SUPPORTING INFORMATION

Heterolytic Activation of E-H Bonds Across Pt-P Bonds in Pt NHP (N-heterocyclic Phosphenium/Phosphido) Complexes

Baofei Pan, Mark W. Bezpalko, Bruce M. Foxman, Christine M. Thomas*

Department of Chemistry, Brandeis University, 415 South Street MS 015, Waltham, Massachusetts, 02454.

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Gaussian 09 Full Reference

Gaussian 09, Revision **A.1**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Scheme S1. Calculated energetics for the reaction of **1** with PhSH.

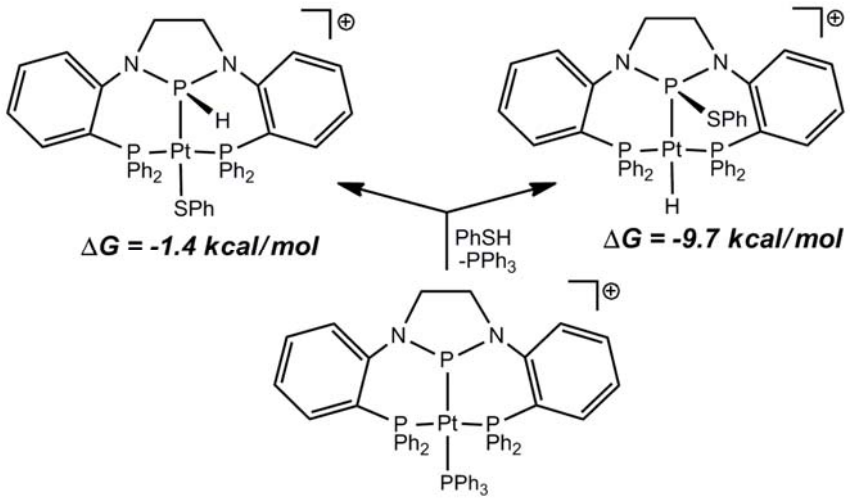
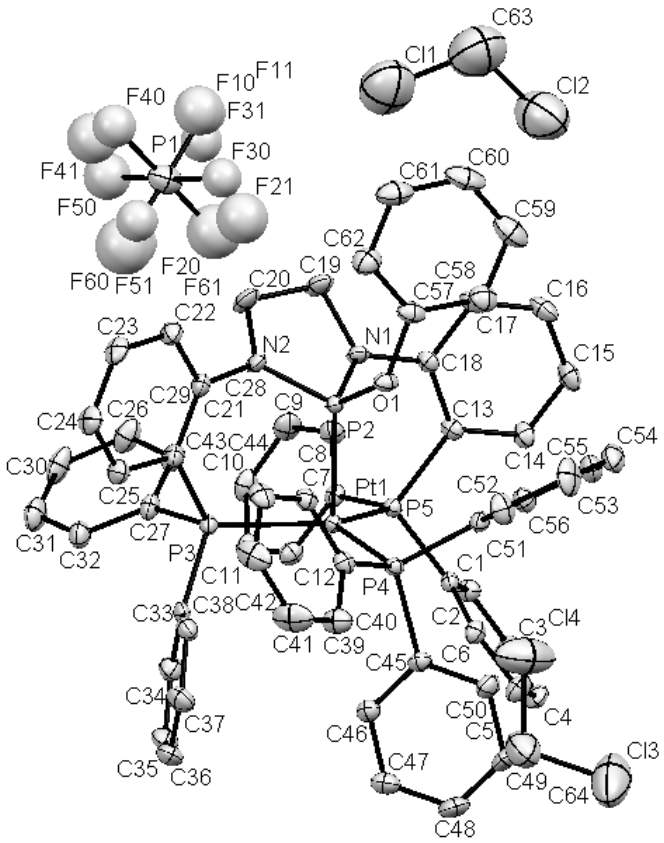


Figure S1 Fully-Labelled Elipsoid Representation of **4** • 2DCM



X-Ray data collection, solution, and refinement for 4 • 2DCM**.** Data collection was carried out at 120K, using a frame time of 20 sec and a detector distance of 60 mm. The optimized strategy used for data collection consisted of three phi and five omega scan sets, with 0.5° steps in phi or omega; completeness was 99.0%. A total of 2115 frames were collected. Final cell constants were obtained from the xyz centroids of 9788 reflections after integration.

From the systematic absences, the observed metric constants and intensity statistics, space group $P2_1/c$ was chosen initially; subsequent solution and refinement confirmed the correctness of this choice. The structure was solved using *SuperFlip*,[1] and refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* program.[2] All ordered non-hydrogen atoms were refined using anisotropic displacement parameters. The Fluorine ions on the PF_6 molecule are disordered. Occupancies of the major component (F(10)/F(20)/F(30)/F(40)/F(50)/F(60)) and minor component (F(11)/F(21)/F(31)/F(41)/F(51)/F(61)) were constrained to sum to 1.0; the major component occupancy refined to a value of 0.586(4). Disordered component atoms were refined by using isotropic displacement parameters. The U_{ij}'s of atoms C(63) and Cl(1) were refined using thermal similarity restraints (details appear in the CIF file). After location of H atoms on electron-density difference maps, the H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C---H in the range 0.93--0.98 Å and U_{iso} (H) in the range 1.2-1.5 times U_{eq} of the parent atom), after which the positions were refined

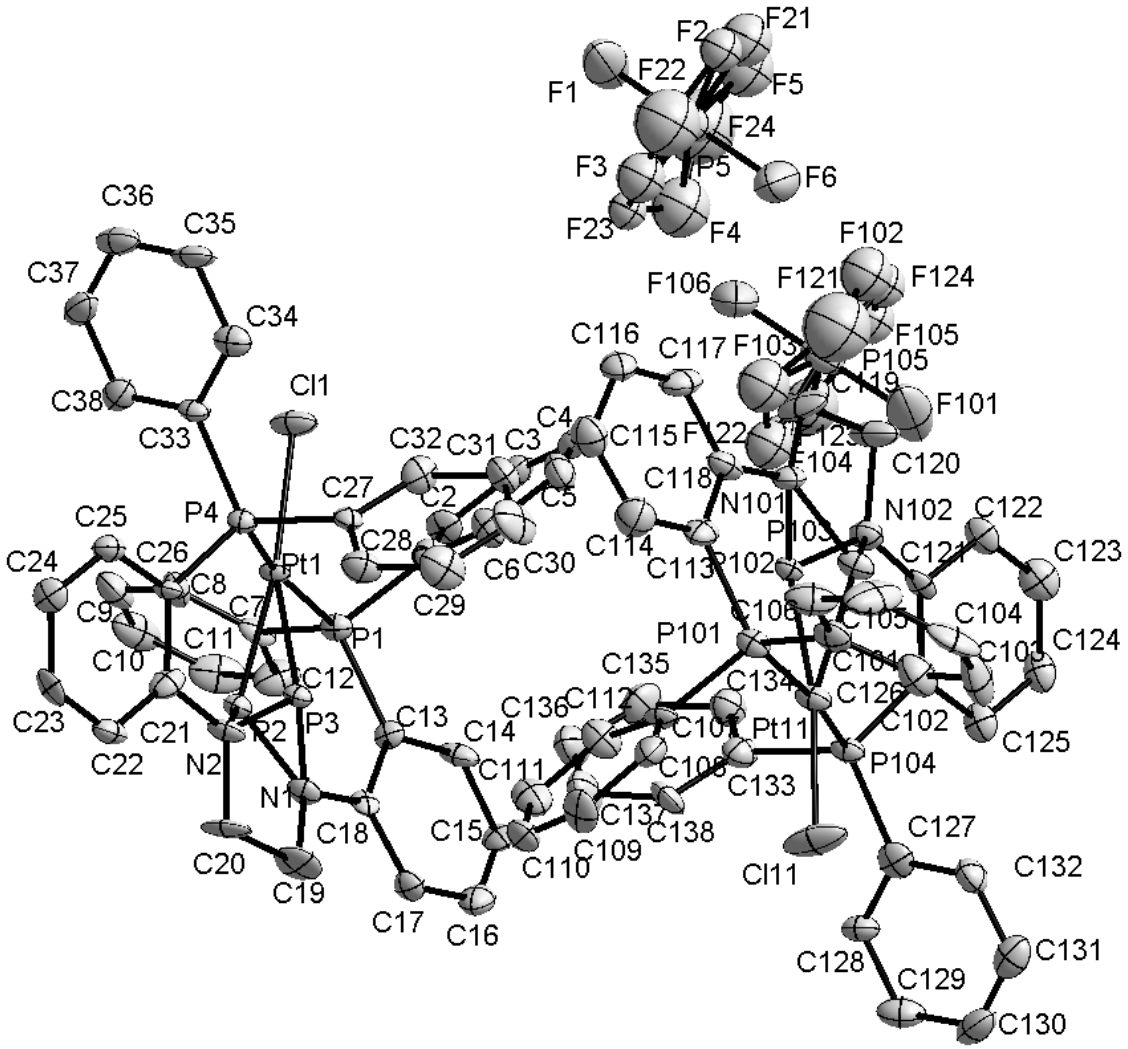
[1] Palatinus, L.; Chapuis, G.; *J. Appl. Cryst.* **2007**, 40, 786.

[2] Betteridge, P. W.; Carruthers, J. R.; Cooper, R. I.; Prout, K.; Watkin, D. J. *J. Appl. Cryst.* **2003**, *36*, 1487; Prout, C.K;. Pearce, L.J. CAMERON, Chemical Crystallography Laboratory, Oxford, UK, 1996.

with riding constraints.[3] The final least-squares refinement converged to R_1 = 0.0418 ($I > 2\sigma(I)$, 14355 data) and wR_2 = 0.1067 (F^2, 17579 data, 743 parameters). The final CIF is available as supporting material.

[3] Cooper, R. I.; Thompson, A. L.; Watkin, D. J. *J. Appl. Cryst.* **2010**, *43*, 1100–1107.

Figure S2 Fully-Labelled Elipsoid Representation of $\mathbf{6}^{\mathbf{PF6}}$.

