

**SUPPLEMENTARY DATA**

Naphthalimide-Based Platinum(II) and Palladium(II) N-Heterocyclic Carbene Complexes:

Synthesis and Structural Elucidation

M. Dangalov <sup>a,\*</sup>, P. Petrov <sup>b</sup>, N. G. Vassilev <sup>a</sup>

<sup>a</sup> *Institute of Organic Chemistry with Center of Phytochemistry, 9, Acad. G. Bonchev Str., 1113 Sofia, Bulgaria,* <sup>b</sup> *Department of Organic Chemistry, Faculty of Chemistry and Pharmacy, Sofia University St. Kliment Ohridsky, 1, James Bourchier Blvd., 1164, Sofia, Bulgaria*

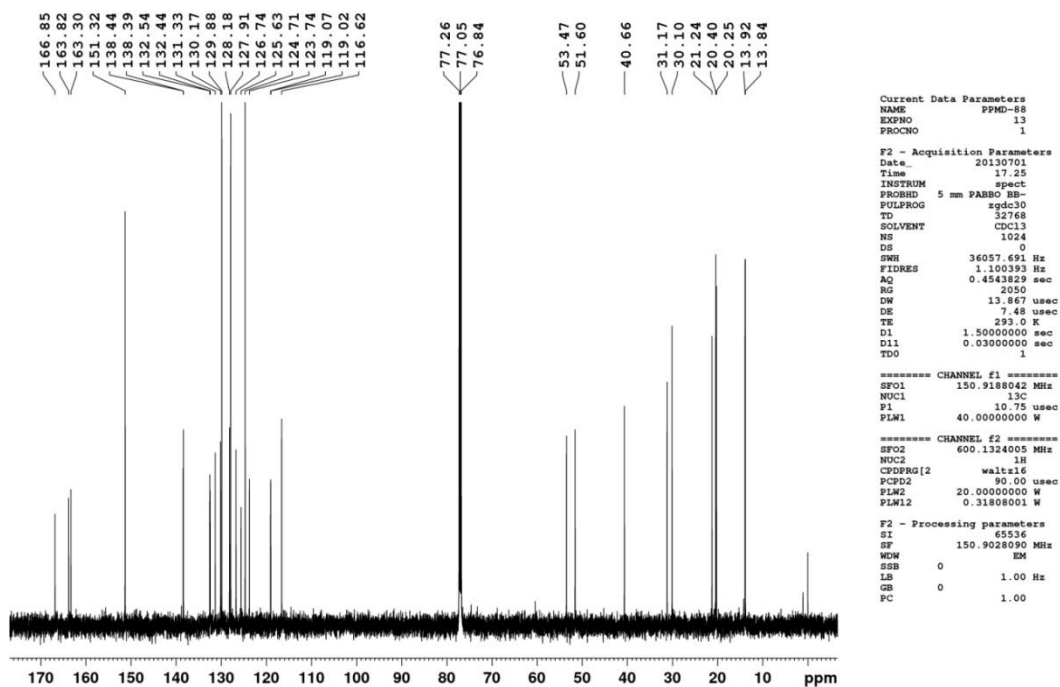
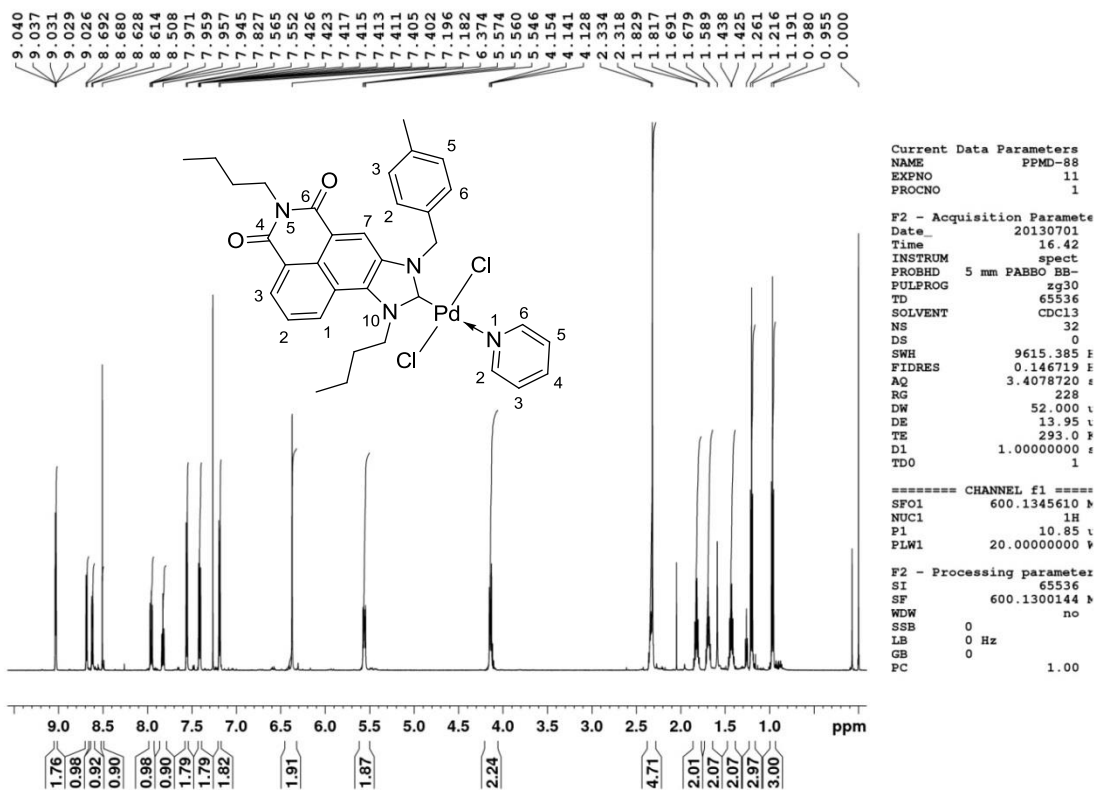
**Contents:**

