1.203657	-0.576455
52	6	3.308805	0.399954	-0.377896
53	6	3.933319	-0.096751	-1.532721
54	6	3.970944	0.269634	0.857449
55	6	5.187740	-0.713988	-1.458615
56	1	3.430993	-0.003296	-2.491836
57	6	5.220387	-0.348700	0.934228
58	1	3.518141	0.671594	1.760981
59	6	5.831153	-0.842968	-0.225638
60	1	5.656947	-1.093575	-2.361748
61	1	5.721345	-0.438195	1.894301
62	1	6.804835	-1.320887	-0.165314
63	6	1.918899	2.822046	0.289650
64	6	3.183149	3.439170	0.300622
65	6	0.822371	3.542429	0.801295
66	6	3.349152	4.722022	0.832069
67	1	4.045571	2.916211	-0.101738
68	6	0.991341	4.821584	1.337733
69	1	-0.178283	3.119727	0.773188
70	6	2.256480	5.416813	1.357832
71	1	4.336597	5.175286	0.834978
72	1	0.129520	5.353381	1.730656
73	1	2.386754	6.412379	1.771624

E(RTPSSh) = -2035.12633576 Hartree
Zero-point correction = 0.565369
Thermal correction to Energy = 0.599244
Thermal correction to Enthalpy = 0.600188
Thermal correction to Gibbs Free Energy = 0.496370
Sum of electronic and zero-point Energies = -2034.560967
Sum of electronic and thermal Energies = -2034.527091
Sum of electronic and thermal Enthalpies = -2034.526147
Sum of electronic and thermal Free Energies = -2034.629965

Table S5. Optimized Cartesian coordinates (Å) obtained for **L2** with DFT calculations TPSSh/6-31+G(d,p) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-3.059204	1.218064	-2.126049
2	5	-2.300742	2.169249	-0.838884
3	1	-1.193314	2.557653	-0.993085
4	5	-2.799140	1.433586	0.706402
5	1	-2.033393	1.335408	1.607089
6	5	-3.856035	0.058970	0.341711
7	1	-3.794610	-0.979944	0.901217
8	5	-4.818017	1.391763	-1.989733
9	1	-5.464217	1.227859	-2.969098
10	5	-3.758470	2.774199	-1.648953
11	1	-3.705842	3.703944	-2.383445
12	5	-3.598851	2.907481	0.122761
13	1	-3.423050	3.945546	0.670561

14	5	-4.558662	1.593760	0.865702
15	1	-5.067411	1.684362	1.933763
16	5	-5.317245	0.674900	-0.446469
17	1	-6.301233	0.018749	-0.375203
18	5	-5.160981	2.435803	-0.592822
19	1	-6.118731	3.135013	-0.570105
20	6	-2.484768	0.471576	-0.670015
21	6	-4.028528	0.026243	-1.356913
22	7	-1.474442	-0.450362	-0.867905
23	15	-0.377314	-0.972277	0.164531
24	6	0.590518	-2.193484	-0.771262
25	6	1.467947	-3.071655	-0.114544
26	6	0.472755	-2.235656	-2.168843
27	6	2.214997	-3.992507	-0.852003
28	1	1.563010	-3.046030	0.967756
29	6	1.221573	-3.161764	-2.901081
30	1	-0.208687	-1.545325	-2.655789
31	6	2.089654	-4.040177	-2.244717
32	1	2.891430	-4.670695	-0.340625
33	1	1.124603	-3.197025	-3.982340
34	1	2.667884	-4.760817	-2.816042
35	6	-0.967636	-1.853997	1.662874
36	6	-1.525715	-3.135599	1.503263
37	6	-0.975855	-1.258009	2.934229
38	6	-2.069629	-3.810549	2.596857
39	1	-1.530691	-3.604951	0.523162
40	6	-1.525150	-1.934484	4.027721
41	1	-0.566097	-0.262998	3.078168
42	6	-2.070684	-3.210338	3.861224
43	1	-2.493723	-4.801273	2.462651
44	1	-1.529841	-1.461813	5.005347
45	1	-2.497766	-3.733943	4.711363
46	1	-2.509519	0.901720	-3.122520
47	6	0.794070	0.308684	0.791514
48	1	0.169365	1.102991	1.215774
49	1	1.413055	-0.118504	1.588950
50	15	1.833853	1.081156	-0.579655
51	6	3.433271	0.159437	-0.369563
52	6	3.931828	-0.523478	-1.490646
53	6	4.179060	0.135199	0.822373
54	6	5.141845	-1.223251	-1.422214
55	1	3.365218	-0.509672	-2.417808
56	6	5.385469	-0.564829	0.893614
57	1	3.829330	0.681323	1.695185
58	6	5.869554	-1.246509	-0.230053
59	1	5.512739	-1.746944	-2.298805
60	1	5.953136	-0.570339	1.820126
61	1	6.811126	-1.785553	-0.175193
62	6	2.259037	2.706469	0.200898
63	6	2.702576	3.711267	-0.678488
64	6	2.167384	3.009488	1.570225
65	6	3.063981	4.973882	-0.202224
66	1	2.755852	3.502622	-1.744311
67	6	2.516825	4.277188	2.046874
68	1	1.819442	2.262581	2.278884
69	6	2.969846	5.261009	1.163148

70	1	3.403100	5.735768	-0.898181
71	1	2.433351	4.494468	3.108114
72	1	3.237762	6.245819	1.534349
73	6	-4.091490	-1.335464	-2.018004
74	1	-4.342718	-1.230144	-3.075445
75	1	-3.111192	-1.815078	-1.927144
76	1	-4.845024	-1.956455	-1.528934

E(RTPSSh) = -2074.44943147 Hartree
Zero-point correction = 0.593300
Thermal correction to Energy = 0.628786
Thermal correction to Enthalpy = 0.629730
Thermal correction to Gibbs Free Energy = 0.524088
Sum of electronic and zero-point Energies = -2073.856131
Sum of electronic and thermal Energies = -2073.820645
Sum of electronic and thermal Enthalpies = -2073.819701
Sum of electronic and thermal Free Energies = -2073.925343

Table S6. Optimized Cartesian coordinates (Å) obtained for **L3** with DFT calculations TPSSh/6-31+G(d,p) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-2.553389	1.809603	-1.912904
2	5	-1.290877	2.788322	-1.147237
3	1	-0.217037	2.807326	-1.644011
4	5	-1.507389	2.594285	0.608118
5	1	-0.583899	2.497441	1.347284
6	5	-2.897998	1.519773	0.853675
7	1	-2.904239	0.684734	1.686350
8	5	-4.140739	2.507969	-1.510772
9	1	-5.037283	2.327776	-2.262427
10	5	-2.745699	3.567166	-1.794195
11	1	-2.684327	4.244629	-2.765639
12	5	-2.098208	4.060054	-0.206611
13	1	-1.561340	5.103886	-0.028948
14	5	-3.085750	3.267039	1.054609
15	1	-3.260837	3.732680	2.131782
16	5	-4.355210	2.334036	0.243273
17	1	-5.403176	2.034192	0.705724
18	5	-3.853541	3.897703	-0.432395
19	1	-4.594285	4.823777	-0.423392
20	6	-1.752181	1.293724	-0.460856
21	6	-3.554760	1.147217	-0.681912
22	7	-1.035210	0.133660	-0.593482
23	15	-0.025507	-0.580854	0.415618
24	6	0.421429	-2.142554	-0.398052
25	6	1.156983	-3.121202	0.290772
26	6	0.044169	-2.358420	-1.731377
27	6	1.509538	-4.309809	-0.351480
28	1	1.446203	-2.963852	1.326663
29	6	0.401075	-3.550258	-2.368939
30	1	-0.529872	-1.592058	-2.241947

31	6	1.131412	-4.524766	-1.681541
32	1	2.077060	-5.064502	0.184674
33	1	0.105240	-3.717390	-3.400530
34	1	1.405092	-5.450862	-2.179035
35	6	-0.650768	-1.049562	2.075887
36	6	-1.564934	-2.114700	2.170444
37	6	-0.321552	-0.323076	3.232162
38	6	-2.127051	-2.452724	3.402460
39	1	-1.837230	-2.675820	1.280880
40	6	-0.889427	-0.662065	4.463865
41	1	0.367376	0.514366	3.180338
42	6	-1.790324	-1.727081	4.551010
43	1	-2.827945	-3.280019	3.465411
44	1	-0.630523	-0.091448	5.350764
45	1	-2.230613	-1.989363	5.508524
46	1	-2.331693	1.178533	-2.883916
47	6	1.546529	0.326205	0.747144
48	1	1.269579	1.311324	1.135720
49	1	2.107695	-0.200554	1.527051
50	15	2.609836	0.595873	-0.796028
51	6	3.918385	-0.689428	-0.539036
52	6	4.241195	-1.508368	-1.632976
53	6	4.602642	-0.885390	0.675173
54	6	5.220425	-2.502294	-1.519023
55	1	3.717584	-1.367689	-2.574818
56	6	5.576816	-1.878890	0.792714
57	1	4.389026	-0.246197	1.528739
58	6	5.887193	-2.690453	-0.306075
59	1	5.457289	-3.127636	-2.375061
60	1	6.099090	-2.015407	1.735716
61	1	6.647069	-3.461401	-0.214785
62	6	3.483841	2.146043	-0.272701
63	6	4.883764	2.270024	-0.303332
64	6	2.717345	3.289755	0.024862
65	6	5.498375	3.493609	-0.015032
66	1	5.500352	1.410573	-0.548304
67	6	3.333125	4.507873	0.320693
68	1	1.631556	3.241526	0.013625
69	6	4.727917	4.614528	0.304525
70	1	6.582294	3.565519	-0.038887
71	1	2.719866	5.373768	0.553164
72	1	5.206849	5.562674	0.530566
73	6	-4.136497	-0.224908	-0.873523
74	6	-4.130329	-0.852459	-2.129391
75	6	-4.748297	-0.886455	0.204543
76	6	-4.707158	-2.113187	-2.299268
77	1	-3.679082	-0.352553	-2.977865
78	6	-5.330203	-2.144318	0.032275
79	1	-4.779103	-0.410771	1.178585
80	6	-5.307664	-2.766498	-1.219540
81	1	-4.691127	-2.580030	-3.279908
82	1	-5.805952	-2.633712	0.877497
83	1	-5.760189	-3.744797	-1.353689

E(RTPSSh) = -2266.20615717 Hartree

```
Zero-point correction = 0.645732
Thermal correction to Energy = 0.684615
Thermal correction to Enthalpy = 0.685559
Thermal correction to Gibbs Free Energy = 0.571729
Sum of electronic and zero-point Energies = -2265.560425
Sum of electronic and thermal Energies = -2265.521542
Sum of electronic and thermal Enthalpies = -2265.520598
Sum of electronic and thermal Free Energies = -2265.634429
```