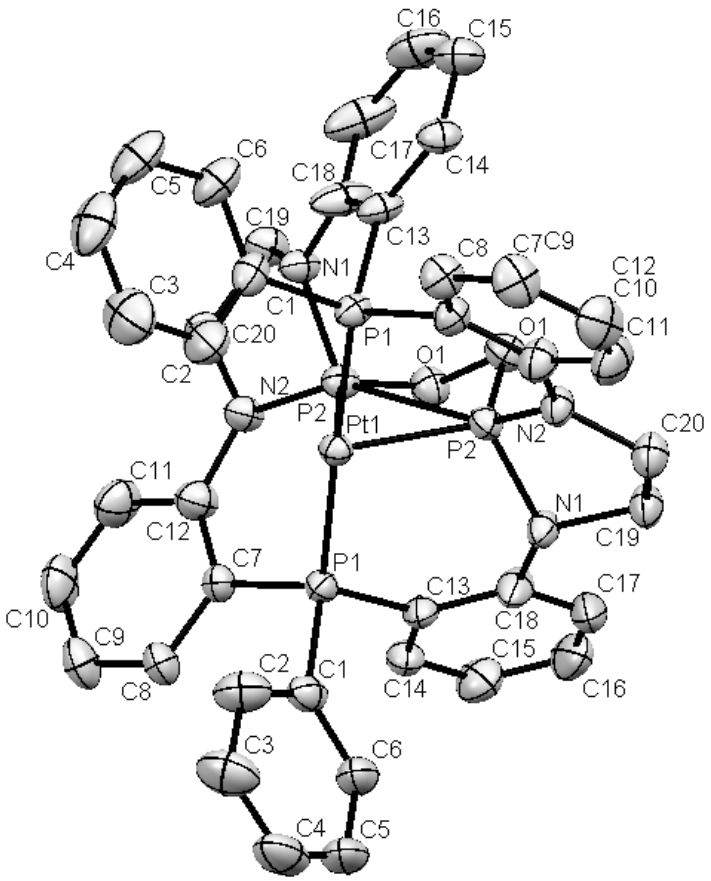


X-Ray data collection, solution, and refinement for $\mathbf{6}^{PF6}$. Data collection was carried out at 120K, using a frame time of 10 sec and a detector distance of 60 mm. The optimized strategy used for data collection consisted of five phi and two omega scan sets, with 0.5° steps in phi or omega; completeness was 99.6%. A total of 2081 frames were collected. Final cell constants were obtained from the xyz centroids of 9915 reflections after integration.

From the apparent systematic absences, the observed metric constants and intensity statistics, space group $P2_1/n$ (Z' = 1) was chosen initially; subsequent solution and refinement led to a disordered structure that converged, with modeling, to R_1 = 0.0756 and wR_2 = 0.1667. The presence of a dozen unexplainable peaks in the range 2.0-4.4 $e^-/Å^3$ as well as a large number of reflections for which I_{h0l} (h + l odd) was significant (282 out of 1113 with I/sigma(I) > 3.0) suggested that an attempt at solving the structure in $P2_1$ or $P2_1/m$ would be a worthy endeavor. Success was achieved only in $P2_1$ (Z' = 2), and the final refinement completed in that space group. The structure was solved using *Sir92*,**Error! Reference source not found.** and refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* program.**Error! Reference source not found.** The asymmetric unit contains two Pt-complex cations and two PF_6^- anions in a nearly centrosymmetric arrangement. The two cations were numbered in a similar fashion, with atoms in the second cation assigned numbers 100 greater than the counterpart atoms in the first cation; the anion pair was treated in a like fashion. In each cation the central P atoms were disordered. Occupancies were constrained to sum to 1.0. For atoms P(2) and P(3) bonded to Pt(1), the major occupancy [P(2)] refined to 0.940(5). For atoms P(102) and P(103) bonded to Pt(101), the major occupancy [P(102)] refined to 0.524(6). In each anion a set of four F atoms was disordered by an approximate rotation of 45º. The sum of major and minor components was constrained to sum to 1.0. For the fluorine set bonded to P(5), [major

atoms F(2, 3, 4, 5)/minor F(21, 22, 23, 24)], the major component occupancy refined to 0.615(10). For the fluorine set bonded to P(105), [major atoms F(102, 103, 104, 105)/minor F(121, 122, 123, 124)], the major component occupancy refined to 0.549(10). All ordered non-hydrogen atoms were refined using anisotropic displacement parameters. After location of H atoms on electron-density difference maps, the H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C---H in the range 0.93--0.98 Å and U_{iso} (H) in the range 1.2-1.5 times U_{eq} of the parent atom), after which the positions were refined with riding constraints.**Error! Reference source not found.** Flack parameter refinement led to a value of 0.500(7). Accordingly, the Flack parameter was reset to zero, and the structure was refined as an inversion twin, with the sum of the two components constrained to sum to 1.0 (twin law: 1 0 0 / 0 -1 0 / 0 0 1). The final result, 0.500(7), confirms the 1:1 twin ratio. The final least-squares refinement converged to R_1 = 0.0419 ($I > 2\sigma(I)$, 17543 data) and wR_2 = 0.0835 (F^2, 21159 data, 952 parameters). CheckCIF reported one Alert A and two Alert B items, related to the hypothesis that the true space group is in fact $P2_1/n$. The two molecules in the asymmetric unit are nearly related by an *n*-glide operation; however, it is apparent that the condition is inexact, as 25% of the data for which the condition I(*h0l*), *h*+*l* odd absent applies, has an I/sigma(I) value greater than 3.0. For these Alerts, the punch line is that if we have no *n* glide, we have no $\bar{1}$ either. Finally, it is important to point out that CheckCIF ignores disordered atoms in its assessment of missed symmetry. Here, it is the disordered atoms that validate the choice of $P2_1$. For example, the occupancies of the disordered central P atoms are 94/6 in one molecule and 52/48 in the other. The final CIF file, available as supporting material, contains validation reply form items which reiterates our treatment of this issue and adds some additional information.

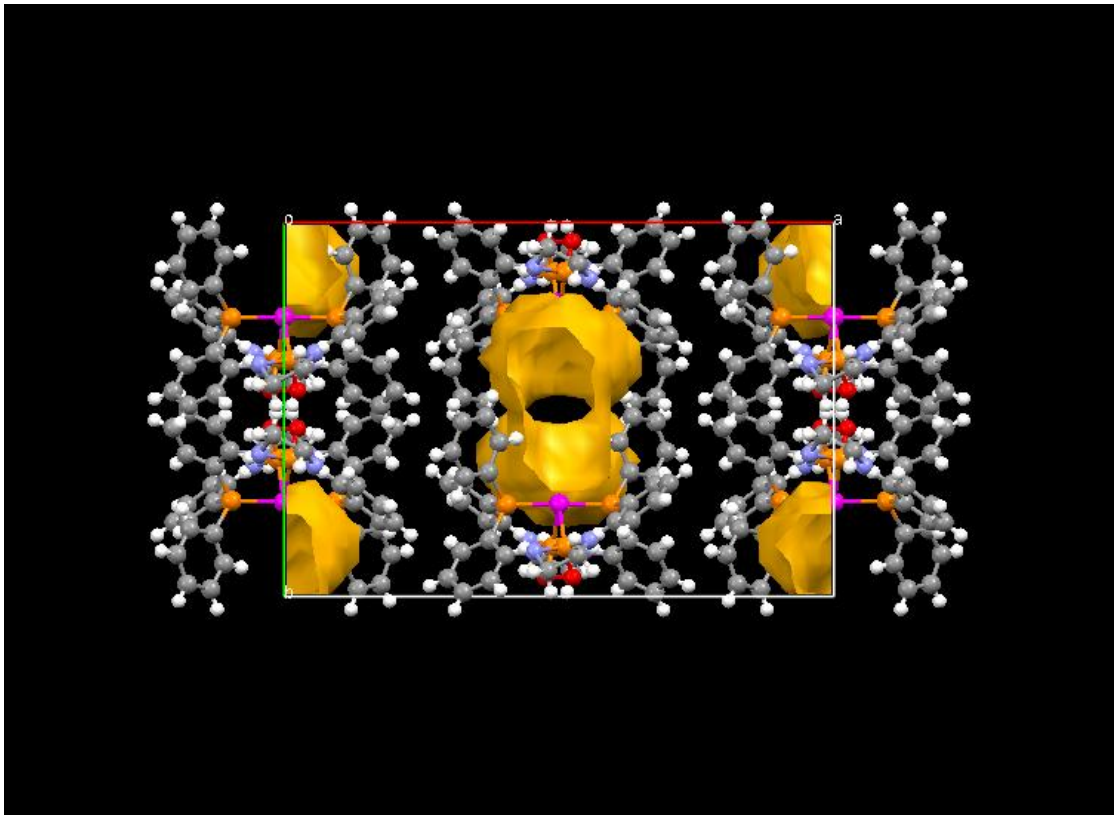
Figure S3 Fully-Labelled Elipsoid Representation of **7.**



X-Ray data collection, solution, and refinement for 7. Data collection was carried out at 120K, using a frame time of 10 sec and a detector distance of 60 mm. The optimized strategy used for data collection consisted of three phi and five omega scan sets, with 0.5° steps in phi or omega; completeness was 99.7%. A total of 2604 frames were collected. Final cell constants were obtained from the xyz centroids of 9905 reflections after integration.