**I. <sup>1</sup>H and <sup>13</sup>C NMR spectra of complexes**

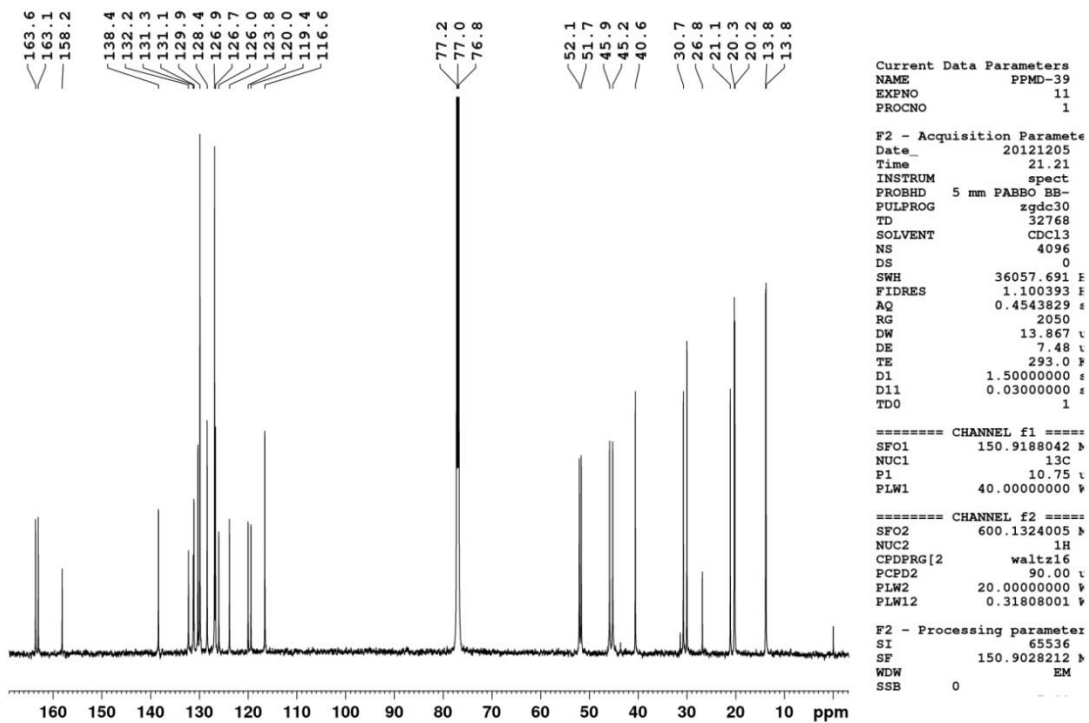
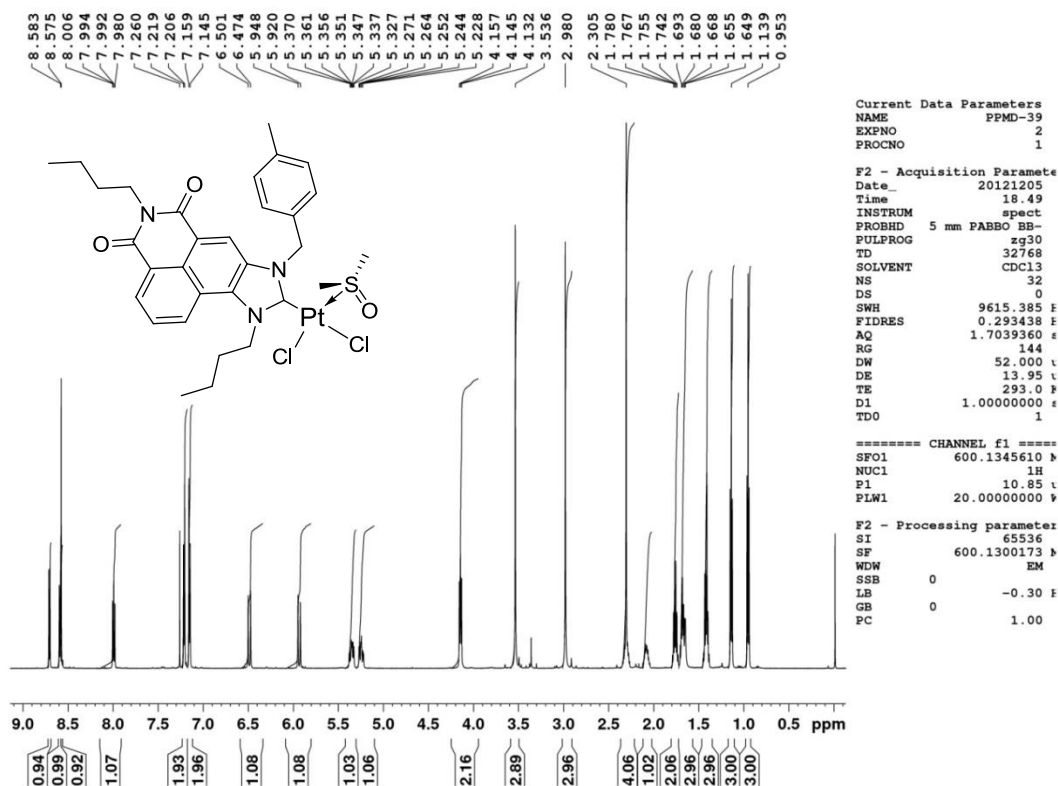
**II. DFT calculations**