Table S7. Optimized Cartesian coordinates (Å) obtained for **L4** with DFT calculations TPSSh/6-31+G(d,p) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-2.831428	1.944097	-0.890398
2	5	-3.407323	1.140137	0.587352
3	1	-2.847952	1.262551	1.629416
4	5	-4.168712	-0.392875	0.097409
5	1	-4.123083	-1.429859	0.665830
6	1	-3.878063	-1.308692	-2.134101
7	5	-4.238838	2.321644	-1.914802
8	1	-4.158235	3.179905	-2.725639
9	5	-4.358773	2.465376	-0.150335
10	1	-4.452400	3.528256	0.369137
11	5	-5.188637	1.013023	0.464283
12	1	-5.882528	1.028732	1.426437
13	5	-5.580093	-0.019111	-0.925875
14	1	-6.448652	-0.815430	-1.036987
15	5	-4.997547	0.790180	-2.394879
16	1	-5.372212	0.544497	-3.488091
17	5	-5.704922	1.745751	-1.089587
18	1	-6.750932	2.282182	-1.240544
19	6	-3.304568	0.917220	-2.136528
20	1	-2.683343	0.772617	-3.011681
21	7	-1.434289	-0.595119	-0.840526
22	15	-0.300619	-1.045795	0.152361
23	6	0.798347	-2.202768	-0.727812
24	6	1.804557	-2.913106	-0.052944
25	6	0.628073	-2.378848	-2.108102
26	6	2.629888	-3.794127	-0.754505
27	1	1.937415	-2.789854	1.018916
28	6	1.457591	-3.260371	-2.808036
29	1	-0.159682	-1.823527	-2.608390
30	6	2.456498	-3.968361	-2.132462
31	1	3.405239	-4.342902	-0.228180
32	1	1.321400	-3.396592	-3.877142
33	1	3.098213	-4.655938	-2.676124
34	6	-0.841473	-1.954749	1.655875
35	6	-1.238221	-3.298224	1.528272
36	6	-0.978752	-1.319942	2.901174
37	6	-1.748548	-3.993509	2.626006
38	1	-1.145079	-3.800594	0.569232
39	6	-1.491920	-2.017231	3.999157

40	1	-0.696060	-0.279014	3.024083
41	6	-1.875181	-3.354302	3.864426
42	1	-2.048355	-5.031461	2.514715
43	1	-1.594732	-1.513150	4.955590
44	1	-2.274241	-3.894668	4.717790
45	1	-1.835817	2.569746	-1.027438
46	6	0.774233	0.310864	0.801940
47	1	0.103892	1.019285	1.301469
48	1	1.471281	-0.081663	1.551058
49	15	1.678532	1.257010	-0.560559
50	6	3.352783	0.469725	-0.485675
51	6	3.928903	0.064574	-1.700363
52	6	4.074341	0.262942	0.704821
53	6	5.192536	-0.536961	-1.728892
54	1	3.379661	0.216895	-2.625707
55	6	5.334128	-0.338950	0.679487
56	1	3.659429	0.590725	1.655133
57	6	5.895327	-0.741381	-0.539198
58	1	5.622356	-0.846547	-2.677260
59	1	5.880927	-0.488332	1.606547
60	1	6.876261	-1.207850	-0.557991
61	6	1.968537	2.859766	0.326703
62	6	3.238824	3.458514	0.396046
63	6	0.862371	3.585176	0.811279
64	6	3.400937	4.729514	0.958021
65	1	4.108540	2.932414	0.014577
66	6	1.027241	4.850450	1.379620
67	1	-0.140975	3.173949	0.733633
68	6	2.298945	5.428060	1.457806
69	1	4.393172	5.169885	1.005219
70	1	0.158705	5.386766	1.751182
71	1	2.426638	6.413678	1.895650
72	5	-2.621785	0.153759	-0.677804
73	6	-4.060257	-0.393694	-1.584533

E(RTPSSh) = -2035.16828676 Hartree
Zero-point correction = 0.567131
Thermal correction to Energy = 0.601133
Thermal correction to Enthalpy = 0.602077
Thermal correction to Gibbs Free Energy = 0.498661
Sum of electronic and zero-point Energies = -2034.601156
Sum of electronic and thermal Energies = -2034.567154
Sum of electronic and thermal Enthalpies = -2034.566210
Sum of electronic and thermal Free Energies = -2034.669626

Table S8. Optimized Cartesian coordinates (Å) obtained for **L5** with DFT calculations TPSSh/6-31+G(d,p) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-2.573693	1.992022	-1.056313
2	5	-3.001487	1.480606	0.591900
3	1	-2.293659	1.692300	1.524950

4	5	-3.947959	-0.021198	0.447829
5	1	-3.913845	-0.956256	1.174247
6	5	-4.072362	2.354399	-1.940161
7	1	-4.034520	3.064584	-2.886333
8	5	-3.928883	2.776699	-0.222539
9	1	-3.854549	3.908743	0.126011
10	5	-4.782195	1.525102	0.717906
11	1	-5.327263	1.752744	1.747163
12	5	-5.453334	0.348138	-0.423750
13	1	-6.395569	-0.356419	-0.286204
14	5	-5.018740	0.860383	-2.060994
15	1	-5.566512	0.501635	-3.045013
16	5	-5.450529	2.072134	-0.853281
17	1	-6.459379	2.685892	-0.956975
18	6	-3.305579	0.835831	-2.043925
19	1	-2.829786	0.503696	-2.959227
20	7	-1.378869	-0.611631	-0.768166
21	15	-0.216455	-1.045549	0.203317
22	6	0.857631	-2.218892	-0.685202
23	6	1.864349	-2.937316	-0.019567
24	6	0.678071	-2.388307	-2.065396
25	6	2.679505	-3.821136	-0.729544
26	1	2.006212	-2.816953	1.051437
27	6	1.496876	-3.273411	-2.773433
28	1	-0.106240	-1.823433	-2.560387
29	6	2.495481	-3.990165	-2.106727
30	1	3.455580	-4.375653	-0.210366
31	1	1.353541	-3.404176	-3.842262
32	1	3.129534	-4.679598	-2.656981
33	6	-0.726575	-1.927158	1.733971
34	6	-1.107161	-3.278425	1.647502
35	6	-0.862942	-1.258837	2.961810
36	6	-1.600201	-3.948833	2.768539
37	1	-1.014359	-3.807091	0.702625
38	6	-1.359157	-1.930983	4.082950
39	1	-0.593867	-0.210886	3.051383
40	6	-1.725887	-3.276363	3.989237
41	1	-1.886441	-4.993614	2.689364
42	1	-1.461775	-1.401192	5.025381
43	1	-2.111166	-3.797392	4.860766
44	1	-1.555600	2.474112	-1.419465
45	6	0.876552	0.316916	0.806785
46	1	0.219390	1.043493	1.297383
47	1	1.577027	-0.066725	1.557237
48	15	1.777372	1.222735	-0.585844
49	6	3.455113	0.445374	-0.487135
50	6	4.038489	0.021480	-1.692007
51	6	4.172774	0.262937	0.709747
52	6	5.304863	-0.574746	-1.704677
53	1	3.492587	0.154919	-2.622244
54	6	5.435124	-0.334153	0.700376
55	1	3.752668	0.605580	1.652503
56	6	6.003360	-0.755490	-0.508594
57	1	5.740294	-0.898640	-2.645695
58	1	5.978539	-0.464623	1.632276
59	1	6.986327	-1.217996	-0.514960

60	6	2.055447	2.854155	0.251204
61	6	3.324275	3.454244	0.330250
62	6	0.938495	3.593419	0.688058
63	6	3.474199	4.742291	0.856049
64	1	4.202002	2.916693	-0.015271
65	6	1.091424	4.875583	1.220569
66	1	-0.062838	3.179051	0.601920
67	6	2.361473	5.455615	1.308847
68	1	4.465283	5.184298	0.911921
69	1	0.214876	5.422684	1.555763
70	1	2.479785	6.454452	1.718522
71	5	-2.486202	0.250620	-0.585739
72	6	-4.091223	-0.317838	-1.214151
73	6	-4.080293	-1.729103	-1.775879
74	1	-4.360584	-1.731793	-2.832286
75	1	-3.079049	-2.154796	-1.660581
76	1	-4.798306	-2.338649	-1.223767

E(RTPSSh) = -2074.49159837 Hartree
Zero-point correction = 0.594427
Thermal correction to Energy = 0.630283
Thermal correction to Enthalpy = 0.631227
Thermal correction to Gibbs Free Energy = 0.523772
Sum of electronic and zero-point Energies = -2073.897171
Sum of electronic and thermal Energies = -2073.861315
Sum of electronic and thermal Enthalpies = -2073.860371
Sum of electronic and thermal Free Energies = -2073.967827

Table S9. Optimized Cartesian coordinates (Å) obtained for [Pd**L1**Cl_2] with DFT calculations TPSSh/6-31G(d) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	2.179689	-2.272668	-0.128096
2	5	2.904602	-1.278672	1.137646
3	1	2.254381	-1.012704	2.097395
4	5	3.887880	-0.007960	0.359734
5	1	3.927673	1.083482	0.804567
6	5	3.774514	-0.210032	-1.393739
7	1	3.617280	0.680538	-2.151212
8	5	3.481214	-3.050536	-1.033924
9	1	3.214540	-4.039442	-1.626551
10	5	3.606677	-2.859346	0.727486
11	1	3.512687	-3.782873	1.467712
12	5	4.663026	-1.453952	1.038433
13	1	5.331032	-1.367885	2.016914
14	5	5.201060	-0.796809	-0.536143
15	1	6.244538	-0.250831	-0.682427
16	5	4.465681	-1.787609	-1.807356
17	1	4.853479	-1.942132	-2.914627
18	5	5.029915	-2.561123	-0.309973
19	1	5.967710	-3.287914	-0.309692
20	6	2.416762	-0.560410	-0.345285