From the systematic absences, the observed metric constants and intensity statistics, space group *C*2/*c* was chosen initially; subsequent solution and refinement confirmed the correctness of this choice. The structure was solved using *SIR-92*,1 and refined (full-matrix-least squares) using the Oxford University *Crystals for Windows* program.2 All non-hydrogen atoms were refined using anisotropic displacement parameters. After location of H atoms on electron-density difference maps, the H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C---H in the range 0.93--0.98 Å and U_{iso} (H) in the range 1.2-1.5 times U_{eq} of the parent atom), after which the positions were refined with riding constraints.3 The Pt(L)H complex is situated on a crystallographic 2 axis and is disordered. Minor disorder in the phenyl rings attached to P could not be resolved. The main result of the disorder is production of two distinct orientations for the $C_2H_4N_2P{=}O$ moiety [atoms C(19), H(191), H(192), C(20), H(201), H(202), N(1), N(2), P(2), O(1); occupancies fixed at 0.5, as required by symmetry]. The hydride ion, (presence verified by NMR), is also required to be disordered and could not be located. Attempts to solve and refine the structure as an undisordered molecule in space group *Cc* were unsuccessful; the results of the attempts in *Cc* simply reinforced the choice of *C*2/*c* as the correct space group. Finally, during the structure solution, electron density difference maps revealed that there were considerable disordered

solvent molecules, which could not be successfully modeled. From history, the remaining solvate was likely ether or THF in a volume of 553.9 Å^3 per unit cell (15.3%). It appeared that the cavity areas contained about four ether and/or THF molecules, located near the centers of symmetry at (0, 0, 0) and (½, ½ , 0) as shown in the *ab* projection below.[4] Modeling with or without restraints was unsuccessful, as



was step by step acquisition of peaks using successive electron density difference maps. Thus, the structure factors were modified using the PLATON SQUEEZE[5,6] technique, in order to produce a

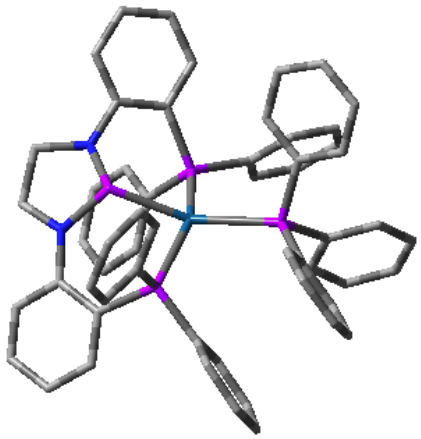
[4] Macrae, C. F; Bruno, I. J.; Chisholm, J. A.; Edgington, P. R.; McCabe, P.; Pidcock, E.; Rodriguez-Monge, L.; Taylor, R.; van de Streek, J.; Wood, P. A. *J. Appl. Cryst.*, **41**, 466-470, 2008

[5] (a) Spek, A. L. Acta Crystallogr., Sect A **1990**, A46, C34. (b) PLATON, A Multipurpose Crystallographic Tool, Utrecht University, Utrecht, The Netherlands, Spek, A. L. 1998

[6] v. d. Sluis, P.; Spek, A. Acta Crystallogr., Sect. A **1990**, A46, 194-201ss

"solvate-free" structure factor set. PLATON reported a total electron density of 174 e^- per unit cell, likely representing *ca.* four THF or ether molecules, consistent with our earlier observations. Use of the SQUEEZE technique resulted in a decrease of *ca*. 1.7 % in *R.* The final least-squares refinement converged to R_1 = 0.0242 ($I > 2\sigma(I)$, 4020 data) and wR_2 = 0.0605 (F^2, 5303 data, 231 parameters). The final CIF is available as supporting material.

XYZ Coordinates for Calculated Optimized Geometry of **1**.



Tag	Symbol	X	Y	Z
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4	P	0.966895	2.086166	0.178604
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6	N	-0.69746	-3.61222	0.456875
7	C	-3.04426	1.775505	-0.95486
8	C	-3.76905	1.793013	-2.16944
9	C	-4.24583	3.005927	-2.69967
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13	C	-3.45989	-0.03018	1.313358
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17	C	-4.21599	-1.51976	3.114128
18	C	-3.38131	-1.28229	1.99836
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22	C	-4.11348	-3.04896	-3.16421
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28	C	0.128615	-5.30708	-1.07692
29	C	1.039182	-5.80066	-2.01231
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32	C	1.436471	-3.24421	-0.83121
33	C	2.7658	-1.99433	1.44626
34	C	2.536437	-1.24179	2.619359
35	C	3.227309	-1.54184	3.806904
36	C	4.152335	-2.60227	3.837018
37	C	4.375897	-3.36843	2.675606
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40	C	4.466863	-0.82811	-1.01868
41	C	5.364227	-0.36898	-2.00125
42	C	4.894564	0.016635	-3.26976
43	C	3.51473	-0.04243	-3.55113
44	C	2.616787	-0.49724	-2.5723
45	C	2.815648	2.311761	0.213642
46	C	3.532838	1.991342	1.39201
47	C	4.922712	2.18191	1.460212
48	C	5.62317	2.692614	0.349775
49	C	4.9209	2.999385	-0.82952
50	C	3.528954	2.805838	-0.90145
51	C	0.477037	3.19814	-1.22435
52	C	0.548111	4.609009	-1.15789
53	C	0.239268	5.392034	-2.28321
54	C	-0.14039	4.778464	-3.49332
55	C	-0.21999	3.375814	-3.56707
56	C	0.083008	2.592479	-2.4385
57	C	0.48918	2.949375	1.759572
58	C	1.138675	4.133137	2.192792
59	C	0.756912	4.763567	3.388703
60	C	-0.27161	4.21873	4.18352
61	C	-0.90748	3.031692	3.776766
62	C	-0.52866	2.403557	2.57525
63	H	-3.97239	0.872039	-2.70472
64	H	-4.80419	2.998528	-3.63222
65	H	-4.38251	5.153388	-2.43396
66	H	-3.0792	5.141703	-0.29887
67	H	-2.22637	3.027925	0.629969
68	H	-4.44156	1.901987	1.276498
69	H	-5.85616	1.479813	3.254302
70	H	-5.74148	-0.73321	4.425111

71	H	-4.15751	-2.4721	3.633783
72	H	-5.16019	-0.96097	-0.66379
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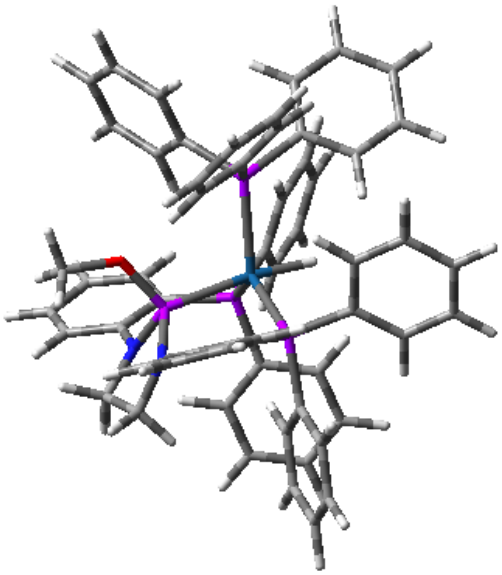
74	H	-4.50202	-3.79089	-3.85727
75	H	-2.06825	-3.21276	-3.86678
76	H	-1.18264	-1.52337	-2.27163
77	H	-3.90618	-3.87422	1.37815
78	H	-2.66821	-4.1173	2.634902
79	H	-2.44015	-4.49727	-0.37873
80	H	-1.7064	-5.4412	0.946255
81	H	-0.72118	-5.92688	-0.82359
82	H	0.873509	-6.7816	-2.45056
83	H	2.880069	-5.40553	-3.10447
84	H	3.201474	-3.195	-2.08913
85	H	1.799548	-0.44429	2.614545
86	H	3.03452	-0.96033	4.704846
87	H	4.682321	-2.83863	4.756189
88	H	5.077445	-4.19824	2.696302
89	H	3.851139	-3.68809	0.609663
90	H	4.847718	-1.1201	-0.04552
91	H	6.425279	-0.31606	-1.77258
92	H	5.591797	0.360749	-4.02933
93	H	3.1435	0.256979	-4.52786
94	H	1.555813	-0.55679	-2.80465
95	H	3.010737	1.622948	2.27007
96	H	5.453033	1.94291	2.37861
97	H	6.696691	2.853995	0.406678
98	H	5.449893	3.39405	-1.69329
99	H	3.00907	3.058646	-1.81969
100	H	0.839298	5.105852	-0.23844
101	H	0.298674	6.475492	-2.21687
102	H	-0.37561	5.386252	-4.36337
103	H	-0.52418	2.89417	-4.49287
104	H	0.001508	1.509842	-2.49827
105	H	1.965053	4.54737	1.622543
106	H	1.266764	5.670384	3.703867
107	H	-0.56173	4.705673	5.110968
108	H	-1.68989	2.591084	4.389265
109	H	-1.015	1.47628	2.285674
110	Pt	-0.10767	-0.22533	0.167257

XYZ Coordinates for Calculated Optimized Geometry of **5**.



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5	P	-2.47571	0.117809	-0.46765
6	O	0.207905	0.386688	3.101872
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8	N	0.412431	-2.20209	2.361701
9	C	-3.13631	1.472283	-1.55349
10	C	-4.44411	1.406059	-2.09753
11	C	-4.92555	2.435953	-2.92234
12	C	-4.11073	3.547547	-3.21885
13	C	-2.80895	3.615734	-2.69103
14	C	-2.32522	2.583258	-1.86596
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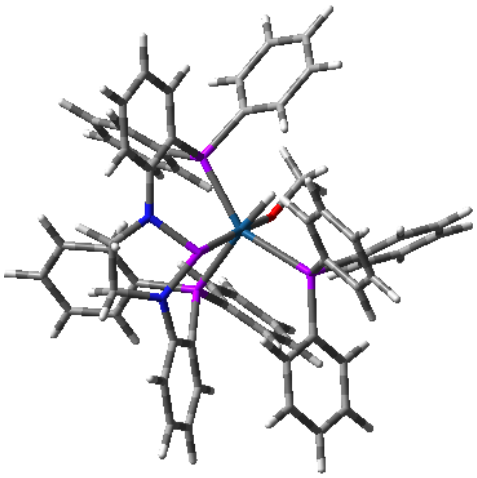
21	C	-3.37066	0.323148	1.164738
22	C	-4.47555	1.202734	1.248923
23	C	-5.25713	1.311731	2.411492
24	C	-4.94621	0.520084	3.529319