# I. <sup>1</sup>H and <sup>13</sup>C NMR spectra of complexes

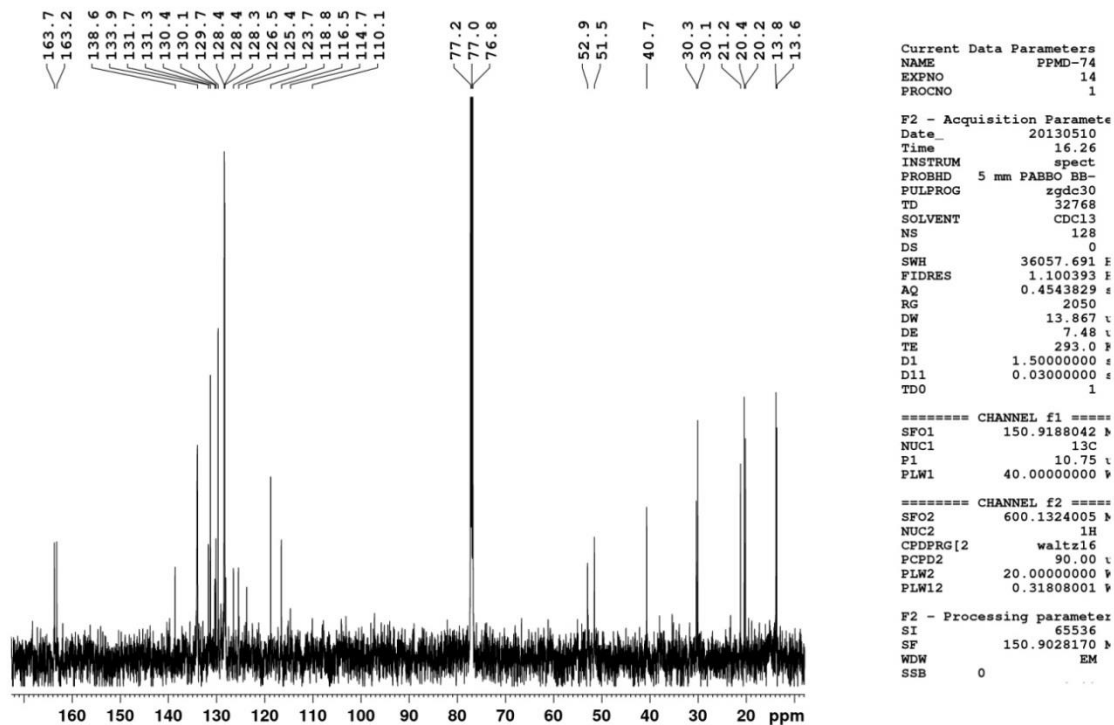
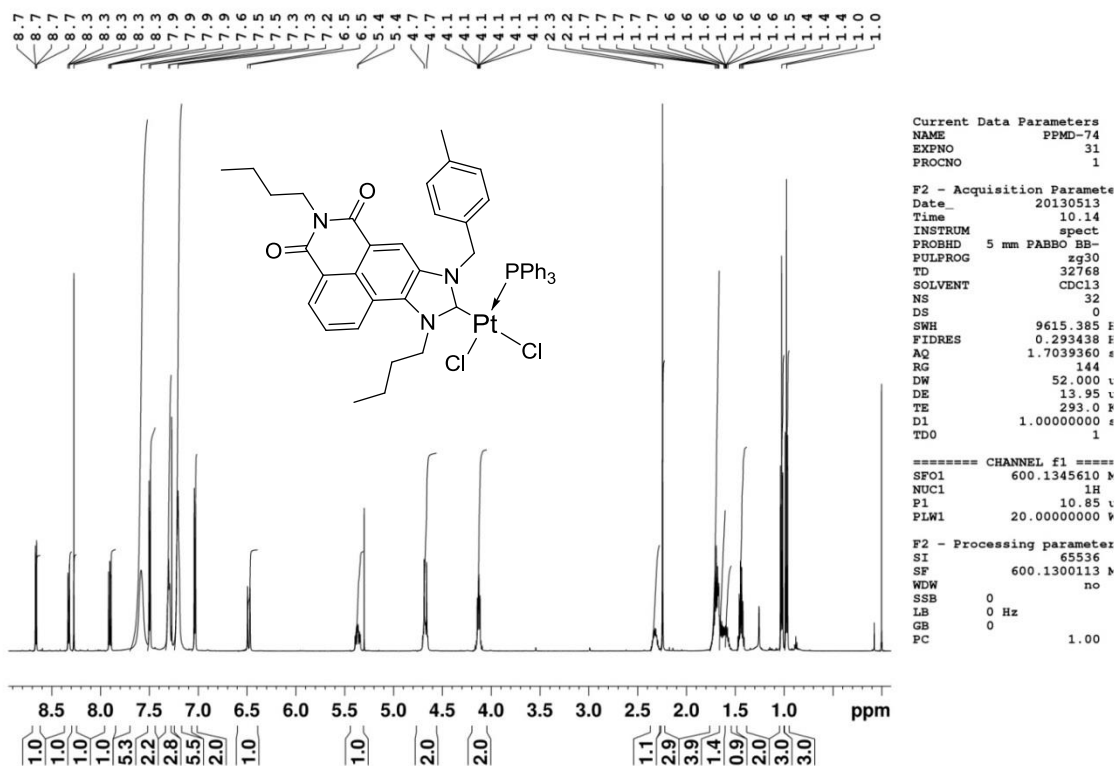
## *trans*-[(NHC)Pd(Pyr)(Cl)<sub>2</sub>, complex 1