21	6	2.791797	-1.592701	-1.576185
22	1	2.094345	-1.546639	-2.412629
23	7	1.235609	0.222561	-0.545190
24	15	0.626138	1.304623	0.521980
25	6	-0.339254	2.506447	-0.426187
26	6	-1.158267	3.422669	0.257291
27	6	-0.217620	2.568633	-1.823876
28	6	-1.869774	4.384358	-0.459256
29	1	-1.242418	3.390850	1.340759
30	6	-0.935129	3.538017	-2.530748
31	1	0.408332	1.853350	-2.350514
32	6	-1.760019	4.439558	-1.853416
33	1	-2.509227	5.085998	0.068118
34	1	-0.850222	3.575991	-3.612412
35	1	-2.317872	5.187751	-2.409718
36	6	1.761153	2.301431	1.532147
37	6	2.360790	3.428088	0.939501
38	6	2.054584	1.979369	2.867300
39	6	3.256892	4.206654	1.670298
40	1	2.130857	3.688424	-0.089314
41	6	2.947739	2.767342	3.595046
42	1	1.605369	1.112507	3.340474
43	6	3.552472	3.876016	2.996776
44	1	3.723124	5.070015	1.205263
45	1	3.174338	2.511085	4.625581
46	1	4.251413	4.483699	3.564115
47	1	1.053939	-2.634566	-0.129467
48	6	-0.512718	0.426891	1.678637
49	1	0.100028	-0.202926	2.330446
50	1	-1.112646	1.103052	2.295109
51	15	-1.588202	-0.643593	0.577137
52	6	-3.197740	0.229278	0.614780
53	6	-3.714592	0.819981	-0.547129
54	6	-3.895027	0.353000	1.831209
55	6	-4.916387	1.531798	-0.489605
56	1	-3.186581	0.702426	-1.487536
57	6	-5.094160	1.064667	1.880490
58	1	-3.512074	-0.120123	2.732484
59	6	-5.605010	1.655335	0.719110
60	1	-5.314847	1.981212	-1.394447
61	1	-5.632030	1.151346	2.820523
62	1	-6.541840	2.204467	0.758333
63	6	-1.865482	-2.198904	1.495080
64	6	-3.082391	-2.878644	1.306562
65	6	-0.864511	-2.783335	2.289235
66	6	-3.298872	-4.108991	1.929060
67	1	-3.848632	-2.450853	0.668479
68	6	-1.090364	-4.012438	2.911706
69	1	0.101431	-2.303004	2.414543
70	6	-2.308141	-4.674939	2.736092
71	1	-4.241629	-4.626467	1.777234
72	1	-0.309791	-4.453224	3.524870
73	1	-2.479860	-5.633080	3.218258
74	46	-0.514170	-0.692118	-1.416992
75	17	-2.365886	-1.823499	-2.204970
76	17	0.395005	-0.505264	-3.586298

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---------------------------------------------------------------------
E(RTPSSh) =  -3083.00627493 Hartree
Zero-point correction = 0.572709
Thermal correction to Energy = 0.611272
Thermal correction to Enthalpy = 0.612217
Thermal correction to Gibbs Free Energy = 0.501199
Sum of electronic and zero-point Energies = -3082.433566
Sum of electronic and thermal Energies = -3082.395003
Sum of electronic and thermal Enthalpies = -3082.394058
Sum of electronic and thermal Free Energies = -3082.505076
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Table S10. Optimized Cartesian coordinates (Å) obtained for [Pd**L2**Cl_2] with DFT calculations TPSSh/6-31G(d) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	2.508208	-1.962227	-1.341075
2	5	2.077903	-2.257230	0.355112
3	1	0.969754	-2.590345	0.606190
4	5	2.879765	-1.006329	1.320330
5	1	2.318133	-0.513832	2.239743
6	5	3.797492	0.032629	0.207319
7	1	3.852339	1.208978	0.284910
8	5	4.262050	-2.189513	-1.507640
9	1	4.673476	-2.484901	-2.578108
10	5	3.329252	-3.236127	-0.418589
11	1	3.134038	-4.376502	-0.680646
12	5	3.569417	-2.635315	1.243149
13	1	3.532785	-3.344152	2.195309
14	5	4.631227	-1.198045	1.166573
15	1	5.359835	-0.874781	2.046540
16	5	5.068065	-0.950949	-0.535398
17	1	6.027910	-0.384485	-0.938446
18	5	4.921392	-2.601034	0.092594
19	1	5.877833	-3.295122	0.201600
20	6	2.264337	-0.657891	-0.235925
21	6	3.604185	-0.633538	-1.349085
22	7	1.174129	0.212614	-0.513157
23	15	0.548432	1.261951	0.594469
24	6	-0.417636	2.511528	-0.290040
25	6	-1.234226	3.376238	0.461197
26	6	-0.299185	2.679510	-1.678435
27	6	-1.945127	4.390558	-0.178865
28	1	-1.316014	3.264801	1.539558
29	6	-1.014744	3.701942	-2.308609
30	1	0.311083	1.998959	-2.265970
31	6	-1.836390	4.552341	-1.564710
32	1	-2.582722	5.050421	0.401986
33	1	-0.932800	3.818353	-3.384870
34	1	-2.393180	5.341722	-2.061977
35	6	1.651449	2.256138	1.653995
36	6	2.311635	3.354846	1.072617
37	6	1.798657	2.010063	3.028328
38	6	3.125913	4.174667	1.852207

39	1	2.186103	3.567188	0.014825
40	6	2.607420	2.841011	3.806406
41	1	1.292350	1.172540	3.497117
42	6	3.275364	3.918110	3.219197
43	1	3.639110	5.015011	1.394496
44	1	2.717182	2.642192	4.868235
45	1	3.907706	4.559867	3.825807
46	1	1.755258	-2.058025	-2.240867
47	6	-0.579526	0.305388	1.690904
48	1	0.050470	-0.365851	2.284782
49	1	-1.178330	0.935256	2.355239
50	15	-1.638421	-0.720201	0.524544
51	6	-3.282345	0.087713	0.617598
52	6	-3.705400	0.917290	-0.432157
53	6	-4.111216	-0.094796	1.738145
54	6	-4.937712	1.570273	-0.350223
55	1	-3.081926	1.029191	-1.313214
56	6	-5.341867	0.559972	1.812359
57	1	-3.810492	-0.763872	2.539873
58	6	-5.755129	1.394574	0.768991
59	1	-5.261679	2.204555	-1.170195
60	1	-5.981386	0.407578	2.677412
61	1	-6.717515	1.896097	0.824478
62	6	-1.815243	-2.335332	1.364389
63	6	-2.067812	-3.466658	0.568973
64	6	-1.710836	-2.476519	2.759263
65	6	-2.219360	-4.718094	1.169532
66	1	-2.141355	-3.357641	-0.509640
67	6	-1.861235	-3.732723	3.351036
68	1	-1.509967	-1.615043	3.391471
69	6	-2.115485	-4.854094	2.556626
70	1	-2.409146	-5.588429	0.548290
71	1	-1.774123	-3.833995	4.429187
72	1	-2.225460	-5.831530	3.017788
73	46	-0.584884	-0.585436	-1.485824
74	17	-2.452667	-1.553312	-2.437100
75	17	0.303770	-0.160949	-3.624938
76	6	3.532839	0.348366	-2.502172
77	1	3.488394	-0.186593	-3.451791
78	1	2.624222	0.949344	-2.418779
79	1	4.413110	0.996420	-2.482006

E(RTPSSh) = -3122.32114533 Hartree
Zero-point correction = 0.600451
Thermal correction to Energy = 0.640827
Thermal correction to Enthalpy = 0.641771
Thermal correction to Gibbs Free Energy = 0.527722
Sum of electronic and zero-point Energies = -3121.720694
Sum of electronic and thermal Energies = -3121.680319
Sum of electronic and thermal Enthalpies = -3121.679374
Sum of electronic and thermal Free Energies = -3121.793423

Table S11. Optimized Cartesian coordinates (Å) obtained for [Pd**L3**Cl_2] with DFT calculations TPSSh/6-31G(d) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	-2.114023	2.203591	-1.384496
2	5	-0.977822	2.941964	-0.227836
3	1	0.170350	2.970025	-0.518950
4	5	-1.519733	2.450763	1.387368
5	1	-0.753305	2.150194	2.245112
6	5	-2.962448	1.436412	1.157423
7	1	-3.190353	0.480546	1.802210
8	5	-3.720707	2.931693	-1.137347
9	1	-4.464085	2.960333	-2.057944
10	5	-2.258577	3.920293	-0.958145
11	1	-1.990447	4.758480	-1.753130
12	5	-1.905847	4.074777	0.783716
13	1	-1.374273	5.027900	1.252834
14	5	-3.128255	3.122809	1.670937
15	1	-3.488874	3.379191	2.773116
16	5	-4.255816	2.446379	0.478728
17	1	-5.376687	2.135364	0.701804
18	5	-3.588169	4.070521	0.225636
19	1	-4.290060	5.025285	0.290013
20	6	-1.613051	1.389520	0.060350
21	6	-3.351867	1.399622	-0.507100
22	7	-0.851875	0.216729	-0.129549
23	15	-0.320782	-0.771238	1.079384
24	6	0.023272	-2.384931	0.340227
25	6	0.718373	-3.349611	1.091566
26	6	-0.473195	-2.699760	-0.934781
27	6	0.931375	-4.620127	0.558109
28	1	1.091339	-3.116709	2.085796
29	6	-0.253789	-3.977400	-1.457424
30	1	-0.995672	-1.949297	-1.520882
31	6	0.446486	-4.932852	-0.717194
32	1	1.476478	-5.361997	1.134210
33	1	-0.624588	-4.212859	-2.450097
34	1	0.617367	-5.922547	-1.131786
35	6	-1.396705	-1.143360	2.500955
36	6	-2.398154	-2.118592	2.336482
37	6	-1.245460	-0.505570	3.742911
38	6	-3.245715	-2.432548	3.397967
39	1	-2.518270	-2.619784	1.380989
40	6	-2.093995	-0.829882	4.803044
41	1	-0.480839	0.250113	3.888741
42	6	-3.095721	-1.788570	4.630687
43	1	-4.020140	-3.182041	3.263934
44	1	-1.973529	-0.330848	5.759866
45	1	-3.756410	-2.036556	5.456395
46	1	-1.740007	1.761080	-2.405935
47	6	1.243528	-0.072181	1.757204
48	1	0.989087	0.831382	2.318600
49	1	1.766108	-0.768529	2.419765
50	15	2.282125	0.362634	0.258332
51	6	3.582328	-0.928967	0.318618
52	6	3.672219	-1.918352	-0.671027
53	6	4.466171	-0.956258	1.413741