25	C	-3.83065	-0.32979	3.489236
26	C	-3.02139	-0.42626	2.333741
27	C	-1.82514	-2.49597	3.230758
28	C	-0.54851	-3.25445	2.804514
29	C	1.814008	-2.48256	2.171299
30	C	2.560652	-2.91643	3.286334
31	C	3.925875	-3.22214	3.169416
32	C	4.564454	-3.07141	1.925619
33	C	3.830142	-2.63234	0.811058
34	C	2.450681	-2.34021	0.902691
35	C	0.720673	-3.58935	-0.94599
36	C	-0.67247	-3.79096	-0.93941
37	C	-1.20963	-5.07875	-1.13885
38	C	-0.35515	-6.17603	-1.34378
39	C	1.042518	-5.98239	-1.34785
40	C	1.577985	-4.70054	-1.14648
41	C	2.642331	-1.63035	-1.97104
42	C	2.469863	-2.25556	-3.22758
43	C	3.326507	-1.94879	-4.30107
44	C	4.366637	-1.01525	-4.13583
45	C	4.537462	-0.38043	-2.88977
46	C	3.677614	-0.6766	-1.81832
47	C	2.977231	2.031994	0.61239
48	C	4.035019	2.651907	-0.09156
49	C	5.364389	2.521593	0.355908
50	C	5.654617	1.776059	1.51358
51	C	4.604382	1.161186	2.224531
52	C	3.27763	1.28494	1.778069
53	C	1.30155	3.199277	-1.46123
54	C	1.641516	2.567183	-2.68219
55	C	1.751493	3.312728	-3.86836
56	C	1.510916	4.701353	-3.85861
57	C	1.164244	5.336978	-2.65189
58	C	1.06463	4.593562	-1.45978
59	C	0.501925	3.337924	1.347388
60	C	1.327208	4.243542	2.055312
61	C	0.769616	5.148416	2.976949
62	C	-0.62065	5.166784	3.201273
63	C	-1.44837	4.267209	2.502717
64	C	-0.88972	3.357381	1.587855
65	C	0.10706	0.213096	4.560985
66	H	0.010807	0.305719	-1.81581
67	H	-5.08058	0.548999	-1.89586

68	H	-5.92862	2.368691	-3.33573
69	H	-4.48383	4.3416	-3.86066
70	H	-2.16395	4.458611	-2.92402
71	H	-1.31001	2.636627	-1.49251
72	H	-4.52695	-1.91875	0.505465
73	H	-5.62919	-3.82529	-0.62396
74	H	-5.10619	-4.3522	-3.01141
75	H	-3.43412	-2.96139	-4.24717
76	H	-2.30197	-1.0724	-3.1161
77	H	-4.74497	1.804986	0.388647
78	H	-6.10388	1.99165	2.431835
79	H	-5.5518	0.573493	4.430107
80	H	-3.58094	-0.91482	4.369425
81	H	-2.7224	-3.09842	3.057161
82	H	-1.77933	-2.24411	4.301095
83	H	-0.75699	-3.94413	1.976656
84	H	-0.13919	-3.82915	3.642294
85	H	2.064038	-3.01004	4.249471
86	H	4.482728	-3.56434	4.037604
87	H	5.621474	-3.29887	1.818754
88	H	4.339302	-2.53588	-0.14222
89	H	-1.33488	-2.94786	-0.78581
90	H	-2.28762	-5.21389	-1.14011
91	H	-0.76763	-7.16972	-1.49963
92	H	1.709508	-6.82633	-1.50437
93	H	2.657203	-4.57194	-1.14462
94	H	1.676052	-2.98132	-3.37702
95	H	3.181796	-2.44125	-5.25925
96	H	5.032679	-0.78503	-4.96338
97	H	5.334195	0.345759	-2.75054
98	H	3.818957	-0.16183	-0.87286
99	H	3.832321	3.238738	-0.98171
100	H	6.16514	3.009724	-0.19424
101	H	6.680536	1.679023	1.859631
102	H	4.817734	0.586323	3.122325
103	H	2.476418	0.817889	2.343565
104	H	1.816039	1.495168	-2.71094
105	H	2.017282	2.81123	-4.79539
106	H	1.590815	5.276766	-4.77745
107	H	0.977936	6.407929	-2.63244
108	H	0.803151	5.105361	-0.53888
109	H	2.401962	4.24384	1.89884
110	H	1.418305	5.836514	3.513247

111	H	-1.05098	5.868787	3.911185
112	H	-2.52241	4.268707	2.671326
113	H	-1.54006	2.659588	1.070766
114	H	0.683202	1.028702	5.002225
115	H	-0.93938	0.291103	4.874869
116	H	0.529712	-0.75213	4.864854

XYZ Coordinates for Calculated Optimized Geometry of $[(PPP)Pt(PPh_3)(MeO)(H)]^+$.



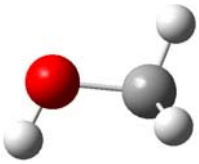
Tag	Symbol	X	Y	Z
1	Pt	-0.07062	-0.41847	0.029938
2	P	-0.12755	0.056181	-2.36455
3	P	0.188838	2.062038	0.433705
4	P	2.338177	-1.20043	-0.12436
5	P	-2.4031	-1.02593	0.11365
6	N	-1.84879	0.266236	-2.8002
7	N	0.077341	1.789995	-2.60535
8	C	-2.6215	-2.64278	1.006732
9	C	-3.54879	-2.76917	2.064953
10	C	-3.75264	-4.01338	2.691276
11	C	-3.03824	-5.14787	2.267683
12	C	-2.11727	-5.03151	1.207277
13	C	-1.91076	-3.79033	0.584463
14	C	-3.51804	0.124368	1.018404
15	C	-4.83269	0.402653	0.583097
16	C	-5.66302	1.237596	1.352965
17	C	-5.18942	1.789601	2.558824
18	C	-3.87755	1.510505	2.990979
19	C	-3.03572	0.685506	2.225165
20	C	-3.18945	-1.40077	-1.52221
21	C	-4.23366	-2.35941	-1.53683
22	C	-4.95134	-2.66102	-2.70349
23	C	-4.62188	-1.99804	-3.89881
24	C	-3.58325	-1.05815	-3.91527
25	C	-2.84882	-0.73716	-2.74241
26	C	-1.92019	1.278424	-3.88848
27	C	-0.96129	2.411191	-3.4773

28	C	1.145006	2.628242	-2.15517
29	C	1.920348	3.328093	-3.10683
30	C	2.895223	4.253361	-2.70413
31	C	3.116895	4.480521	-1.33383
32	C	2.359599	3.781872	-0.37873
33	C	1.369983	2.852459	-0.76653
34	C	-1.23045	3.249888	0.251094
35	C	-2.41184	2.882412	-0.42164
36	C	-3.44215	3.820806	-0.62045
37	C	-3.29783	5.141088	-0.1593
38	C	-2.11091	5.521665	0.499106
39	C	-1.08352	4.586014	0.699554
40	C	0.859138	2.406476	2.119667
41	C	-0.01305	2.783122	3.165792
42	C	0.473221	2.966519	4.471357
43	C	1.837446	2.770797	4.756129
44	C	2.710106	2.380945	3.722746
45	C	2.223852	2.19146	2.417565
46	C	3.754361	-0.03692	-0.42251
47	C	4.759722	0.205855	0.540756
48	C	5.855959	1.033043	0.231413
49	C	5.962879	1.624432	-1.0403
50	C	4.963663	1.386443	-2.00408
51	C	3.865727	0.567424	-1.69814
52	C	2.814548	-2.12457	1.400848
53	C	2.789607	-1.44924	2.644149
54	C	3.214877	-2.10505	3.811422
55	C	3.649152	-3.44368	3.759294
56	C	3.649764	-4.12761	2.529222
57	C	3.238948	-3.47306	1.353701
58	C	2.586633	-2.42283	-1.5061
59	C	3.909782	-2.74324	-1.90551
60	C	4.146193	-3.71152	-2.89499
61	C	3.067466	-4.3779	-3.50906
62	C	1.751782	-4.06501	-3.12423
63	C	1.5147	-3.09536	-2.1323
64	H	-4.11263	-1.90952	2.410411
65	H	-4.46693	-4.08974	3.506796
66	H	-3.19542	-6.10755	2.752903
67	H	-1.56174	-5.90197	0.868475
68	H	-1.19975	-3.73082	-0.2354
69	H	-5.21187	-0.02401	-0.3411
70	H	-6.6744	1.449048	1.015661

71	H	-5.83515	2.429748	3.154633
72	H	-3.51277	1.932615	3.924278
73	H	-2.01374	0.473421	2.543568
74	H	-4.49581	-2.87911	-0.62117
75	H	-5.74811	-3.39811	-2.67611
76	H	-5.15984	-2.21959	-4.81698
77	H	-3.32839	-0.57655	-4.85309
78	H	-2.94685	1.646239	-3.98593
79	H	-1.61204	0.856724	-4.85926
80	H	-1.48603	3.196025	-2.91945
81	H	-0.51352	2.866165	-4.36874
82	H	1.748733	3.145263	-4.16464
83	H	3.472528	4.792361	-3.45092
84	H	3.862729	5.200431	-1.00846
85	H	2.526338	3.991782	0.672171
86	H	-2.5277	1.877169	-0.80731
87	H	-4.3533	3.516701	-1.12958
88	H	-4.09409	5.865211	-0.31174
89	H	-1.98485	6.542026	0.851723
90	H	-0.1739	4.90261	1.202133
91	H	-1.06872	2.942412	2.97009
92	H	-0.21103	3.261936	5.262727
93	H	2.213974	2.920406	5.7648
94	H	3.766468	2.226605	3.929632
95	H	2.917068	1.883096	1.641496
96	H	4.715592	-0.26881	1.514964
97	H	6.628493	1.198075	0.978096
98	H	6.815493	2.253934	-1.2814
99	H	5.039082	1.833708	-2.99107
100	H	3.1206	0.374845	-2.46557
101	H	2.385213	-0.44596	2.708441
102	H	3.191054	-1.57533	4.760331
103	H	3.972806	-3.94947	4.665474
104	H	3.972304	-5.16439	2.47996
105	H	3.257275	-4.01676	0.415106
106	H	4.757919	-2.24391	-1.44716
107	H	5.167878	-3.94473	-3.18283
108	H	3.251195	-5.12455	-4.27721
109	H	0.910281	-4.56442	-3.59733
110	H	0.490239	-2.86387	-1.86347
111	H	-0.09851	-1.99178	-0.20228
112	O	-0.03667	-0.4932	2.240479
113	C	-0.28539	-1.64776	3.07586

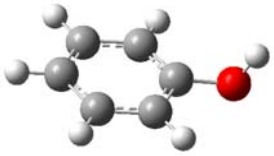
114	H	0.274165	-1.52457	4.016059
115	H	-1.35126	-1.74966	3.336113
116	H	0.04125	-2.59505	2.618097

XYZ Coordinates for Calculated Optimized Geometry of MeOH.