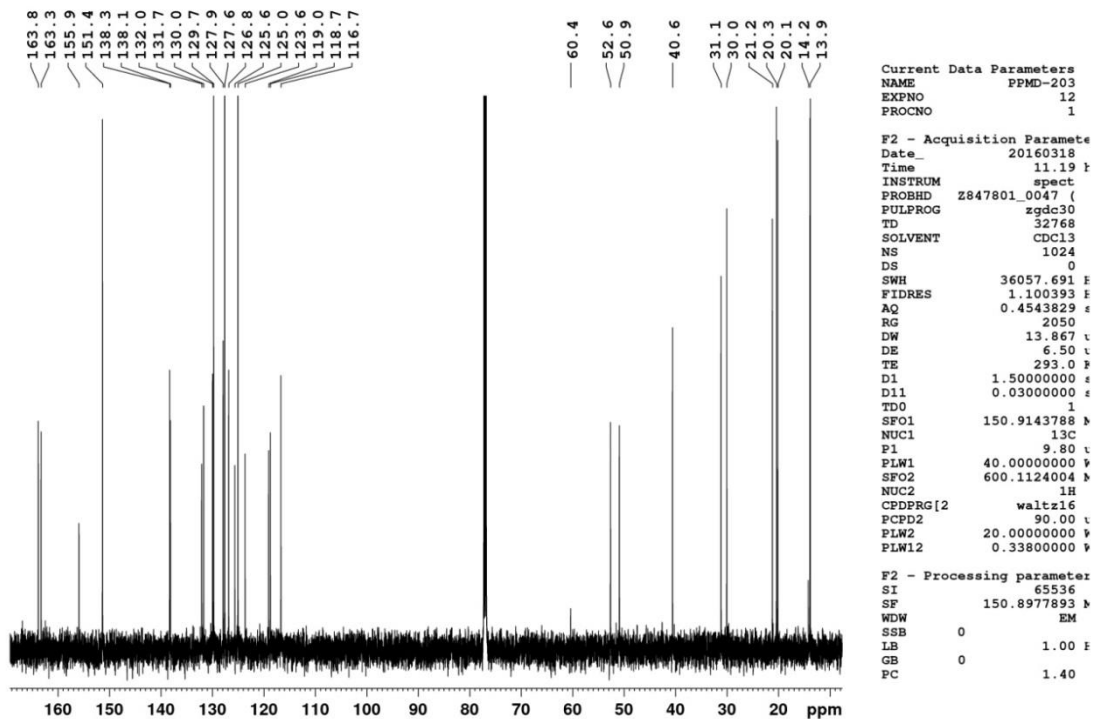
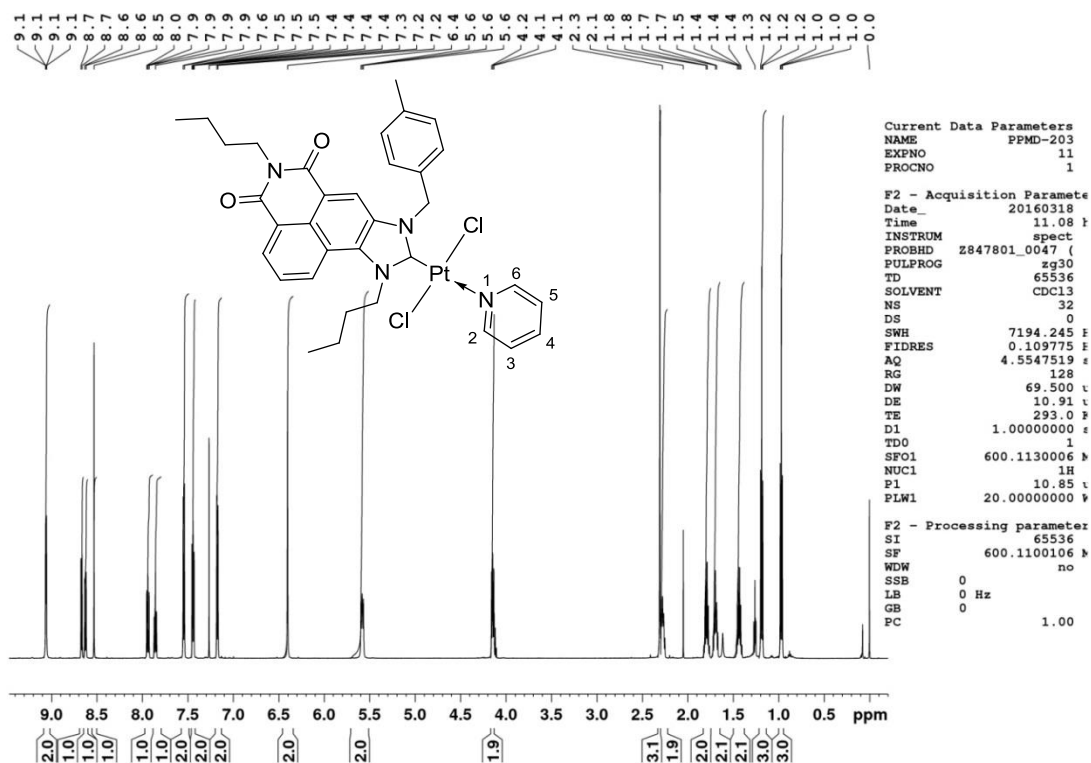
*cis*-[(NHC)Pt(DMSO)(Cl)<sub>2</sub>], complex 2