54	6	4.636050	-2.925516	-0.560705
55	1	3.005796	-1.885130	-1.526470
56	6	5.426188	-1.963366	1.516113
57	1	4.417068	-0.181725	2.175639
58	6	5.511178	-2.949925	0.527517
59	1	4.704623	-3.684915	-1.334204
60	1	6.110430	-1.973374	2.360061
61	1	6.262659	-3.731083	0.604266
62	6	3.153295	1.914953	0.671971
63	6	4.422476	2.135837	0.106631
64	6	2.553462	2.927810	1.438255
65	6	5.086715	3.342292	0.332212
66	1	4.879263	1.371547	-0.513414
67	6	3.226598	4.130178	1.663154
68	1	1.555397	2.801969	1.846632
69	6	4.494485	4.338113	1.113905
70	1	6.065770	3.504178	-0.109370
71	1	2.752828	4.905297	2.258390
72	1	5.014060	5.276459	1.286014
73	46	0.859683	0.277526	-1.497503
74	17	2.757706	0.578420	-2.778172
75	17	-0.387521	-0.235015	-3.429385
76	6	-3.944248	0.125723	-1.035891
77	6	-3.691800	-0.306509	-2.346635
78	6	-4.812476	-0.628348	-0.225580
79	6	-4.285536	-1.475616	-2.828950
80	1	-3.015942	0.248394	-2.984804
81	6	-5.408883	-1.790737	-0.714788
82	1	-5.034756	-0.295031	0.782763
83	6	-5.144314	-2.220989	-2.018752
84	1	-4.069145	-1.797384	-3.843371
85	1	-6.086437	-2.354243	-0.078705
86	1	-5.609150	-3.126294	-2.400050

E(RTPSSh) = -3314.06471076 Hartree
Zero-point correction = 0.652717
Thermal correction to Energy = 0.696478
Thermal correction to Enthalpy = 0.697422
Thermal correction to Gibbs Free Energy = 0.574450
Sum of electronic and zero-point Energies = -3313.411994
Sum of electronic and thermal Energies = -3313.368233
Sum of electronic and thermal Enthalpies = -3313.367289
Sum of electronic and thermal Free Energies = -3313.490261

Table S12. Optimized Cartesian coordinates (Å) obtained for [Pd**L4**Cl_2] with DFT calculations TPSSh/6-31G(d) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	2.600301	-2.153387	0.553282
2	5	3.478151	-0.759803	1.208349
3	1	3.177979	-0.270894	2.248382
4	5	4.053048	0.213875	-0.171056
5	1	4.107140	1.394385	-0.241911

6	1	3.187972	-0.161243	-2.430334
7	5	3.731657	-3.138815	-0.396333
8	1	3.490338	-4.281204	-0.590308
9	5	4.274700	-2.358234	1.101759
10	1	4.522305	-2.993788	2.073895
11	5	5.174061	-0.884656	0.658294
12	1	6.072931	-0.460248	1.307931
13	5	5.196454	-0.772154	-1.114646
14	1	5.991260	-0.236522	-1.809968
15	5	4.306544	-2.162067	-1.766642
16	1	4.401353	-2.562742	-2.872895
17	5	5.332807	-2.365192	-0.340208
18	1	6.331876	-3.001038	-0.406733
19	6	2.726422	-1.974716	-1.119650
20	1	1.923763	-2.232402	-1.805141
21	7	1.160554	0.194334	-0.401485
22	15	0.514539	1.338079	0.539854
23	6	-0.419021	2.524114	-0.465859
24	6	-1.223521	3.493637	0.158363
25	6	-0.294638	2.503281	-1.864359
26	6	-1.913878	4.426199	-0.615159
27	1	-1.309857	3.526582	1.241899
28	6	-0.989561	3.444094	-2.630468
29	1	0.320762	1.747297	-2.345911
30	6	-1.798196	4.399498	-2.009907
31	1	-2.540946	5.170029	-0.132349
32	1	-0.899546	3.419620	-3.712264
33	1	-2.338804	5.125760	-2.610591
34	6	1.637300	2.358374	1.544671
35	6	2.305653	3.424936	0.915790
36	6	1.843447	2.126192	2.914363
37	6	3.177490	4.232991	1.644931
38	1	2.141791	3.621447	-0.139718
39	6	2.710546	2.943834	3.641455
40	1	1.339042	1.308649	3.419290
41	6	3.379969	3.993628	3.007624
42	1	3.695273	5.049358	1.150373
43	1	2.865483	2.756389	4.699746
44	1	4.056987	4.625838	3.574844
45	1	1.615433	-2.647724	0.988134
46	6	-0.675297	0.510173	1.681636
47	1	-0.085919	-0.074911	2.394718
48	1	-1.324042	1.198466	2.231348
49	15	-1.664830	-0.633416	0.572944
50	6	-3.291138	0.203029	0.474967
51	6	-3.747350	0.737729	-0.738207
52	6	-4.068020	0.347903	1.639306
53	6	-4.968632	1.417176	-0.782038
54	1	-3.159049	0.600522	-1.639455
55	6	-5.285995	1.026368	1.587427
56	1	-3.730492	-0.083285	2.578873
57	6	-5.736297	1.562285	0.375539
58	1	-5.320481	1.823508	-1.725777
59	1	-5.885363	1.129770	2.487759
60	1	-6.687803	2.085544	0.335485
61	6	-1.982865	-2.151313	1.541776

62	6	-3.128347	-2.902879	1.220584
63	6	-1.091103	-2.636396	2.512107
64	6	-3.383657	-4.105047	1.881393
65	1	-3.806059	-2.552131	0.449128
66	6	-1.355634	-3.838389	3.172135
67	1	-0.178765	-2.099247	2.752430
68	6	-2.502831	-4.572491	2.860872
69	1	-4.269870	-4.678178	1.624932
70	1	-0.659601	-4.201365	3.922826
71	1	-2.704427	-5.509001	3.373055
72	46	-0.478509	-0.773327	-1.345969
73	17	-2.248546	-1.966672	-2.236379
74	17	0.666328	-0.706222	-3.417731
75	5	2.416201	-0.528403	-0.201554
76	6	3.555036	-0.646062	-1.531795

E(RTPSSh) = -3083.05864922 Hartree
Zero-point correction = 0.574196
Thermal correction to Energy = 0.613015
Thermal correction to Enthalpy = 0.613960
Thermal correction to Gibbs Free Energy = 0.501211
Sum of electronic and zero-point Energies = -3082.484453
Sum of electronic and thermal Energies = -3082.445634
Sum of electronic and thermal Enthalpies = -3082.444690
Sum of electronic and thermal Free Energies = -3082.557438

Table S13. Optimized Cartesian coordinates (Å) obtained for [Pd**L5**Cl_2] with DFT calculations TPSSh/6-31G(d) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	5	2.265768	-2.305033	0.007980
2	5	2.918525	-1.300962	1.314874
3	1	2.327297	-1.141344	2.338194
4	5	3.854502	0.010656	0.562078
5	1	3.949436	1.134077	0.921389
6	5	3.617689	-3.023366	-0.879479
7	1	3.443702	-4.006717	-1.514327
8	5	3.711276	-2.844127	0.884458
9	1	3.668803	-3.788481	1.603138
10	5	4.695819	-1.402435	1.234387
11	1	5.373354	-1.298886	2.204530
12	5	5.219037	-0.710237	-0.317109
13	1	6.181874	-0.055059	-0.536084
14	5	4.560042	-1.715428	-1.614246
15	1	4.978683	-1.736919	-2.719026
16	5	5.135373	-2.475204	-0.129339
17	1	6.116283	-3.142099	-0.141304
18	6	2.868469	-1.589065	-1.404377
19	1	2.268777	-1.541231	-2.312904
20	7	1.111342	0.297611	-0.428126
21	15	0.421615	1.334738	0.608025
22	6	-0.571035	2.546154	-0.303064
23	6	-1.406537	3.434108	0.397035

24	6	-0.472343	2.623133	-1.701651
25	6	-2.152886	4.382528	-0.301857
26	1	-1.475276	3.389860	1.481301
27	6	-1.223049	3.579104	-2.392382
28	1	0.164513	1.927386	-2.242006
29	6	-2.062562	4.452780	-1.696788
30	1	-2.804756	5.062232	0.239084
31	1	-1.153275	3.629233	-3.474803
32	1	-2.647559	5.190357	-2.239329
33	6	1.519284	2.321163	1.672853
34	6	2.058821	3.513330	1.155727
35	6	1.869515	1.909781	2.969364
36	6	2.944408	4.271703	1.921269
37	1	1.783722	3.846684	0.159252
38	6	2.752576	2.675496	3.732649
39	1	1.471725	0.989792	3.384514
40	6	3.292787	3.853111	3.209195
41	1	3.358945	5.189271	1.514130
42	1	3.021242	2.348432	4.732603
43	1	3.982265	4.444929	3.804346
44	1	1.194552	-2.808282	-0.039944
45	6	-0.710592	0.381719	1.709449
46	1	-0.084168	-0.241615	2.355799
47	1	-1.360941	1.004754	2.330564
48	15	-1.692323	-0.706628	0.540203
49	6	-3.333386	0.106888	0.514139
50	6	-3.835019	0.660257	-0.672395
51	6	-4.074959	0.219333	1.705168
52	6	-5.065086	1.324766	-0.664317
53	1	-3.272790	0.549231	-1.593502
54	6	-5.302206	0.883046	1.705289
55	1	-3.703147	-0.225649	2.625312
56	6	-5.797322	1.437491	0.519455
57	1	-5.450800	1.745947	-1.588131
58	1	-5.873684	0.961195	2.626097
59	1	-6.755531	1.949996	0.520366
60	6	-1.951607	-2.285670	1.422752
61	6	-3.150175	-2.989723	1.211368
62	6	-0.945028	-2.858407	2.218630
63	6	-3.345595	-4.233092	1.815028
64	1	-3.919369	-2.570330	0.571241
65	6	-1.149910	-4.100431	2.822147
66	1	0.009493	-2.358884	2.357177
67	6	-2.351011	-4.787263	2.625281
68	1	-4.274694	-4.769698	1.645971
69	1	-0.365542	-4.532548	3.436678
70	1	-2.506273	-5.755377	3.093046
71	46	-0.530812	-0.683159	-1.396632
72	17	-2.274262	-1.904977	-2.301815
73	17	0.517374	-0.424712	-3.505862
74	5	2.298590	-0.519831	-0.159923
75	6	3.778798	-0.264215	-1.112617
76	6	3.718838	0.879034	-2.117219
77	1	4.521770	0.780528	-2.851490
78	1	2.755313	0.874294	-2.634612
79	1	3.839481	1.827513	-1.587424