Tag	Symbol	X	Y	Z
1	C	0.687346	-0.02177	0.000003
2	H	1.088605	0.994617	-0.00111
3	H	1.052174	-0.54681	-0.89657
4	H	1.052296	-0.54491	0.897636
5	O	-0.76437	0.122619	0.000001
6	H	-1.20223	-0.75325	0.000024

XYZ Coordinates for Calculated Optimized Geometry of PhOH.

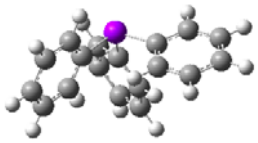


Tag	Symbol	X	Y	Z
1	C	-1.16858	1.218919	0.005298
2	C	0.239288	1.223193	-0.01241
3	C	0.933549	-5.4E-05	-0.01204
4	C	0.239171	-1.22325	-0.01231
5	C	-1.16868	-1.21886	0.005329
6	C	-1.8754	0.000073	0.017944
7	H	-1.70976	2.162225	0.003928
8	H	0.801035	2.153014	-0.03868
9	H	0.800925	-2.15306	-0.03846
10	H	-1.70997	-2.1621	0.004015
11	H	-2.96249	0.0001	0.029422
12	O	2.351903	-0.00026	-0.08866
13	H	2.768901	0.001762	0.798144

XYZ Coordinates for Calculated Optimized Geometry of PhSH.

Tag	Symbol	X	Y	Z
1	C	-1.62265	1.218858	0.004307
2	C	-0.21359	1.221324	-0.00842
3	C	0.48642	-1E-06	-0.00595
4	C	-0.2136	-1.22132	-0.00833
5	C	-1.62265	-1.21885	0.004347
6	C	-2.32836	0.000005	0.012284
7	H	-2.16209	2.162929	0.003986
8	H	0.335839	2.158219	-0.02386
9	H	0.335843	-2.15821	-0.02362
10	H	-2.1621	-2.16292	0.004073
11	H	-3.41576	0.000005	0.020129
12	S	2.349063	-8.1E-05	-0.07847
13	H	2.569819	0.001217	1.285388

XYZ Coordinates for Calculated Optimized Geometry of PPh_3



Tag	Symbol	X	Y	Z
1	P	-3.7E-05	-0.01737	-1.26603
2	C	-0.09354	1.662577	-0.46994
3	C	-1.05684	1.992616	0.510813
4	C	-1.08053	3.278779	1.084972
5	C	-0.14078	4.249752	0.6921
6	C	0.827015	3.925628	-0.27992
7	C	0.850306	2.645115	-0.85842
8	C	-1.41075	-0.93267	-0.47148
9	C	-2.71924	-0.73999	-0.97803
10	C	-3.81691	-1.3953	-0.39441
11	C	-3.6254	-2.26527	0.697712
12	C	-2.32786	-2.46968	1.202674
13	C	-1.22783	-1.8051	0.626501

14	C	1.506906	-0.74808	-0.45858
15	C	1.970888	-0.29315	0.798457
16	C	3.089072	-0.89166	1.407199
17	C	3.757114	-1.95703	0.773
18	C	3.303202	-2.41388	-0.47903
19	C	2.190686	-1.80992	-1.0909
20	H	-1.78511	1.256003	0.834604
21	H	-1.8246	3.513882	1.842086
22	H	-0.15812	5.240835	1.138341
23	H	1.559891	4.667501	-0.58739
24	H	1.610555	2.404274	-1.5959
25	H	-2.88342	-0.08428	-1.82867
26	H	-4.81453	-1.23225	-0.79406
27	H	-4.47411	-2.77615	1.145414
28	H	-2.16866	-3.13742	2.045764
29	H	-0.23663	-1.97164	1.03659
30	H	1.471494	0.528801	1.303019
31	H	3.433028	-0.52896	2.372616
32	H	4.619065	-2.42117	1.245847
33	H	3.813932	-3.23224	-0.98048
34	H	1.86464	-2.16307	-2.06363

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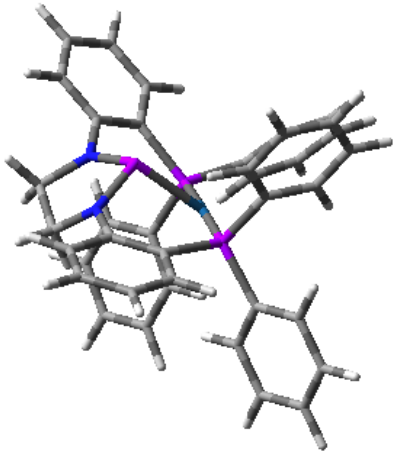
XYZ Coordinates for Calculated Optimized Geometry of $[(PPP)Pt]^{+}$.

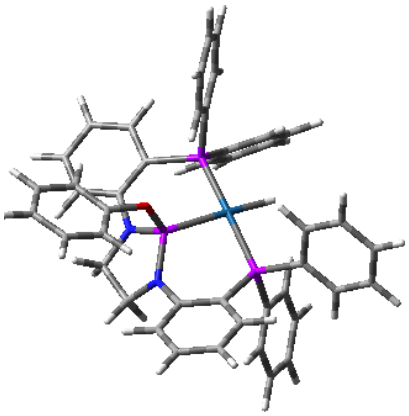


Tag	Symbol	X	Y	Z
1	Pt	0.029538	-0.30191	-0.0354
2	P	-2.32146	-0.3614	0.040819
3	P	0.141119	1.692984	-1.21788
4	P	2.378669	-0.27242	0.008439
5	N	-1.33557	2.48509	-0.81439
6	N	1.022715	2.750569	-0.18225
7	C	-3.03121	-2.01915	-0.33933
8	C	-4.13533	-2.55097	0.365361
9	C	-4.63883	-3.82231	0.032334
10	C	-4.05069	-4.56816	-1.00694
11	C	-2.94879	-4.0427	-1.71126
12	C	-2.43594	-2.77795	-1.37637
13	C	-3.14281	0.80768	-1.14443
14	C	-4.35397	0.453811	-1.7816
15	C	-5.03325	1.364975	-2.60861
16	C	-4.50375	2.652594	-2.81459
17	C	-3.2845	3.010997	-2.21666
18	C	-2.59339	2.101142	-1.38977
19	C	-2.99023	0.112414	1.696102
20	C	-4.12193	0.944463	1.854006
21	C	-4.59867	1.256282	3.141539
22	C	-3.95626	0.736918	4.281242
23	C	-2.82788	-0.09407	4.130545
24	C	-2.34368	-0.39974	2.847179
25	C	-1.18867	3.719011	0.008336
26	C	0.153251	3.548683	0.743275

27	C	2.43121	2.651805	0.063405
28	C	3.144715	3.864973	0.234914
29	C	4.520866	3.875518	0.485552
30	C	5.229899	2.659597	0.560898
31	C	4.540973	1.45426	0.38686
32	C	3.142143	1.41415	0.143022
33	C	3.070579	-1.02255	-1.52844
34	C	2.758077	-2.37842	-1.80082
35	C	3.205647	-2.98634	-2.98475
36	C	3.958618	-2.24693	-3.91988
37	C	4.262285	-0.89853	-3.66021
38	C	3.823328	-0.28705	-2.47
39	C	3.096145	-1.22554	1.416534
40	C	4.219833	-2.07247	1.280382
41	C	4.734054	-2.74891	2.401556
42	C	4.136278	-2.58505	3.665774
43	C	3.014253	-1.74453	3.806578
44	C	2.492546	-1.07273	2.688006
45	H	-4.59656	-1.98894	1.17277
46	H	-5.48467	-4.22633	0.582157
47	H	-4.44214	-5.54948	-1.26187
48	H	-2.48923	-4.61741	-2.51096
49	H	-1.57559	-2.38472	-1.91457
50	H	-4.77605	-0.53491	-1.62713
51	H	-5.96539	1.072339	-3.08313
52	H	-5.0227	3.363315	-3.45182
53	H	-2.85227	3.990048	-2.40737
54	H	-4.6346	1.348443	0.98564
55	H	-5.47011	1.896436	3.251414
56	H	-4.32881	0.975687	5.273915
57	H	-2.32886	-0.49912	5.006963
58	H	-1.4668	-1.03555	2.741189
59	H	-2.02158	3.801021	0.714828
60	H	-1.17616	4.615402	-0.62791
61	H	0.02043	2.994921	1.683876
62	H	0.605732	4.516993	0.968814
63	H	2.611743	4.806519	0.13941
64	H	5.039857	4.822365	0.606987
65	H	6.29897	2.653849	0.751012
66	H	5.095028	0.522271	0.459074
67	H	2.167981	-2.95929	-1.09457
68	H	2.966565	-4.02854	-3.17932
69	H	4.300958	-2.71707	-4.83795

70	H	4.839819	-0.32163	-4.37758
71	H	4.072425	0.753896	-2.28728
72	H	4.689563	-2.21448	0.311011
73	H	5.59718	-3.3993	2.287331
74	H	4.537199	-3.1081	4.529959
75	H	2.54837	-1.61701	4.780189
76	H	1.621068	-0.43078	2.803172

XYZ Coordinates for Calculated Optimized Geometry of $[(PP(OPh)P)Pt(H)]^{+}$.