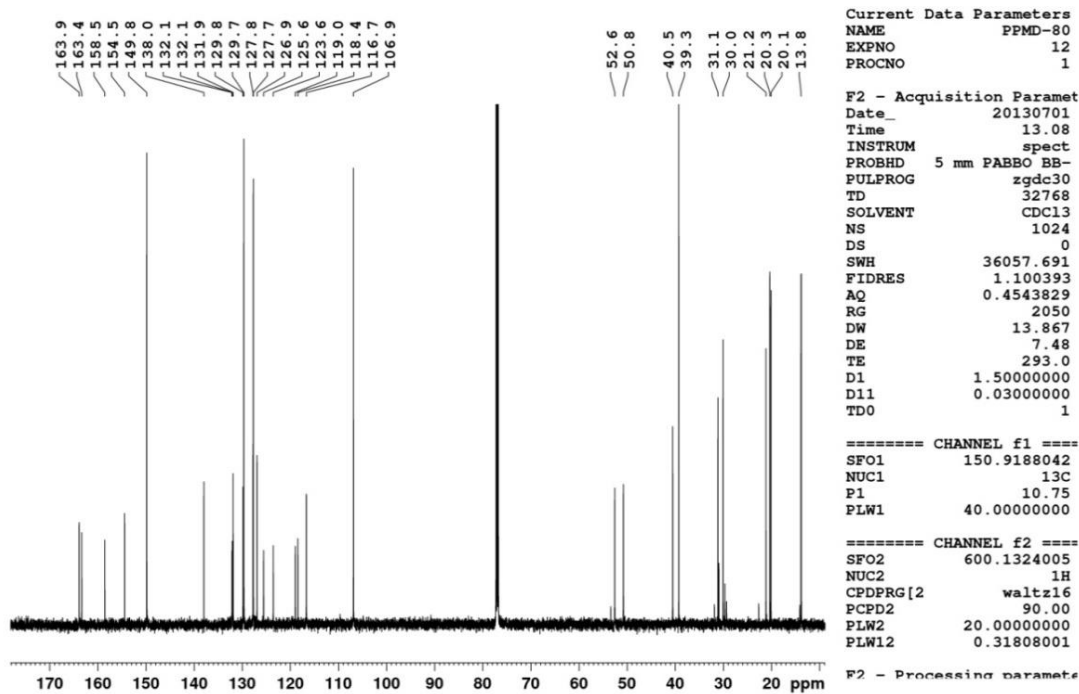
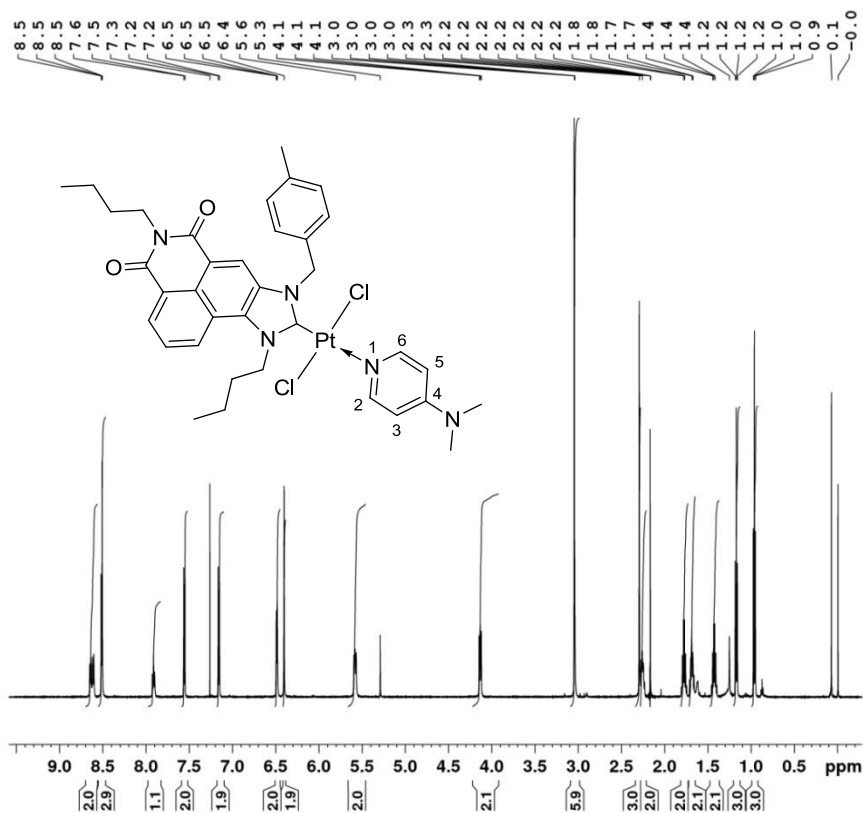
*cis*-[(NHC)Pt(PPh<sub>3</sub>)(Cl)<sub>2</sub>], complex 3