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---------------------------------------------------------------------
E(RTPSSh) = -3122.37698369 Hartree
Zero-point correction = 0.602413
Thermal correction to Energy = 0.642805
Thermal correction to Enthalpy = 0.643749
Thermal correction to Gibbs Free Energy = 0.529010
Sum of electronic and zero-point Energies = -3121.774570
Sum of electronic and thermal Energies = -3121.734179
Sum of electronic and thermal Enthalpies = -3121.733235
Sum of electronic and thermal Free Energies = -3121.847974
```

Table S14. Optimized Cartesian coordinates (Å) obtained for [ClPd**L1**(μ-Cl)$_2$Pd**L1**Cl] with DFT calculations TPSSh/6-31G(d) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	46	1.525616	0.541137	-0.704919
2	17	2.400064	0.350605	-2.841390
3	17	0.402293	0.780619	1.363857
4	15	5.805452	0.116832	-0.382293
5	15	3.226686	1.927524	-0.173395
6	7	4.786421	-0.880587	0.314022
7	5	3.136175	-2.936491	0.331001
8	1	2.265808	-2.158464	0.159247
9	5	4.365096	-3.348283	-0.870821
10	1	4.280593	-2.872316	-1.950007
11	5	5.941269	-3.420309	-0.036619
12	1	6.919467	-3.009306	-0.559797
13	5	5.682119	-3.064382	1.674684
14	1	6.386140	-2.369360	2.320348
15	5	3.068896	-4.237364	1.536517
16	1	2.065956	-4.357124	2.155927
17	5	3.321601	-4.613972	-0.178789
18	1	2.474234	-5.131307	-0.831824
19	5	5.063116	-4.917514	-0.415326
20	1	5.469352	-5.661190	-1.247776
21	5	5.880249	-4.736206	1.163943
22	1	6.861001	-5.335092	1.463163
23	5	4.640244	-4.320667	2.363861
24	1	4.686707	-4.491365	3.535869
25	5	4.256066	-5.477779	1.074509
26	1	4.072184	-6.625370	1.318361
27	6	4.748566	-2.265803	0.415207
28	6	4.001736	-2.847089	1.801862
29	6	4.850694	1.577389	-0.994035
30	1	5.493110	2.460616	-0.898765
31	1	4.611742	1.412629	-2.049387
32	6	6.740663	-0.438425	-1.851647
33	6	6.038182	-0.689021	-3.045132
34	1	4.964257	-0.525885	-3.097573
35	6	6.717309	-1.170591	-4.165491
36	1	6.167641	-1.361414	-5.082466
37	6	8.092740	-1.413169	-4.104747
38	1	8.617114	-1.789657	-4.978651

39	6	8.791907	-1.180842	-2.917236
40	1	9.858423	-1.379882	-2.862853
41	6	8.120745	-0.698784	-1.791902
42	1	8.668826	-0.533111	-0.869749
43	6	7.042113	0.869701	0.744989
44	6	7.011682	0.542595	2.106429
45	1	6.274367	-0.167530	2.463789
46	6	7.914159	1.136137	2.993691
47	1	7.883510	0.874799	4.047487
48	6	8.848399	2.062677	2.526517
49	1	9.550919	2.522545	3.216068
50	6	8.879145	2.402430	1.169121
51	1	9.604443	3.123841	0.803123
52	6	7.979479	1.811581	0.281194
53	1	8.018088	2.073113	-0.773959
54	6	2.750442	3.578554	-0.806784
55	6	3.402717	4.222576	-1.868802
56	1	4.263791	3.768569	-2.348618
57	6	2.934158	5.455176	-2.333794
58	1	3.444150	5.944859	-3.158639
59	6	1.813940	6.048721	-1.748521
60	1	1.448571	7.002868	-2.117416
61	6	1.154813	5.407965	-0.693575
62	1	0.274001	5.855997	-0.243440
63	6	1.615658	4.177849	-0.226151
64	1	1.088408	3.675596	0.580856
65	6	3.605155	2.217423	1.596342
66	6	4.107853	3.463708	2.010171
67	1	4.241357	4.265250	1.289327
68	6	4.422088	3.680694	3.352897
69	1	4.809091	4.646617	3.664883
70	6	4.224529	2.664728	4.292477
71	1	4.454672	2.841328	5.339618
72	6	3.719334	1.426589	3.886774
73	1	3.549316	0.640414	4.616997
74	6	3.413147	1.199377	2.543290
75	1	3.016795	0.243865	2.222431
76	46	-1.526143	-0.540240	0.702333
77	17	-2.399480	-0.351043	2.839444
78	17	-0.403679	-0.778373	-1.367076
79	15	-5.805277	-0.117280	0.382716
80	15	-3.226615	-1.927696	0.171691
81	7	-4.786718	0.880450	-0.313878
82	5	-3.136297	2.936543	-0.326633
83	1	-2.266058	2.158479	-0.154419
84	5	-4.366782	3.347162	0.873964
85	1	-4.283392	2.870290	1.952830
86	5	-5.941909	3.419848	0.037820
87	1	-6.920712	3.008257	0.559433
88	5	-5.680634	3.065406	-1.673421
89	1	-6.383784	2.370888	-2.320572
90	5	-3.067659	4.238374	-1.531023
91	1	-2.063972	4.358821	-2.149086
92	5	-3.322525	4.613548	0.184292
93	1	-2.476036	5.130358	0.838876
94	5	-5.064366	4.916774	0.419014

95	1	-5.471633	5.659737	1.251593
96	5	-5.879515	4.736784	-1.161451
97	1	-6.859928	5.335833	-1.461461
98	5	-4.637996	4.322314	-2.360173
99	1	-4.683013	4.493962	-3.532099
100	5	-4.255464	5.478367	-1.069401
101	1	-4.071332	6.626172	-1.312062
102	6	-4.748576	2.265798	-0.413490
103	6	-4.000069	2.848283	-1.798616
104	6	-4.850375	-1.578369	0.993114
105	1	-5.492757	-2.461552	0.897248
106	1	-4.611202	-1.414428	2.048535
107	6	-6.739957	0.437143	1.852738
108	6	-6.037451	0.686176	3.046525
109	1	-4.963595	0.522559	3.098836
110	6	-6.716430	1.166879	4.167352
111	1	-6.166718	1.356500	5.084551
112	6	-8.091742	1.410139	4.106788
113	1	-8.615999	1.785937	4.981060
114	6	-8.790942	1.179371	2.918989
115	1	-9.857366	1.378943	2.864751
116	6	-8.119936	0.698173	1.793203
117	1	-8.668056	0.533658	0.870868
118	6	-7.042525	-0.869412	-0.744423
119	6	-7.012772	-0.541348	-2.105645
120	1	-6.275621	0.169034	-2.462843
121	6	-7.915692	-1.134279	-2.992861
122	1	-7.885588	-0.872211	-4.046494
123	6	-8.849699	-2.061143	-2.525852
124	1	-9.552557	-2.520541	-3.215372
125	6	-8.879784	-2.401812	-1.168671
126	1	-9.604913	-3.123460	-0.802803
127	6	-7.979664	-1.811584	-0.280788
128	1	-8.017785	-2.073786	0.774217
129	6	-2.749095	-3.578347	0.805101
130	6	-3.400925	-4.222757	1.867154
131	1	-4.262406	-3.769376	2.346825
132	6	-2.931443	-5.454941	2.332302
133	1	-3.441094	-5.944936	3.157173
134	6	-1.810726	-6.047661	1.747154
135	1	-1.444602	-7.001463	2.116193
136	6	-1.152070	-5.406539	0.692132
137	1	-0.270883	-5.853924	0.242088
138	6	-1.613858	-4.176835	0.224533
139	1	-1.087001	-3.674279	-0.582541
140	6	-3.606163	-2.218137	-1.597737
141	6	-4.108564	-3.464786	-2.010850
142	1	-4.241065	-4.266229	-1.289705
143	6	-4.423785	-3.682235	-3.353264
144	1	-4.810558	-4.648426	-3.664708
145	6	-4.227488	-2.666399	-4.293257
146	1	-4.458435	-2.843371	-5.340158
147	6	-3.722546	-1.427929	-3.888273
148	1	-3.553542	-0.641818	-4.618797
149	6	-3.415384	-1.200256	-2.545087
150	1	-3.019268	-0.244474	-2.224766

151	1	-3.675825	2.068173	-2.475671
152	1	3.678365	-2.066376	2.478641

E(RTPSSh) = -6166.01987087 Hartree
Zero-point correction = 1.145701
Thermal correction to Energy = 1.225843
Thermal correction to Enthalpy = 1.226787
Thermal correction to Gibbs Free Energy = 1.018692
Sum of electronic and zero-point Energies = -6164.874170
Sum of electronic and thermal Energies = -6164.794028
Sum of electronic and thermal Enthalpies = -6164.793084
Sum of electronic and thermal Free Energies = -6165.001179

Table S15. Optimized Cartesian coordinates (Å) obtained for [ClPd**L2**(μ-Cl)$_2$Pd**L2**Cl] with DFT calculations TPSSh/6-31G(d) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	46	1.549635	0.679007	-0.872695
2	17	2.569770	0.211569	-2.897371
3	17	0.263412	1.233761	1.035029
4	15	5.881018	0.107726	-0.240676
5	15	3.300609	2.003098	-0.335404
6	7	4.912633	-0.932283	0.457282
7	5	3.170063	-2.908507	0.452396
8	1	2.321682	-2.086055	0.461007
9	5	4.236397	-3.216936	-0.926586
10	1	4.053875	-2.611255	-1.925341
11	5	5.882805	-3.449099	-0.276022
12	1	6.832956	-3.025973	-0.837499
13	5	5.792240	-3.288324	1.483492
14	1	6.592790	-2.702621	2.130527
15	5	3.147871	-4.356491	1.476184
16	1	2.200618	-4.521682	2.170149
17	5	3.209494	-4.514788	-0.286859
18	1	2.276141	-4.912025	-0.906387
19	5	4.900043	-4.852176	-0.741074
20	1	5.186121	-5.496423	-1.697312
21	5	5.875431	-4.894573	0.755672
22	1	6.853995	-5.556734	0.877751
23	5	4.783805	-4.599118	2.115897
24	1	4.945442	-4.923599	3.245364
25	5	4.220143	-5.567798	0.741876
26	1	4.006597	-6.730098	0.863149
27	6	4.801023	-2.311456	0.415125
28	6	4.147931	-3.037294	1.857765
29	6	4.948063	1.507258	-1.020791
30	1	5.604897	2.385476	-1.002352
31	1	4.753137	1.230801	-2.061561
32	6	6.946298	-0.437528	-1.621492
33	6	6.347933	-0.775075	-2.849906
34	1	5.273451	-0.679101	-2.986294