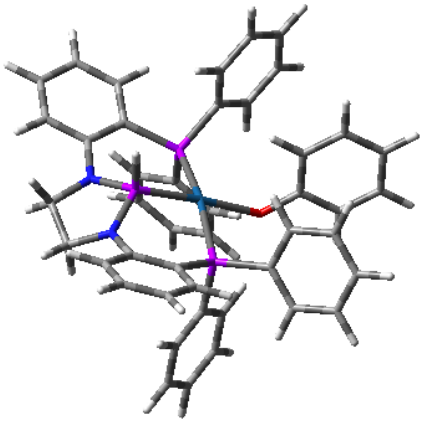


Tag	Symbol	X	Y	Z
1	Pt	-0.15685	-0.76058	0.28226
2	P	0.178805	1.400853	-0.37916
3	P	-2.49165	-0.50086	0.139655
4	P	2.140355	-1.19166	0.111792
5	O	0.661737	2.418266	0.856043
6	N	1.259281	1.56776	-1.69142
7	N	-1.09995	2.135969	-1.22119
8	C	2.977828	-1.16039	1.756862
9	C	4.020199	-2.05044	2.103154
10	C	4.64493	-1.95183	3.359519
11	C	4.240703	-0.96359	4.277156
12	C	3.202531	-0.07462	3.93596
13	C	2.569446	-0.17227	2.684895
14	C	2.480817	-2.84612	-0.6345
15	C	2.950057	-2.99621	-1.95758
16	C	3.105173	-4.28032	-2.51395
17	C	2.795791	-5.42393	-1.75625
18	C	2.318434	-5.27917	-0.43731
19	C	2.152357	-4.00046	0.11764
20	C	3.114987	0.012931	-0.92835
21	C	4.507175	-0.26034	-0.97016
22	C	5.404419	0.487368	-1.74125
23	C	4.908539	1.558596	-2.50447
24	C	3.546063	1.876442	-2.46247
25	C	2.623201	1.132869	-1.67901
26	C	0.770984	2.5388	-2.71761
27	C	-0.77148	2.536258	-2.6199
28	C	-2.41578	2.301021	-0.6611

29	C	-3.02533	3.569529	-0.78599
30	C	-4.29341	3.8271	-0.24516
31	C	-4.96492	2.817733	0.467055
32	C	-4.36906	1.553822	0.60018
33	C	-3.10782	1.255609	0.028061
34	C	-3.12678	-1.29876	-1.40022
35	C	-2.59641	-2.55584	-1.78095
36	C	-3.08203	-3.21248	-2.92472
37	C	-4.09231	-2.62051	-3.70832
38	C	-4.61661	-1.36709	-3.34028
39	C	-4.13968	-0.70826	-2.19183
40	C	-3.41446	-1.25143	1.543443
41	C	-4.62586	-1.95528	1.358728
42	C	-5.29114	-2.51476	2.465413
43	C	-4.7579	-2.36973	3.760328
44	C	-3.54796	-1.67166	3.947373
45	C	-2.87408	-1.12064	2.844394
46	C	0.996479	3.80692	0.761378
47	C	2.316657	4.173478	0.453374
48	C	2.652765	5.54036	0.432933
49	C	1.679895	6.517726	0.721832
50	C	0.364444	6.125638	1.040527
51	C	0.013395	4.762672	1.062043
52	H	-0.40454	-2.32624	0.633538
53	H	4.339222	-2.82558	1.411767
54	H	5.44177	-2.64386	3.619002
55	H	4.725568	-0.88943	5.247083
56	H	2.884522	0.68867	4.641206
57	H	1.76694	0.518128	2.435884
58	H	3.196862	-2.12647	-2.55856
59	H	3.467059	-4.38221	-3.53362
60	H	2.920512	-6.41464	-2.18545
61	H	2.071889	-6.15762	0.153201
62	H	1.757848	-3.90573	1.126412
63	H	4.898629	-1.08935	-0.38756
64	H	6.460944	0.238277	-1.74711
65	H	5.578109	2.155564	-3.11789
66	H	3.19966	2.729679	-3.0335
67	H	1.092668	2.219148	-3.71348
68	H	1.168815	3.544075	-2.52253
69	H	-1.21224	1.813801	-3.31901
70	H	-1.16541	3.529602	-2.85402
71	H	-2.48808	4.366755	-1.29158

72	H	-4.73954	4.811276	-0.35961
73	H	-5.9372	3.007529	0.912013
74	H	-4.90016	0.784857	1.152129
75	H	-1.80793	-3.01552	-1.19153
76	H	-2.66998	-4.17828	-3.20474
77	H	-4.46376	-3.12855	-4.59447
78	H	-5.39581	-0.90407	-3.9401
79	H	-4.56	0.256393	-1.92339
80	H	-5.04399	-2.08199	0.363778
81	H	-6.218	-3.06198	2.315455
82	H	-5.27388	-2.80271	4.613318
83	H	-3.12759	-1.56705	4.94399
84	H	-1.92751	-0.60541	2.99357
85	H	3.065046	3.410297	0.261295
86	H	3.673035	5.83756	0.205333
87	H	1.946713	7.570855	0.712156
88	H	-0.38377	6.875949	1.282102
89	H	-0.98959	4.443402	1.328987

XYZ Coordinates for Calculated Optimized Geometry of $[(PP(H)P)Pt(OPh)]^{+}$.

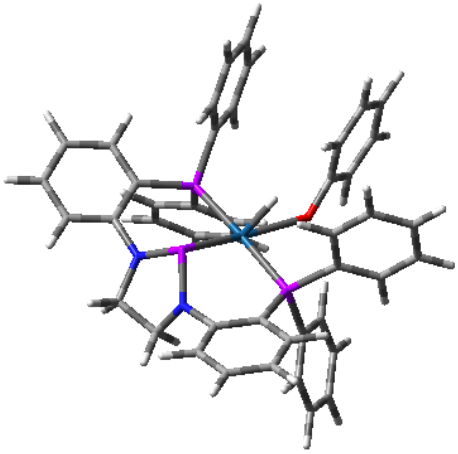


Tag	Symbol	X	Y	Z
1	Pt	0.005459	-0.00697	-0.23853
2	P	0.02415	-1.99763	-1.1896
3	P	-2.37423	-0.1502	-0.0003
4	P	2.37958	-0.09804	0.0197
5	N	1.2215	-3.10748	-0.6757
6	N	-1.26538	-3.05707	-0.85826
7	C	3.259772	1.328155	-0.74152
8	C	3.822763	2.357786	0.041391
9	C	4.440345	3.457861	-0.58281
10	C	4.50185	3.536836	-1.98525
11	C	3.940195	2.508973	-2.77039
12	C	3.317135	1.413395	-2.15389
13	C	2.782071	-0.12054	1.821511
14	C	3.735029	-1.0159	2.361626
15	C	4.0308	-0.98674	3.736185
16	C	3.383441	-0.06649	4.582044
17	C	2.428244	0.820255	4.048125
18	C	2.118346	0.79445	2.677184
19	C	3.229252	-1.59533	-0.67764
20	C	4.618963	-1.46943	-0.92645
21	C	5.411069	-2.55935	-1.3147
22	C	4.811653	-3.8221	-1.45886
23	C	3.434869	-3.97463	-1.24213
24	C	2.622523	-2.87949	-0.86039
25	C	0.664673	-4.4886	-0.57
26	C	-0.82135	-4.31452	-0.18792
27	C	-2.62267	-2.76777	-1.2237

28	C	-3.37089	-3.76733	-1.88274
29	C	-4.69196	-3.53082	-2.29223
30	C	-5.27753	-2.2709	-2.07376
31	C	-4.53982	-1.26746	-1.42561
32	C	-3.21739	-1.49248	-0.97314
33	C	-2.67656	-0.58843	1.763675
34	C	-2.01478	0.173034	2.759453
35	C	-2.22841	-0.11802	4.117491
36	C	-3.09047	-1.16687	4.495538
37	C	-3.74421	-1.9266	3.507075
38	C	-3.54052	-1.64046	2.144397
39	C	-3.31592	1.38369	-0.3531
40	C	-4.31128	1.857362	0.531664
41	C	-5.03093	3.024206	0.218404
42	C	-4.76398	3.722537	-0.97473
43	C	-3.76918	3.254597	-1.85501
44	C	-3.04411	2.092278	-1.54558
45	C	-0.08412	3.061857	0.138637
46	C	-0.38606	4.198056	0.929114
47	C	-0.37575	5.481085	0.357765
48	C	-0.06856	5.659394	-1.00766
49	C	0.22868	4.530348	-1.79412
50	C	0.221059	3.24147	-1.23118
51	H	3.787767	2.311577	1.12526
52	H	4.86745	4.248713	0.027578
53	H	4.979157	4.388155	-2.46317
54	H	3.986991	2.563642	-3.85484
55	H	2.888915	0.627033	-2.77271
56	H	4.247627	-1.7324	1.728316
57	H	4.765207	-1.6779	4.141275
58	H	3.618191	-0.043	5.643158
59	H	1.923549	1.531547	4.697015
60	H	1.362334	1.462437	2.270786
61	H	5.091171	-0.49917	-0.80565
62	H	6.473161	-2.42383	-1.49354
63	H	5.406029	-4.68336	-1.75161
64	H	2.991147	-4.95334	-1.38546
65	H	1.207398	-5.04557	0.200066
66	H	0.751533	-5.02739	-1.52598
67	H	-0.94181	-4.22451	0.899514
68	H	-1.40815	-5.1699	-0.53322
69	H	-2.90876	-4.72709	-2.09643
70	H	-5.24874	-4.31593	-2.79641

71	H	-6.29276	-2.06949	-2.40206
72	H	-5.00357	-0.30063	-1.25881
73	H	-1.34686	0.979832	2.46601
74	H	-1.72255	0.470468	4.878456
75	H	-3.25136	-1.38822	5.547517
76	H	-4.41366	-2.73382	3.792647
77	H	-4.06001	-2.23009	1.394727
78	H	-4.52103	1.333077	1.459524
79	H	-5.79131	3.386776	0.904882
80	H	-5.31734	4.627495	-1.21134
81	H	-3.54552	3.801462	-2.76656
82	H	-2.26408	1.753028	-2.22206
83	H	-0.62735	4.056273	1.979548
84	H	-0.6096	6.34317	0.978893
85	H	-0.0596	6.654325	-1.44459
86	H	0.473791	4.651124	-2.84754
87	H	0.459475	2.373844	-1.84313
88	H	0.098777	-1.96151	-2.62437
89	O	-0.08807	1.827754	0.762451

XYZ Coordinates for Calculated Optimized Geometry of transition state prior to $[(PP(H)P)Pt(OPh)]^{+}$.