*trans*-[(NHC)Pt(C<sub>5</sub>H<sub>5</sub>N)(Cl)<sub>2</sub>], complex 4



*trans*-[(NHC)Pt((CH<sub>3</sub>)<sub>2</sub>NC<sub>5</sub>H<sub>4</sub>N)(Cl)<sub>2</sub>], complex 5



## II. DFT calculations

All calculations were performed with Gaussian09 program package [1] at the DFT level of theory. Geometry optimizations were performed by using density functional theory [2-4] with B3LYP functionals [5, 6]. As for the basis sets, we used 6-31G(d) sets for C, H, N, O, S, P and Cl [7]. For Pd we used LANL2DZ basis sets [8], whose core parts were represented by effective core potentials (ECP). Solvent was included implicitly to the optimizations via the SMD [9] model with the built in parameters for solvent  $\text{CHCl}_3$ . The nature of all critical points was confirmed by means of the vibrational analysis, and ZPV energies were evaluated. The thermal and entropy corrections to Gibbs free energy to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at the same level.

1. M. J. T. Frisch, 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., in *Gaussian, Inc.*, Wallingford CT, 2009.
2. P. Hohenberg, W. Kohn (1964) *Phys. Rev. B* 136:864-871.
3. W. Kohn, L. J. Sham (1965) *Phys. Rev. A* 140:1133-1138.
4. R. G. Parr, W. Yang (1989) *Density-Functional Theory of Atoms and Molecules* (Oxford Univ Press, Oxford).
5. A. D. Becke (1993) *J. Chem. Phys.* 98:5648-5652.
6. C. Lee, W. Yang, R. G. Parr (1988) *Phys. Rev. B* 37:785-789.
7. P. C. Hariharan, J. A. Pople (1973) *Theor. Chim. Acta* 28:213-222.
8. W. R. Wadt, P. J. Hay (1985) *J. Chem. Phys.* 82:284-298.
9. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*, **2009**, *113*, 6378-6396.

Archive Entries of complex **1** in THF:

*trans*:

```
1\1\GINC-WN29\FOpt\RB3LYP\GenECP\C34H36Cl2N4O2Pd1\NVASILEV\04-Feb-2017
\0\#p b3lyp/genecp opt=tight freq test SCRF(SMD,Solvent=TetraHydroFur
an)\Title Card Required\0,1\C,1.4245446986,-0.3308368918,-0.36335536
23\C,-0.5792266763,-1.3638042962,-0.2333799998\N,0.8024381333,-1.51155
52883,-0.0919727317\C,1.5478030622,-2.7245611298,0.2924038774\H,2.5759
567799,-2.5640048548,-0.0383886717\H,1.1535987349,-3.5615799081,-0.289
5787086\C,1.5221048454,-2.9996486543,1.7997197551\H,1.967272778,-2.139
5524549,2.3138556011\H,0.4871901136,-3.0827046123,2.1547412445\C,2.295
1182033,-4.277666697,2.1513247153\H,3.321829205,-4.1968188249,1.767787
8011\C,0.1220860758,3.0103922728,-0.1557953479\C,-0.7062723403,4.01094
76307,-0.6735367967\C,0.422699124,3.0292688674,1.2145798192\C,-1.22447
68078,5.0091609435,0.1561371136\H,-0.9497422299,4.014120277,-1.7338347
184\C,-0.1016145221,4.0231110091,2.0379502354\H,1.0725252324,2.2664105
318,1.6366828289\C,-0.933545102,5.0326089966,1.5249313166\H,-1.8685316
251,5.775713067,-0.2684685648\H,0.1421756038,4.0202589744,3.0983495265
\C,0.7143783021,1.9654528818,-1.0814170769\H,1.8008470944,2.0663541652
,-1.1427853765\H,0.3129915994,2.0811457809,-2.0926611668\C,-1.48453626
75,6.1105347353,2.4275528536\H,-1.996478556,5.6813514068,3.2976815806\
H,-0.6835557749,6.754243124,2.8144559126\H,-2.198614726,6.7493727899,1
.8977755109\C,-2.0508573439,0.5064978941,-0.8588727113\C,-3.1398729242
,-0.3350177569,-0.7429674157\C,-2.9806569634,-1.7028980893,-0.36957404
76\H,-2.1939003199,1.5424445401,-1.1389310223\C,-1.6078911692,-3.63509
9288,0.2501064114\C,-2.7461914606,-4.4140302577,0.3415977896\C,-4.0122
174329,-3.8627573009,0.0887668308\H,-4.9087837372,-4.4680088587,0.1645
328478\C,-4.1303883327,-2.527639081,-0.2623094109\H,-0.650888855,-4.09
23207232,0.4576988071\H,-2.6587496814,-5.4608291956,0.6158314387\C,-0.
7835173337,-0.0298517831,-0.5981473795\N,0.4687158102,0.5752946338,-0.
6582941828\C,-4.4841246119,0.227661664,-1.016777043\C,-5.4878715738,-1
```