35	6	7.131988	-1.264026	-3.895396
36	1	6.662313	-1.527454	-4.838438

37	6	8.511035	-1.421512	-3.727002
38	1	9.117405	-1.804695	-4.542959
39	6	9.108781	-1.092677	-2.507402
40	1	10.178957	-1.220344	-2.371337
41	6	8.331428	-0.605297	-1.454846
42	1	8.800725	-0.364297	-0.506143
43	6	6.991590	0.936331	0.956387
44	6	6.991712	0.505911	2.289120
45	1	6.335556	-0.307542	2.579488
46	6	7.827530	1.119333	3.226645
47	1	7.820619	0.779465	4.258270
48	6	8.667664	2.164550	2.837320
49	1	9.318140	2.640464	3.565910
50	6	8.675821	2.598048	1.506605
51	1	9.333383	3.406657	1.199849
52	6	7.841608	1.988361	0.569116
53	1	7.870643	2.319364	-0.466679
54	6	2.969903	3.620772	-1.130062
55	6	3.626091	4.044952	-2.296125
56	1	4.395231	3.431600	-2.753983
57	6	3.278459	5.259981	-2.893128
58	1	3.792334	5.579387	-3.795373
59	6	2.272081	6.053800	-2.338994
60	1	2.001167	6.995323	-2.808208
61	6	1.604524	5.629420	-1.185081
62	1	0.810918	6.234805	-0.757081
63	6	1.945727	4.418216	-0.583688
64	1	1.412201	4.087395	0.303286
65	6	3.601256	2.414524	1.422505
66	6	4.258552	3.612262	1.757531
67	1	4.548550	4.313574	0.980189
68	6	4.527276	3.911745	3.093582
69	1	5.033350	4.839430	3.345272
70	6	4.134883	3.027167	4.103169
71	1	4.332156	3.269791	5.143731
72	6	3.481548	1.837129	3.774306
73	1	3.162800	1.153519	4.555852
74	6	3.217032	1.526766	2.437939
75	1	2.700546	0.609802	2.180601
76	6	3.834792	-2.103879	3.009689
77	46	-1.514269	-0.341336	0.516024
78	17	-2.359370	-0.123658	2.660465
79	17	-0.406285	-0.579405	-1.561111
80	15	-5.843584	-0.298885	0.375012
81	15	-3.087623	-1.912866	0.118167
82	7	-5.014047	0.913880	-0.215027
83	5	-3.642605	3.154853	0.108983
84	1	-2.665689	2.495225	0.169727
85	5	-4.900756	3.187754	1.349383
86	1	-4.734919	2.557058	2.335591
87	5	-6.474995	3.180201	0.508349
88	1	-7.388894	2.555787	0.926482
89	5	-6.157404	3.156747	-1.230476
90	1	-6.763661	2.494188	-2.001258
91	5	-3.756790	4.644987	-0.842332
92	1	-2.778642	5.011828	-1.404582

93	5	-4.049912	4.680333	0.904621
94	1	-3.276886	5.187164	1.650076
95	5	-5.815838	4.695832	1.155423
96	1	-6.320043	5.218378	2.095778
97	5	-6.602998	4.673097	-0.447697
98	1	-7.661618	5.166700	-0.663629
99	5	-5.324789	4.652200	-1.671445
100	1	-5.405686	5.016649	-2.797417
101	5	-5.102677	5.610716	-0.197326
102	1	-5.081955	6.797493	-0.239944
103	6	-5.138417	2.290321	-0.095323
104	6	-4.459695	3.201372	-1.400733
105	6	-4.714771	-1.645313	0.958029
106	1	-5.280636	-2.584056	0.919561
107	1	-4.460691	-1.422418	1.998654
108	6	-6.900479	-0.044482	1.847331
109	6	-6.290676	0.218854	3.087965
110	1	-5.207526	0.250650	3.174339
111	6	-7.077258	0.468621	4.213582
112	1	-6.598211	0.674707	5.166190
113	6	-8.471558	0.462572	4.113135
114	1	-9.080203	0.659527	4.991270
115	6	-9.082257	0.212325	2.881445
116	1	-10.165263	0.217158	2.797207
117	6	-8.302436	-0.037093	1.750552
118	1	-8.784202	-0.217618	0.794868
119	6	-6.912656	-1.130459	-0.860748
120	6	-6.998475	-0.597707	-2.153028
121	1	-6.431097	0.294861	-2.394171
122	6	-7.805559	-1.211004	-3.115619
123	1	-7.867782	-0.788605	-4.114395
124	6	-8.528088	-2.361468	-2.793564
125	1	-9.156431	-2.837037	-3.541560
126	6	-8.445079	-2.902512	-1.505511
127	1	-9.008783	-3.795713	-1.250866
128	6	-7.641110	-2.291577	-0.542807
129	1	-7.600055	-2.709122	0.460823
130	6	-2.477345	-3.479601	0.843572
131	6	-3.009621	-4.039863	2.014964
132	1	-3.840675	-3.567154	2.527850
133	6	-2.458369	-5.210099	2.544296
134	1	-2.876654	-5.635676	3.452150
135	6	-1.372450	-5.823015	1.915765
136	1	-0.942033	-6.728887	2.333004
137	6	-0.830195	-5.263019	0.753902
138	1	0.024789	-5.724207	0.269558
139	6	-1.374565	-4.094886	0.220693
140	1	-0.939012	-3.656574	-0.673381
141	6	-3.495418	-2.350688	-1.613799
142	6	-3.975357	-3.638716	-1.913186
143	1	-4.059979	-4.386370	-1.129682
144	6	-4.328394	-3.966264	-3.222847
145	1	-4.695385	-4.963947	-3.446646
146	6	-4.197470	-3.019194	-4.243370
147	1	-4.460335	-3.281867	-5.264366
148	6	-3.719332	-1.740099	-3.950881

149	1	-3.603159	-1.004663	-4.741714
150	6	-3.371394	-1.403520	-2.640554
151	1	-2.984917	-0.417321	-2.415867
152	6	-3.863155	2.409461	-2.547500
153	1	2.759350	-2.085945	3.203650
154	1	4.355977	-2.435232	3.911698
155	1	4.165113	-1.093962	2.750524
156	1	-4.181199	2.844487	-3.498466
157	1	-2.771652	2.413792	-2.496115
158	1	-4.214624	1.376174	-2.487158

E(RTPSSh) = -6244.65458284 Hartree
Zero-point correction = 1.201536
Thermal correction to Energy = 1.285251
Thermal correction to Enthalpy = 1.286195
Thermal correction to Gibbs Free Energy = 1.070487
Sum of electronic and zero-point Energies = -6243.453047
Sum of electronic and thermal Energies = -6243.369332
Sum of electronic and thermal Enthalpies = -6243.368388
Sum of electronic and thermal Free Energies = -6243.584096

Table S16. Optimized Cartesian coordinates (Å) obtained for [ClPd**L3**(μ-Cl)$_2$Pd**L3**Cl] with DFT calculations TPSSh/6-31G(d) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	46	1.488818	0.795406	-0.790082
2	17	2.345509	0.974039	-2.937873
3	17	0.385764	0.689335	1.297420
4	15	5.689608	0.414119	-0.457599
5	15	3.079421	2.248466	-0.125605
6	7	4.686527	-0.774824	-0.127689
7	5	3.197008	-2.914767	-0.490205
8	1	2.249357	-2.222560	-0.376086
9	5	4.260275	-2.815121	-1.903452
10	1	3.984404	-2.041281	-2.754057
11	5	5.922802	-2.990008	-1.290140
12	1	6.827215	-2.370059	-1.728742
13	5	5.815675	-3.200939	0.466865
14	1	6.581762	-2.683817	1.205558
15	5	3.327900	-4.551421	0.197277
16	1	2.406470	-4.971487	0.812651
17	5	3.392909	-4.320913	-1.554884
18	1	2.497023	-4.677247	-2.250197
19	5	5.104631	-4.369869	-2.049346
20	1	5.455270	-4.760623	-3.115008
21	5	6.090088	-4.605180	-0.576620
22	1	7.141938	-5.156952	-0.578582
23	5	4.988647	-4.739382	0.795975
24	1	5.208362	-5.290346	1.821969
25	5	4.526102	-5.448259	-0.762395
26	1	4.446269	-6.626781	-0.887855
27	6	4.739084	-2.125783	-0.413908
28	6	4.163982	-3.248454	0.893834

29	6	4.746735	1.955820	-0.869671
30	1	5.396735	2.802954	-0.618172
31	1	4.573835	1.944444	-1.950304
32	6	6.780724	0.269070	-1.918168
33	6	6.184433	0.219823	-3.192489
34	1	5.105082	0.300391	-3.300476
35	6	6.976688	0.034948	-4.326034
36	1	6.508620	-0.007903	-5.305061
37	6	8.362304	-0.104407	-4.200946
38	1	8.975493	-0.251071	-5.085716
39	6	8.957648	-0.064429	-2.937356
40	1	10.032787	-0.182358	-2.835990
41	6	8.171829	0.116854	-1.797173
42	1	8.639686	0.127431	-0.817820
43	6	6.762660	0.908092	0.940568
44	6	6.658830	0.206775	2.148640
45	1	5.948140	-0.609412	2.230050
46	6	7.452622	0.568950	3.240441
47	1	7.363866	0.020498	4.173820
48	6	8.349035	1.634019	3.133149
49	1	8.965813	1.914574	3.982469
50	6	8.451747	2.344867	1.931841
51	1	9.147195	3.175092	1.846095
52	6	7.661144	1.986354	0.839638
53	1	7.758108	2.535475	-0.094346
54	6	2.579475	3.894831	-0.750595
55	6	3.311659	4.627604	-1.695813
56	1	4.247810	4.245536	-2.089683
57	6	2.830979	5.858690	-2.152383
58	1	3.403130	6.417449	-2.887648
59	6	1.621197	6.363788	-1.671790
60	1	1.248811	7.318442	-2.032381
61	6	0.884408	5.635936	-0.730956
62	1	-0.061721	6.018179	-0.359354
63	6	1.356213	4.405557	-0.274929
64	1	0.775805	3.838628	0.448829
65	6	3.360101	2.500634	1.663753
66	6	3.580418	3.791812	2.177128
67	1	3.548619	4.655438	1.520197
68	6	3.828715	3.968002	3.539154
69	1	3.993111	4.968416	3.929646
70	6	3.853558	2.863846	4.395691
71	1	4.035598	3.005451	5.457603
72	6	3.636317	1.580556	3.888655
73	1	3.646550	0.718468	4.547556
74	6	3.388474	1.393908	2.526967
75	1	3.214798	0.396536	2.137349
76	6	3.737305	-2.732461	2.238991
77	6	2.415796	-2.316867	2.468801
78	1	1.707283	-2.280719	1.650041
79	6	1.993014	-1.960137	3.751668
80	1	0.965196	-1.642338	3.899827
81	6	2.883567	-2.022362	4.827218
82	1	2.549897	-1.761250	5.828116
83	6	4.202177	-2.435378	4.609908
84	1	4.899389	-2.501888	5.441160