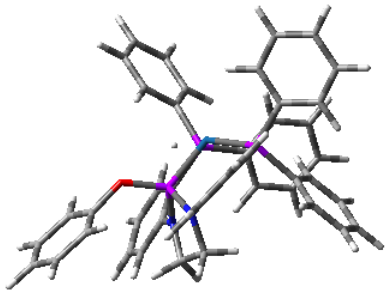
Imaginary frequency: -496.32 cm^{-1}

Tag	Symbol	X	Y	Z
1	Pt	-0.09003	-0.16716	-0.12918
2	P	-0.41167	-2.21497	-1.29515
3	P	-2.47467	0.201994	-0.02816
4	P	2.269963	-0.57558	-0.07235
5	N	0.613783	-3.28709	-0.35572
6	N	-1.80637	-2.91836	-0.55925
7	C	3.256121	0.649546	-1.02012
8	C	4.088394	1.59166	-0.38013
9	C	4.80691	2.527418	-1.1471
10	C	4.699727	2.528266	-2.54907
11	C	3.864401	1.590671	-3.19052
12	C	3.140084	0.658217	-2.43174
13	C	2.795476	-0.51843	1.694843
14	C	3.743402	-1.42472	2.226747
15	C	4.12283	-1.33554	3.577462
16	C	3.561952	-0.34686	4.409086
17	C	2.613074	0.551796	3.884903
18	C	2.223578	0.468036	2.536655
19	C	2.831402	-2.22581	-0.68939
20	C	4.188217	-2.36677	-1.06917
21	C	4.745889	-3.6264	-1.33648
22	C	3.943902	-4.77684	-1.21321
23	C	2.587908	-4.65802	-0.87404

24	C	2.007859	-3.39111	-0.63092
25	C	-0.12856	-4.37691	0.335663
26	C	-1.52156	-3.78994	0.617895
27	C	-3.14027	-2.4864	-0.86785
28	C	-4.06233	-3.45415	-1.32224
29	C	-5.37681	-3.09735	-1.65767
30	C	-5.78016	-1.75076	-1.56623
31	C	-4.87038	-0.77998	-1.1211
32	C	-3.54665	-1.12572	-0.74928
33	C	-2.98175	0.342293	1.737577
34	C	-2.24676	1.218799	2.576254
35	C	-2.6053	1.353851	3.928516
36	C	-3.68002	0.613483	4.459813
37	C	-4.40184	-0.26617	3.630617
38	C	-4.05789	-0.4037	2.273712
39	C	-2.98311	1.733916	-0.90917
40	C	-3.54542	2.83765	-0.23544
41	C	-3.8955	3.996112	-0.95453
42	C	-3.68623	4.060611	-2.34376
43	C	-3.12306	2.958699	-3.01948
44	C	-2.76866	1.801931	-2.30735
45	C	0.752588	3.200245	0.291603
46	C	1.308096	3.974838	1.34425
47	C	1.991879	5.171119	1.063493
48	C	2.150217	5.614982	-0.26433
49	C	1.60693	4.84497	-1.31285
50	C	0.915168	3.653597	-1.04132
51	H	4.179939	1.606088	0.701456
52	H	5.439967	3.254861	-0.64716
53	H	5.256919	3.252241	-3.13762
54	H	3.779071	1.587362	-4.27398
55	H	2.502657	-0.06291	-2.94002
56	H	4.186691	-2.1944	1.603132
57	H	4.853529	-2.03396	3.976577
58	H	3.858526	-0.28045	5.452639
59	H	2.175479	1.314724	4.523375
60	H	1.481649	1.157992	2.141606
61	H	4.818414	-1.48493	-1.14243
62	H	5.78952	-3.70847	-1.62452
63	H	4.365584	-5.76038	-1.40232
64	H	1.971523	-5.55033	-0.82405
65	H	0.389758	-4.65745	1.259204
66	H	-0.21986	-5.26718	-0.30458

67	H	-1.52276	-3.20192	1.549178
68	H	-2.27871	-4.57544	0.7028
69	H	-3.72663	-4.48205	-1.43278
70	H	-6.07179	-3.85538	-2.00825
71	H	-6.78953	-1.45939	-1.8416
72	H	-5.1934	0.255205	-1.05849
73	H	-1.41147	1.782801	2.164273
74	H	-2.04705	2.035099	4.56545
75	H	-3.95109	0.71994	5.507028
76	H	-5.23192	-0.83952	4.034732
77	H	-4.63207	-1.0804	1.648479
78	H	-3.71015	2.806814	0.837038
79	H	-4.32477	4.843842	-0.42764
80	H	-3.95561	4.957538	-2.89502
81	H	-2.96092	3.002292	-4.09323
82	H	-2.3392	0.958148	-2.84453
83	H	1.171638	3.645137	2.371698
84	H	2.398629	5.757976	1.884548
85	H	2.678629	6.540428	-0.47679
86	H	1.718719	5.175277	-2.34347
87	H	0.482287	3.071804	-1.85505
88	H	0.019474	1.06931	-1.06962
89	O	0.02521	2.069727	0.603459

XYZ Coordinates for Calculated Optimized Geometry of transition state prior to $[(PP(OPh)P)Pt(H)]^{+}$.



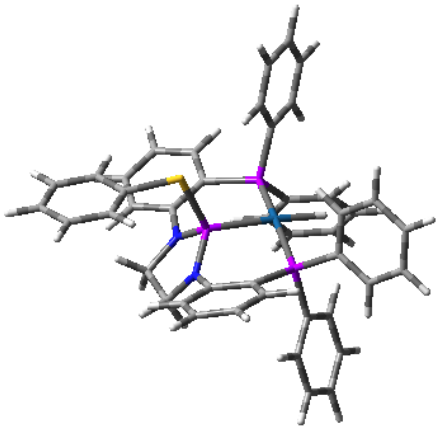
Imaginary frequency: -262.83 cm^{-1}

Tag	Symbol	X	Y	Z
1	Pt	0.240035	-0.30344	-0.77281
2	P	-0.82915	1.534827	-0.16654
3	P	2.523182	0.374077	-0.18444
4	P	-1.32089	-1.87873	-0.12124
5	O	-1.8965	2.34256	-1.15677
6	N	-1.74132	1.131935	1.241008
7	N	0.230644	2.523901	0.709065
8	C	-2.0394	-2.75618	-1.58073
9	C	-2.37	-4.1308	-1.56229
10	C	-2.94418	-4.73588	-2.69525
11	C	-3.19715	-3.97738	-3.85393
12	C	-2.86775	-2.60769	-3.87902
13	C	-2.28846	-2.00032	-2.75204
14	C	-0.7239	-3.21176	1.0147
15	C	-1.18334	-3.35424	2.341926
16	C	-0.64225	-4.3505	3.178197
17	C	0.357527	-5.21544	2.697744
18	C	0.82403	-5.07572	1.373746
19	C	0.293928	-4.0768	0.540978
20	C	-2.7778	-1.12658	0.753962
21	C	-3.92185	-1.95313	0.890717
22	C	-5.06087	-1.54495	1.597277
23	C	-5.07516	-0.26837	2.18844
24	C	-3.97358	0.583158	2.039266
25	C	-2.81615	0.187959	1.320869
26	C	-1.50256	2.103961	2.349907
27	C	-0.04905	2.595704	2.175426

28	C	1.473909	3.060167	0.187459
29	C	1.579351	4.464367	0.126137
30	C	2.747627	5.089857	-0.3388
31	C	3.827825	4.299692	-0.76649
32	C	3.734575	2.897965	-0.71016
33	C	2.576645	2.246106	-0.22555
34	C	2.973943	-0.03447	1.561059
35	C	2.577628	-1.28812	2.081576
36	C	2.934689	-1.66023	3.390042
37	C	3.681658	-0.78049	4.197426
38	C	4.071541	0.474186	3.689177
39	C	3.723184	0.846237	2.377608
40	C	3.955883	-0.16443	-1.21553
41	C	5.220741	-0.48259	-0.67031
42	C	6.265323	-0.91124	-1.51074
43	C	6.06088	-1.01904	-2.89952
44	C	4.800991	-0.70643	-3.44844
45	C	3.751905	-0.29011	-2.61137
46	C	-2.9206	3.266788	-0.77447
47	C	-4.25254	2.826945	-0.75261
48	C	-5.26753	3.757667	-0.46237
49	C	-4.94663	5.104865	-0.20179
50	C	-3.60291	5.526983	-0.24079
51	C	-2.57799	4.607081	-0.53182
52	H	0.183668	1.378304	-1.49617
53	H	-2.17715	-4.73352	-0.67932
54	H	-3.19233	-5.79374	-2.67107
55	H	-3.64071	-4.44779	-4.72753
56	H	-3.05545	-2.01774	-4.7722
57	H	-2.02789	-0.94446	-2.784
58	H	-1.95972	-2.70204	2.72946
59	H	-1.00731	-4.45093	4.197044
60	H	0.767399	-5.98946	3.341402
61	H	1.595342	-5.74056	0.99383
62	H	0.672457	-3.97348	-0.47405
63	H	-3.91674	-2.94188	0.440143
64	H	-5.91486	-2.20947	1.687237
65	H	-5.94438	0.071259	2.745275
66	H	-4.01954	1.58079	2.463182
67	H	-1.63406	1.602954	3.313734
68	H	-2.20093	2.950385	2.292314
69	H	0.658061	1.953566	2.716068
70	H	0.060457	3.623197	2.537638

71	H	0.730006	5.063675	0.444973
72	H	2.805843	6.173954	-0.37848
73	H	4.735149	4.764122	-1.14228
74	H	4.578103	2.306149	-1.052
75	H	1.989277	-1.96757	1.47154
76	H	2.625997	-2.62853	3.774924
77	H	3.954862	-1.0672	5.209698
78	H	4.647942	1.157986	4.307026
79	H	4.034206	1.81684	2.000883
80	H	5.393071	-0.41135	0.399916
81	H	7.23243	-1.15983	-1.08161
82	H	6.869712	-1.34958	-3.54588
83	H	4.634995	-0.79561	-4.51874
84	H	2.776821	-0.06984	-3.04239
85	H	-4.4856	1.78973	-0.97275
86	H	-6.30431	3.432428	-0.45003
87	H	-5.73536	5.820012	0.014527
88	H	-3.3541	6.569554	-0.06132
89	H	-1.54144	4.923358	-0.60287

XYZ Coordinates for Calculated Optimized Geometry of $[(PP(SPh)P)Pt(H)]^{+}$.