.9805632641,-0.5147912483\O,-4.64952452,1.3998517963,-1.3410870124\O,-  
6.4992225919,-2.666540203,-0.4050873988\N,-5.5777355929,-0.6358771922,  
-0.8924151347\C,-6.9202840182,-0.0788635358,-1.149894474\H,-6.81066354  
16,0.6606133775,-1.9445120572\H,-7.5397315939,-0.9010454764,-1.5095413  
214\C,-7.543157082,0.5610596216,0.0958953464\H,-6.8791119748,1.3550811  
411,0.4603819713\H,-7.612493521,-0.1927318204,0.8910397006\C,-8.933661  
2647,1.1418066093,-0.1902712749\H,-8.8607490261,1.8725141347,-1.008313  
4438\H,-9.596199759,0.3415658965,-0.549103856\C,-9.5607638028,1.812385  
6892,1.0352197387\H,-8.9388438622,2.6414279203,1.3959818077\H,-10.5529  
851859,2.2176295957,0.8028561183\H,-9.6780310908,1.1010614385,1.862677  
8612\C,2.3343604348,-4.5483176963,3.6580230378\H,2.8197136329,-3.72443  
44125,4.1960101218\H,1.3234513447,-4.6635866529,4.0692971094\H,2.89124  
50245,-5.4662158267,3.8808674449\H,1.8406093733,-5.1356729304,1.635830  
6275\C,-1.683742513,-2.2641279509,-0.1048074836\C1,3.3710965064,0.5040  
740284,1.9312624727\Pd,3.3967231901,-0.0136063689,-0.4075752903\C1,3.3  
653742271,-0.5532955989,-2.7438842739\N,5.5090390225,0.3335010796,-0.4  
865477076\C,6.0307891662,1.1481443394,-1.4223645487\H,5.3288030426,1.5  
904834129,-2.119306486\C,6.3355979148,-0.2602662993,0.3942523049\H,5.8  
687694648,-0.8948769817,1.1382963034\C,7.3961307465,1.4029749051,-1.50  
59760191\H,7.7695336199,2.0729799698,-2.2733372215\C,7.7130168669,-0.0  
65355405,0.3663551663\H,8.3400186468,-0.5704739475,1.0936395781\C,8.25  
49660939,0.7837791231,-0.5982360265\H,9.3257675933,0.9601862443,-0.641  
3355148\\Version=EM64L-G09RevD.01\State=1-A\HF=-2734.1298301\RMSD=7.40  
0e-09\RMSF=2.042e-06\Dipole=1.6015202,-0.5029238,0.6682676\Quadrupole=  
14.6567092,9.7298334,-24.3865427,-2.0471378,-1.5718994,-10.2504699\PG=  
C01 [X(C34H36C12N4O2Pd1)]\@

**cis:**

1\1\GINC-WN29\FOpt\RB3LYP\GenECP\C34H36C12N4O2Pd1\NVASILEV\06-Feb-2017  
\0\#p b3lyp/genecp opt=tight freq test SCRF(SMD,Solvent=TetraHydroFur

an)\Title Card Required\0,1\C,-1.709783856,-0.144326301,-0.065583837  
5\C,0.2661880687,-1.2413576746,-0.0719588959\N,-1.1025222503,-1.334944  
3505,-0.3346949723\C,-1.8399122438,-2.4989678637,-0.8617060602\H,-2.89  
38723686,-2.3065734427,-0.6492840419\H,-1.5435707984,-3.3776886186,-0.  
2817148605\C,-1.6463648404,-2.7086570075,-2.3674833192\H,-2.0142102145  
, -1.8166968039,-2.8869207184\H,-0.579204069,-2.8019855565,-2.605412008  
2\C,-2.3983746149,-3.952050056,-2.8607613092\H,-3.46348655,-3.85510874  
96,-2.6081706699\C,-0.3209602936,3.1396283973,-0.1123048358\C,0.511990  
3365,4.1137736652,0.4464329933\C,-0.5624522183,3.1721003449,-1.4940096  
114\C,1.0937896846,5.0998136969,-0.355447612\H,0.7086585375,4.10705233  
19,1.5162602989\C,0.0249883192,4.1535345454,-2.2887118058\H,-1.2163369  
66,2.4306841181,-1.9472085355\C,0.8631604029,5.1363822506,-1.735363159  
8\H,1.7402969709,5.8462831915,0.1000150161\H,-0.1739127537,4.161419893  
, -3.3583177582\C,-0.98169405,2.104166969,0.7774252419\H,-2.0669557073,  
2.2317738092,0.7857998548\H,-0.6220562783,2.2009642551,1.8065084529\C,  
1.4845838956,6.2001578535,-2.608655659\H,2.0303991537,5.7573976209,-3.  
4509921606\H,0.7194638012,6.8607813409,-3.0371746417\H,2.1845485373,6.  
8241505046,-2.0434758408\C,1.7384860224,0.5455187212,0.7612878282\C,2.  
8030077856,-0.332910104,0.7116751045\C,2.6307101,-1.6786367238,0.26953  
4079\H,1.8908306049,1.5643360552,1.0946141826\C,1.2553887544,-3.528403  
9911,-0.5598875635\C,2.3690887112,-4.346887759,-0.5810568237\C,3.62383  
53617,-3.856839491,-0.1859004681\H,4.5015726628,-4.4934565782,-0.20369  
9239\C,3.7550035357,-2.5430871653,0.2339351205\H,0.3066979795,-3.93847  
11364,-0.8747478487\H,2.2714027399,-5.3771061692,-0.9091447366\C,0.481  
9643369,0.0683083667,0.3649592128\N,-0.752034737,0.712910116,0.3491084  
529\C,4.1343517671,0.1631908282,1.1392782195\C,5.0987759391,-2.0640003  
652,0.6463892079\O,4.3088509508,1.3151890533,1.5247559796\O,6.08924190  
74,-2.7869356304,0.6098345396\N,5.2004813072,-0.7412188068,1.091660620  
4\C,6.530498057,-0.2594614197,1.5143577317\H,6.3651372087,0.4823667512  
,2.2966949489\H,7.0564599366,-1.1153965002,1.9392216612\C,7.3362789064  
,0.3464967574,0.3599312306\H,6.7712547242,1.1814793084,-0.0739081155\H  
,7.4564326952,-0.4076407146,-0.4285132242\C,8.7150039395,0.8376292459,