85	6	4.625922	-2.788368	3.327180
86	1	5.640514	-3.141762	3.173905
87	46	-1.398452	-0.763191	0.501052
88	17	-2.204075	-1.036513	2.655422
89	17	-0.327678	-0.599790	-1.600269
90	15	-5.695787	-0.589239	0.472429
91	15	-2.990290	-2.178630	-0.234212
92	7	-4.846666	0.732319	0.264732
93	5	-3.456047	2.766426	1.223961
94	1	-2.485751	2.108313	1.103482
95	5	-4.683155	2.401657	2.445539
96	1	-4.485811	1.489470	3.170624
97	5	-6.267499	2.667786	1.676663
98	1	-7.188685	1.953729	1.876333
99	5	-5.967659	3.199331	0.017900
100	1	-6.623413	2.818258	-0.888780
101	5	-3.562809	4.493567	0.825155
102	1	-2.591822	5.029940	0.405347
103	5	-3.827473	3.953542	2.487374
104	1	-3.033714	4.185830	3.339275
105	5	-5.588358	3.892194	2.767442
106	1	-6.073084	4.079770	3.835698
107	5	-6.399019	4.386288	1.253642
108	1	-7.458969	4.921648	1.224195
109	5	-5.145553	4.770402	0.070308
110	1	-5.254110	5.492152	-0.863495
111	5	-4.893793	5.193918	1.774480
112	1	-4.865569	6.331304	2.115205
113	6	-4.955756	1.999888	0.804535
114	6	-4.274438	3.319981	-0.186278
115	6	-4.611819	-2.083099	0.647829
116	1	-5.217937	-2.946150	0.345290
117	1	-4.364854	-2.174174	1.709695
118	6	-6.757202	-0.761906	1.955724
119	6	-6.148988	-0.888983	3.218492
120	1	-5.065875	-0.901937	3.310050
121	6	-6.935888	-0.970996	4.368367
122	1	-6.457364	-1.064088	5.338860
123	6	-8.329633	-0.924645	4.271998
124	1	-8.938656	-0.987182	5.169519
125	6	-8.938852	-0.788751	3.021789
126	1	-10.021315	-0.741869	2.943427
127	6	-8.158432	-0.703140	1.867210
128	1	-8.639519	-0.581959	0.901848
129	6	-6.771942	-0.982356	-0.955825
130	6	-6.816155	-0.084331	-2.029921
131	1	-6.201233	0.809433	-1.995775
132	6	-7.631992	-0.350669	-3.133321
133	1	-7.661040	0.350547	-3.962405
134	6	-8.402115	-1.514789	-3.171459
135	1	-9.036323	-1.720164	-4.029447
136	6	-8.356592	-2.420159	-2.105214
137	1	-8.954752	-3.326702	-2.132312
138	6	-7.544768	-2.156953	-1.001721
139	1	-7.531899	-2.857366	-0.169431
140	6	-2.406913	-3.883150	0.085266

141	6	-3.031676	-4.764389	0.981025
142	1	-3.924352	-4.467352	1.522037
143	6	-2.497841	-6.038628	1.196147
144	1	-2.986553	-6.712409	1.894316
145	6	-1.342280	-6.440757	0.523344
146	1	-0.928372	-7.430045	0.696462
147	6	-0.710966	-5.564528	-0.366210
148	1	0.195389	-5.864321	-0.883175
149	6	-1.234114	-4.289780	-0.580902
150	1	-0.729836	-3.608116	-1.261085
151	6	-3.387788	-2.139338	-2.018879
152	6	-3.678502	-3.326902	-2.713699
153	1	-3.629718	-4.284673	-2.204597
154	6	-4.016510	-3.277527	-4.066949
155	1	-4.235373	-4.198727	-4.599741
156	6	-4.060560	-2.049889	-4.733988
157	1	-4.312499	-2.016131	-5.790555
158	6	-3.773846	-0.868704	-4.045555
159	1	-3.798921	0.088014	-4.557270
160	6	-3.438025	-0.907430	-2.690570
161	1	-3.214161	0.011631	-2.159214
162	6	-3.690366	3.046487	-1.545292
163	6	-2.342894	2.681875	-1.698154
164	1	-1.726570	2.504688	-0.824372
165	6	-1.779579	2.548534	-2.970094
166	1	-0.736702	2.260659	-3.063395
167	6	-2.554191	2.782059	-4.109456
168	1	-2.111160	2.688764	-5.097335
169	6	-3.897510	3.143988	-3.968929
170	1	-4.507095	3.341081	-4.847103
171	6	-4.460800	3.275969	-2.698358
172	1	-5.494916	3.588633	-2.600034

E(RTPSSh) = -6628.15304869 Hartree
Zero-point correction = 1.307492
Thermal correction to Energy = 1.397202
Thermal correction to Enthalpy = 1.398146
Thermal correction to Gibbs Free Energy = 1.172618
Sum of electronic and zero-point Energies = -6626.845557
Sum of electronic and thermal Energies = -6626.755846
Sum of electronic and thermal Enthalpies = -6626.754902
Sum of electronic and thermal Free Energies = -6626.980430

Table S17. Optimized Cartesian coordinates (Å) obtained for [ClPd**L4**(μ-Cl)$_2$Pd**L4**Cl] with DFT calculations TPSSh/6-31G(d) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	46	-1.547206	-0.525907	-0.690776
2	17	-2.437267	-0.278361	-2.812441
3	17	-0.424938	-0.793316	1.376397
4	15	-5.840884	-0.197529	-0.323460
5	15	-3.222531	-1.954855	-0.192722
6	7	-4.973911	0.882982	0.411449

7	5	-3.102198	3.055542	0.227609
8	1	-2.179516	2.322050	0.123737
9	5	-4.333063	3.435169	-1.000527
10	1	-4.259726	3.029763	-2.112385
11	5	-5.887706	3.599475	-0.145094
12	1	-6.958882	3.259088	-0.520828
13	1	-6.190049	2.884359	2.152038
14	5	-2.985577	4.429158	1.356679
15	1	-1.995883	4.579810	1.990226
16	5	-3.253258	4.718791	-0.373272
17	1	-2.403505	5.201127	-1.050268
18	5	-4.985676	5.057293	-0.613058
19	1	-5.388588	5.784622	-1.461203
20	5	-5.776024	4.989065	0.973928
21	1	-6.767589	5.529739	1.333075
22	5	-4.541978	4.612578	2.190422
23	1	-4.658958	4.801269	3.352437
24	5	-4.144401	5.679462	0.845073
25	1	-3.940284	6.832904	1.037887
26	6	-3.951858	3.074390	1.685758
27	6	-4.851680	-1.617246	-1.002959
28	1	-5.469393	-2.521247	-0.942410
29	1	-4.619271	-1.406950	-2.051650
30	6	-6.837520	0.327342	-1.766122
31	6	-6.174287	0.664109	-2.960909
32	1	-5.094359	0.562425	-3.038954
33	6	-6.899815	1.153544	-4.048196
34	1	-6.379407	1.412288	-4.965676
35	6	-8.285146	1.317542	-3.953888
36	1	-8.846091	1.699982	-4.802201
37	6	-8.946964	0.997946	-2.765504
38	1	-10.022152	1.132463	-2.685686
39	6	-8.227975	0.507916	-1.672793
40	1	-8.748737	0.268064	-0.750683
41	6	-7.011792	-1.011985	0.825484
42	6	-7.058335	-0.575059	2.155228
43	1	-6.385909	0.218803	2.465889
44	6	-7.939379	-1.168977	3.062931
45	1	-7.965479	-0.827301	4.093892
46	6	-8.781895	-2.201838	2.645319
47	1	-9.468620	-2.662857	3.349903
48	6	-8.741950	-2.644523	1.318416
49	1	-9.398376	-3.445805	0.990611
50	6	-7.859953	-2.054375	0.411959
51	1	-7.848269	-2.393403	-0.621692
52	6	-2.706318	-3.583523	-0.850446
53	6	-3.335764	-4.212212	-1.935320
54	1	-4.199041	-3.760204	-2.413077
55	6	-2.840630	-5.424397	-2.425408
56	1	-3.332815	-5.902152	-3.267893
57	6	-1.716314	-6.012567	-1.842445
58	1	-1.329963	-6.950680	-2.230666
59	6	-1.079691	-5.386684	-0.764936
60	1	-0.195601	-5.830198	-0.316775
61	6	-1.566864	-4.176482	-0.272588
62	1	-1.056679	-3.684382	0.551381

63	6	-3.591105	-2.266358	1.574813
64	6	-4.034227	-3.534752	1.989028
65	1	-4.126936	-4.342376	1.268611
66	6	-4.341648	-3.764532	3.331188
67	1	-4.681928	-4.747625	3.644089
68	6	-4.197263	-2.738118	4.268946
69	1	-4.421817	-2.923889	5.315771
70	6	-3.753903	-1.477047	3.861774
71	1	-3.626426	-0.681995	4.591176
72	6	-3.453725	-1.236749	2.519358
73	1	-3.110072	-0.260958	2.197349
74	46	1.508324	0.526972	0.731336
75	17	2.395162	0.285862	2.858146
76	17	0.376234	0.819653	-1.324617
77	15	5.802912	0.106100	0.386636
78	15	3.215595	1.910891	0.210696
79	7	4.790886	-0.886173	-0.326229
80	5	3.150747	-2.947463	-0.392647
81	1	2.276121	-2.175773	-0.214317
82	5	4.371932	-3.375252	0.811739
83	1	4.277293	-2.918476	1.898354
84	5	5.954929	-3.426633	-0.010554
85	1	6.927126	-3.020731	0.527469
86	5	5.707365	-3.042239	-1.717502
87	1	6.413980	-2.333871	-2.345678
88	5	3.098355	-4.228546	-1.620211
89	1	2.100653	-4.342057	-2.249163
90	5	3.339090	-4.632756	0.090250
91	1	2.489141	-5.164654	0.728044
92	5	5.079905	-4.933393	0.335429
93	1	5.482540	-5.689394	1.158499
94	5	5.908783	-4.721873	-1.233863
95	1	6.894357	-5.311553	-1.535615
96	5	4.676544	-4.291273	-2.436406
97	1	4.733377	-4.442082	-3.610701
98	5	4.287119	-5.471588	-1.169826
99	1	4.109973	-6.615627	-1.434546
100	6	4.760780	-2.269174	-0.451964
101	6	4.027235	-2.829960	-1.855142
102	6	4.839741	1.548463	1.026683
103	1	5.478783	2.436155	0.952222
104	1	4.599059	1.359988	2.077794
105	6	6.743232	-0.469360	1.844954
106	6	6.042071	-0.749386	3.032631
107	1	4.966965	-0.595095	3.087666
108	6	6.724220	-1.248602	4.143372
109	1	6.175538	-1.462378	5.055876
110	6	8.101485	-1.479492	4.078564
111	1	8.628232	-1.869966	4.944885
112	6	8.799526	-1.217538	2.896552
113	1	9.867569	-1.407312	2.838885
114	6	8.125260	-0.717879	1.780764
115	1	8.672307	-0.529340	0.862386
116	6	7.033277	0.886236	-0.728680
117	6	7.004028	0.580337	-2.095098