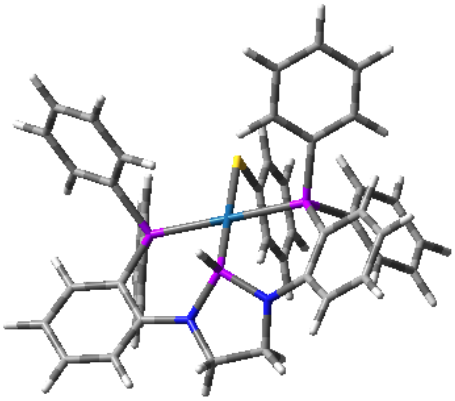


Tag	Symbol	X	Y	Z
1	Pt	-0.20123	-0.85257	0.328914
2	P	0.215663	1.353917	-0.15455
3	P	-2.52096	-0.49607	0.12288
4	P	2.070874	-1.3854	0.097019
5	N	1.37428	1.576042	-1.39461
6	N	-1.01104	2.145505	-1.03106
7	C	2.887853	-1.83031	1.690826
8	C	3.744641	-2.94612	1.825573
9	C	4.348855	-3.22686	3.065059
10	C	4.107998	-2.39701	4.17596
11	C	3.255319	-1.28272	4.045398
12	C	2.643807	-1.00179	2.812202
13	C	2.285181	-2.83429	-1.03137
14	C	2.92351	-2.73165	-2.28673
15	C	3.014474	-3.85503	-3.13107
16	C	2.475977	-5.09037	-2.72963
17	C	1.833791	-5.19812	-1.47866
18	C	1.729926	-4.07761	-0.63919
19	C	3.154576	-0.05736	-0.63563
20	C	4.544208	-0.33497	-0.57015
21	C	5.508084	0.486928	-1.16744
22	C	5.084384	1.633735	-1.86111
23	C	3.722862	1.955841	-1.91581
24	C	2.734697	1.140676	-1.30435
25	C	0.962962	2.633874	-2.36817
26	C	-0.58332	2.647179	-2.36908
27	C	-2.33549	2.337151	-0.50783
28	C	-2.90386	3.62761	-0.58931

29	C	-4.17465	3.899025	-0.06117
30	C	-4.88971	2.881422	0.594326
31	C	-4.33741	1.593331	0.678079
32	C	-3.0762	1.283244	0.114657
33	C	-3.09881	-1.14254	-1.50911
34	C	-2.5377	-2.34277	-2.00884
35	C	-2.98525	-2.88011	-3.22823
36	C	-3.98862	-2.22401	-3.9679
37	C	-4.54394	-1.02547	-3.48091
38	C	-4.10427	-0.48645	-2.25799
39	C	-3.53699	-1.3205	1.415586
40	C	-4.75659	-1.96913	1.117267
41	C	-5.49331	-2.58986	2.143113
42	C	-5.02348	-2.56163	3.470001
43	C	-3.80565	-1.91883	3.77005
44	C	-3.06088	-1.30689	2.747786
45	C	1.16354	4.239297	0.954967
46	C	2.485889	4.53201	0.566254
47	C	2.804979	5.826822	0.113416
48	C	1.810529	6.823621	0.055222
49	C	0.493612	6.52599	0.457838
50	C	0.165639	5.232712	0.909694
51	H	-0.51458	-2.43073	0.550767
52	H	3.937312	-3.60078	0.980344
53	H	5.002961	-4.08958	3.160039
54	H	4.575682	-2.61641	5.132189
55	H	3.064327	-0.63889	4.899778
56	H	1.985588	-0.14028	2.727271
57	H	3.35263	-1.78989	-2.61337
58	H	3.507241	-3.76166	-4.09522
59	H	2.552369	-5.9576	-3.38029
60	H	1.413537	-6.14878	-1.16105
61	H	1.211928	-4.17104	0.312174
62	H	4.879033	-1.22305	-0.04179
63	H	6.561482	0.234471	-1.09635
64	H	5.80839	2.285332	-2.34306
65	H	3.427252	2.865516	-2.42528
66	H	1.346239	2.384151	-3.36249
67	H	1.356296	3.614529	-2.07096
68	H	-0.98521	1.986562	-3.1482
69	H	-0.94914	3.661652	-2.55199
70	H	-2.33508	4.4297	-1.05041
71	H	-4.58963	4.900231	-0.14012

72	H	-5.86339	3.082552	1.031141
73	H	-4.90418	0.816033	1.180765
74	H	-1.75494	-2.85033	-1.45253
75	H	-2.54864	-3.803	-3.60052
76	H	-4.33065	-2.63988	-4.91208
77	H	-5.31738	-0.51271	-4.04673
78	H	-4.54552	0.438645	-1.8991
79	H	-5.12669	-2.00661	0.096278
80	H	-6.42621	-3.09409	1.905465
81	H	-5.59454	-3.04192	4.260236
82	H	-3.4344	-1.90358	4.791205
83	H	-2.10985	-0.83401	2.983629
84	H	3.256749	3.769947	0.635011
85	H	3.826912	6.058623	-0.17536
86	H	2.062699	7.824788	-0.28442
87	H	-0.27083	7.298431	0.435581
88	H	-0.8417	5.00548	1.245809
89	S	0.754766	2.55952	1.632877

XYZ Coordinates for Calculated Optimized Geometry of $[(PP(H)P)Pt(SPh)]^{+}$.



Tag	Symbol	X	Y	Z
1	Pt	0.006463	-0.2172	0.278516
2	P	0.053611	-2.32263	-0.45181
3	P	2.411103	-0.16111	0.275235
4	P	-2.38624	-0.26146	0.295512
5	N	-1.14184	-2.736	-1.60085
6	N	1.346429	-2.75975	-1.46747
7	C	-2.98512	-0.24854	2.040984
8	C	-4.20825	0.349668	2.422865
9	C	-4.64426	0.27966	3.757775
10	C	-3.87174	-0.39175	4.723971
11	C	-2.6523	-0.98888	4.350386
12	C	-2.2099	-0.91348	3.019187
13	C	-3.2322	1.110616	-0.59363
14	C	-3.70909	0.915671	-1.91143
15	C	-4.30548	1.97714	-2.6129
16	C	-4.42999	3.242914	-2.00964
17	C	-3.94835	3.443434	-0.70235
18	C	-3.34629	2.388974	0.003464
19	C	-3.17097	-1.7854	-0.4512
20	C	-4.5589	-1.92804	-0.19838
21	C	-5.32735	-2.95074	-0.76808
22	C	-4.70481	-3.87286	-1.62715
23	C	-3.33109	-3.77464	-1.88131
24	C	-2.5417	-2.74927	-1.30163
25	C	-0.57094	-3.56619	-2.70157
26	C	0.899636	-3.11903	-2.84417
27	C	2.706574	-2.78628	-1.01785
28	C	3.507611	-3.89138	-1.39062

29	C	4.835211	-4.0056	-0.95906
30	C	5.38113	-3.02258	-0.11301
31	C	4.593668	-1.92762	0.267406
32	C	3.258024	-1.76746	-0.1811
33	C	3.160516	1.045146	-0.89987
34	C	3.148844	2.427946	-0.59664
35	C	3.682686	3.352924	-1.50865
36	C	4.220739	2.915937	-2.7342
37	C	4.225175	1.542912	-3.04477
38	C	3.698295	0.610329	-2.1342
39	C	3.046569	0.233534	1.958264
40	C	4.234242	0.971139	2.167598
41	C	4.694567	1.212743	3.474279
42	C	3.981239	0.716543	4.58169
43	C	2.797837	-0.01956	4.378011
44	C	2.330766	-0.2558	3.074664
45	C	-0.11501	3.249203	-0.29008
46	C	-0.11394	4.637058	-0.02042
47	C	-0.18205	5.564364	-1.07657
48	C	-0.25325	5.120895	-2.41241
49	C	-0.25376	3.738563	-2.67923
50	C	-0.18363	2.807138	-1.62717
51	H	-4.81705	0.879249	1.695977
52	H	-5.58267	0.749213	4.040389
53	H	-4.21193	-0.44397	5.754774
54	H	-2.04797	-1.50347	5.092756
55	H	-1.25747	-1.3618	2.745833
56	H	-3.63295	-0.05628	-2.39003
57	H	-4.67245	1.81434	-3.62287
58	H	-4.89192	4.06327	-2.5526
59	H	-4.02781	4.42088	-0.23486
60	H	-2.95159	2.568759	0.997908
61	H	-5.05441	-1.2148	0.452392
62	H	-6.38827	-3.02192	-0.54958
63	H	-5.27921	-4.67218	-2.08743
64	H	-2.86848	-4.51295	-2.52623
65	H	-1.12786	-3.3863	-3.62645
66	H	-0.62256	-4.63862	-2.45932
67	H	0.983547	-2.24773	-3.50769
68	H	1.506276	-3.92866	-3.25746
69	H	3.07811	-4.6794	-2.00229
70	H	5.428745	-4.86424	-1.26078
71	H	6.402196	-3.10713	0.246372

72	H	5.029508	-1.18039	0.921929
73	H	2.717356	2.781184	0.333898
74	H	3.664459	4.411657	-1.26596
75	H	4.630376	3.635909	-3.43785
76	H	4.6423	1.197059	-3.98695
77	H	3.729527	-0.44615	-2.38372
78	H	4.794553	1.368153	1.325993
79	H	5.604316	1.787853	3.624607
80	H	4.338508	0.906737	5.590275
81	H	2.237419	-0.39636	5.229378
82	H	1.403238	-0.80471	2.929476
83	H	-0.06021	4.988014	1.007498
84	H	-0.18014	6.629008	-0.85362
85	H	-0.30675	5.838652	-3.227
86	H	-0.30717	3.382202	-3.70559
87	H	-0.17916	1.742481	-1.84734
88	S	-0.01149	2.119766	1.164508
89	H	0.030078	-3.36028	0.546244