118	1	6.269982	-0.127539	-2.463492

119	6	7.903476	1.191831	-2.973121
120	1	7.873667	0.946910	-4.030870
121	6	8.833541	2.115348	-2.491784
122	1	9.533811	2.589099	-3.174191
123	6	8.862811	2.434295	-1.129318
124	1	9.584649	3.153473	-0.752226
125	6	7.966157	1.825434	-0.250536
126	1	8.003898	2.070789	0.808543
127	6	2.749637	3.559945	0.857370
128	6	3.398199	4.186148	1.932421
129	1	4.248071	3.716889	2.417604
130	6	2.940426	5.420696	2.403004
131	1	3.447698	5.896612	3.237577
132	6	1.835145	6.034303	1.809953
133	1	1.479200	6.990802	2.182103
134	6	1.178962	5.410733	0.742992
135	1	0.309560	5.873972	0.286295
136	6	1.628183	4.178122	0.270746
137	1	1.101578	3.689225	-0.544804
138	6	3.592630	2.214291	-1.557157
139	6	4.108680	3.458696	-1.959976
140	1	4.254101	4.251231	-1.231490
141	6	4.420469	3.686065	-3.301529
142	1	4.817402	4.650680	-3.604975
143	6	4.207916	2.682087	-4.250654
144	1	4.436037	2.866877	-5.296833
145	6	3.689889	1.445701	-3.855799
146	1	3.507741	0.669334	-4.593556
147	6	3.385588	1.208147	-2.513645
148	1	2.977788	0.254375	-2.201681
149	5	-4.728402	2.271549	0.290693
150	6	-5.509994	3.393519	1.479908
151	1	3.706518	-2.038933	-2.521120
152	1	-3.709153	2.389067	2.488787

E(RTPSSh) = -6166.06277737 Hartree
Zero-point correction = 1.147432
Thermal correction to Energy = 1.227638
Thermal correction to Enthalpy = 1.228583
Thermal correction to Gibbs Free Energy = 1.021119
Sum of electronic and zero-point Energies = -6164.915345
Sum of electronic and thermal Energies = -6164.835139
Sum of electronic and thermal Enthalpies = -6164.834195
Sum of electronic and thermal Free Energies = -6165.041658

Table S18. Optimized Cartesian coordinates (Å) obtained for [ClPd**L5**(μ-Cl)$_2$Pd**L5**Cl] with DFT calculations TPSSh/6-31G(d) (0 imaginary frequencies).

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	46	-1.572627	-0.588304	-0.647146
2	17	-2.450318	-0.393879	-2.779133
3	17	-0.439912	-0.843019	1.415910

4	15	-5.924819	-0.308335	-0.320175
5	15	-3.241026	-2.020189	-0.134973
6	7	-5.173361	0.868024	0.396243
7	5	-3.236407	2.981587	0.256428
8	1	-2.330606	2.246306	0.463542
9	5	-4.180349	3.142272	-1.244037
10	1	-3.900004	2.545745	-2.229050
11	5	-5.866338	3.451771	-0.756265
12	1	-6.856649	3.055702	-1.271714
13	1	-6.633692	3.144519	1.525224
14	5	-3.292125	4.533878	1.122588
15	1	-2.435782	4.794615	1.900607
16	5	-3.203293	4.513243	-0.646740
17	1	-2.218941	4.866492	-1.212259
18	5	-4.841280	4.803494	-1.281322
19	1	-5.048108	5.366739	-2.306301
20	5	-5.928435	5.010559	0.105460
21	1	-6.953689	5.602177	0.165270
22	5	-4.968737	4.856932	1.582262
23	1	-5.303795	5.254432	2.645541
24	5	-4.282199	5.672829	0.182113
25	1	-4.081957	6.842730	0.213777
26	6	-4.338592	3.244578	1.519462
27	6	-4.862529	-1.698648	-0.964855
28	1	-5.459766	-2.617602	-0.922051
29	1	-4.617106	-1.482141	-2.008998
30	6	-6.932988	0.093337	-1.794449
31	6	-6.281527	0.408611	-3.001566
32	1	-5.197693	0.356381	-3.073995
33	6	-7.023957	0.819496	-4.109649
34	1	-6.512252	1.064177	-5.035816
35	6	-8.415667	0.924073	-4.025097
36	1	-8.989973	1.245296	-4.889674
37	6	-9.066976	0.622787	-2.826153
38	1	-10.147738	0.709058	-2.755069
39	6	-8.330663	0.212267	-1.712411
40	1	-8.843741	-0.014621	-0.782557
41	6	-7.055936	-1.152836	0.844301
42	6	-7.176737	-0.654354	2.147524
43	1	-6.583201	0.208692	2.432089
44	6	-8.038867	-1.267727	3.060513
45	1	-8.122163	-0.877317	4.070945
46	6	-8.790289	-2.380034	2.674679
47	1	-9.462568	-2.855741	3.383422
48	6	-8.679864	-2.881149	1.372883
49	1	-9.267695	-3.742400	1.067768
50	6	-7.815852	-2.272259	0.461582
51	1	-7.752472	-2.658161	-0.553535
52	6	-2.717513	-3.656626	-0.767198
53	6	-3.224909	-4.203498	-1.955659
54	1	-3.994143	-3.684171	-2.517686
55	6	-2.723814	-5.415605	-2.438574
56	1	-3.121754	-5.830386	-3.360328
57	6	-1.711059	-6.084004	-1.747427
58	1	-1.319155	-7.022301	-2.129410
59	6	-1.193334	-5.538195	-0.567696

60	1	-0.397731	-6.048084	-0.032129
61	6	-1.688647	-4.329061	-0.079639
62	1	-1.274881	-3.902420	0.830253
63	6	-3.631636	-2.303063	1.630669
64	6	-4.133898	-3.546242	2.054661
65	1	-4.251739	-4.359109	1.343882
66	6	-4.467921	-3.744679	3.395296
67	1	-4.852542	-4.708541	3.716524
68	6	-4.296547	-2.711106	4.321001
69	1	-4.543795	-2.872901	5.366641
70	6	-3.799389	-1.474106	3.903098
71	1	-3.652995	-0.672829	4.621863
72	6	-3.469401	-1.265867	2.561965
73	1	-3.079585	-0.309320	2.234810
74	6	-4.232610	2.511205	2.846258
75	46	1.461924	0.524542	0.770581
76	17	2.378231	0.261385	2.879800
77	17	0.317850	0.800434	-1.282768
78	15	5.836915	0.251997	0.431285
79	15	3.135874	1.943715	0.238500
80	7	4.911662	-0.892879	-0.161766
81	5	4.444093	-3.430852	0.598065
82	1	3.806318	-3.012818	1.500286
83	5	6.204225	-3.294431	0.483482
84	1	6.805775	-2.835156	1.390483
85	5	6.605404	-2.848203	-1.194344
86	1	7.470006	-2.065950	-1.412317
87	5	5.086728	-2.721196	-2.089040
88	1	4.840298	-1.863065	-2.866523
89	5	3.928421	-4.759731	-0.453622
90	1	2.893946	-5.286087	-0.208801
91	5	5.434341	-4.891835	0.461776
92	1	5.538447	-5.629895	1.386346
93	5	6.779092	-4.527827	-0.657564
94	1	7.857977	-5.008085	-0.527660
95	5	6.082941	-4.168999	-2.261648
96	1	6.643925	-4.388314	-3.285437
97	5	4.322001	-4.313228	-2.124146
98	1	3.556765	-4.537219	-3.001949
99	5	5.364882	-5.443521	-1.236537
100	1	5.411991	-6.593031	-1.531261
101	6	5.201044	-2.229278	-0.424400
102	6	3.847159	-3.139212	-0.980414
103	6	4.765079	1.618545	1.055823
104	1	5.365528	2.534558	1.001599
105	1	4.522494	1.406818	2.101938
106	6	6.870765	-0.150553	1.885484
107	6	6.222710	-0.464351	3.095243
108	1	5.138214	-0.419169	3.166967
109	6	6.969773	-0.868413	4.201741
110	1	6.463213	-1.108731	5.131932
111	6	8.361453	-0.975230	4.109673
112	1	8.939572	-1.295306	4.972127
113	6	9.007347	-0.682286	2.906024
114	1	10.086577	-0.778278	2.827652
115	6	8.266975	-0.273266	1.794452

116	1	8.773576	-0.062157	0.857922
117	6	6.955500	1.092969	-0.755090
118	6	6.925020	0.719533	-2.105203
119	1	6.259239	-0.074823	-2.424345
120	6	7.739900	1.374034	-3.033318
121	1	7.711585	1.075605	-4.077177
122	6	8.584017	2.406777	-2.620231
123	1	9.217996	2.913503	-3.342607
124	6	8.613231	2.791975	-1.275188
125	1	9.268590	3.595622	-0.950932
126	6	7.802643	2.139577	-0.345514
127	1	7.843023	2.435111	0.700687
128	6	2.622600	3.574018	0.896395
129	6	3.250200	4.203972	1.981772
130	1	4.111339	3.752912	2.464115
131	6	2.756636	5.418757	2.466909
132	1	3.248521	5.897969	3.308741
133	6	1.635607	6.008324	1.878966
134	1	1.252104	6.949701	2.262201
135	6	0.999628	5.380362	0.802381
136	1	0.118592	5.824143	0.348709
137	6	1.484870	4.167314	0.315005
138	1	0.974565	3.675445	-0.508929
139	6	3.487850	2.248731	-1.531522
140	6	3.903606	3.522892	-1.957599
141	1	3.988345	4.337032	-1.243824
142	6	4.193863	3.748504	-3.304037
143	1	4.511755	4.735901	-3.626640
144	6	4.062115	2.712492	-4.233423
145	1	4.273912	2.895350	-5.283346
146	6	3.649862	1.445138	-3.813831
147	1	3.537835	0.639223	-4.533222
148	6	3.365019	1.209361	-2.467258
149	1	3.043514	0.227550	-2.142657
150	6	2.523327	-2.410198	-1.084198
151	5	-4.863566	2.222507	0.112037
152	6	-5.814456	3.525787	0.926277
153	1	2.594213	-1.452841	-0.555460
154	1	2.257999	-2.227469	-2.128373
155	1	1.734379	-3.003856	-0.617184
156	1	-4.574230	1.479859	2.721171
157	1	-3.188585	2.502681	3.168732
158	1	-4.831112	3.006111	3.616442

E(RTPSSh) = -6244.70264478 Hartree
Zero-point correction = 1.203488
Thermal correction to Energy = 1.286948
Thermal correction to Enthalpy = 1.287892
Thermal correction to Gibbs Free Energy = 1.075049
Sum of electronic and zero-point Energies = -6243.499156
Sum of electronic and thermal Energies = -6243.415697
Sum of electronic and thermal Enthalpies = -6243.414753
Sum of electronic and thermal Free Energies = -6243.627595