0.8197160531\H,8.5877957727,1.5851267616,1.6155132412\H,9.2674141792,0  
.0000520894,1.2686869249\C,9.5418640193,1.4419660399,-0.3189379037\H,9  
.0317616223,2.3047891902,-0.7658227926\H,10.5210113214,1.7830893545,0.  
038435383\H,9.7156416182,0.709009802,-1.1170093436\C,-2.2512927297,-4.  
1690869842,-4.3692275035\H,-2.6479549475,-3.3152242132,-4.9319820763\H  
, -1.1989357062,-4.2956417752,-4.6537017455\H,-2.7942997296,-5.06438618  
05,-4.6945407076\H,-2.0331439345,-4.8401301563,-2.3247930179\C,1.34611  
39315,-2.177092653,-0.1399282215\C1,-3.4238379251,0.709134531,-2.48187  
96029\Pd,-3.6852139685,0.2330638161,-0.1657955266\C1,-6.0810154953,0.6  
596515213,-0.2119977938\N,-3.8745317683,-0.1645655521,1.8818017372\C,-  
3.7082288704,-1.408268299,2.370769816\H,-3.422967476,-2.1745933145,1.6  
601909731\C,-4.2337061021,0.8282163072,2.7189451514\H,-4.3736331161,1.  
8067012181,2.2767324099\C,-3.8951635154,-1.7022840883,3.7173277955\H,-  
3.7560713313,-2.720600684,4.0647786227\C,-4.4291450994,0.6093944367,4.  
0785508249\H,-4.7154399404,1.439881964,4.7150460496\C,-4.259643943,-0.  
6770625296,4.5894527183\H,-4.4109106983,-0.8773676142,5.6459178904\\Ve  
rsion=EM64L-G09RevD.01\State=1-A\HF=-2734.1219446\RMSD=4.030e-09\RMSF=  
1.307e-06\Dipole=3.1995229,-2.3921637,4.2555421\Quadrupole=-61.7202707  
,34.2856578,27.4346128,21.7921664,-40.5566393,3.9056202\PG=C01 [X(C34H  
36C12N4O2Pd1)]\@

Archive Entries of complex **2** in THF:

*trans*:

```
1\1\GINC-WN29\FOpt\RB3LYP\GenECP\C31H37C12N3O3Pt1S1\NVASILEV\07-Feb-20
17\0\#\#p b3lyp/genecp opt=tight freq test SCRF(SMD,Solvent=TetraHydroF
uran)\Title Card Required\0,1\C,1.2297797332,-0.2899287254,-0.314154
1056\C,-0.7673406816,-1.3375029149,-0.2170597719\N,0.6129227874,-1.479
106157,-0.0632180364\C,1.354306985,-2.6892001443,0.3406107884\H,2.3898
032001,-2.5220405714,0.0376351894\H,0.9775632188,-3.5285518487,-0.2490
865896\C,1.2879593171,-2.9571525503,1.8477840346\H,1.7140738022,-2.092
0914877,2.3697015835\H,0.243741621,-3.043602084,2.1736444481\C,2.05669
92098,-4.2293712541,2.228583445\H,3.097514156,-4.1393892704,1.88767098
47\C,-0.1066231328,3.0311475933,-0.0419324041\C,-0.9408820513,4.038140
079,-0.5372555057\C,0.1837114127,3.0132860767,1.330537754\C,-1.4755219
404,5.006297619,0.3170889752\H,-1.1763779403,4.0696895895,-1.598820588
1\C,-0.3569168342,3.977245475,2.1784659923\H,0.8380807881,2.2450346608
,1.7351058168\C,-1.1956133547,4.9925017691,1.6883899697\H,-2.124329130
8,5.7782909553,-0.0900259839\H,-0.1210572965,3.9457170495,3.240136719\
C,0.5020893219,2.0188411078,-0.9925996861\H,1.5877505044,2.1336009261,
-1.0448237596\H,0.1029396602,2.1548536572,-2.0020987691\C,-1.765484548
4,6.0376784592,2.617441993\H,-2.266262342,5.578002051,3.4783488402\H,-
0.9765308557,6.6882864932,3.0174345508\H,-2.4935260756,6.6745571952,2.
1045250919\C,-2.2460634526,0.531764028,-0.8288664397\C,-3.3296470678,-
0.3189189575,-0.7361696159\C,-3.1642872582,-1.6917581368,-0.3831858007
\H,-2.3933730314,1.5707202715,-1.0947660806\C,-1.7839182206,-3.6255858
207,0.213078395\C,-2.917351842,-4.4140419331,0.2787504965\C,-4.1848230
389,-3.8667357919,0.0251447162\H,-5.0774663873,-4.4798599224,0.0808175
904\C,-4.309130738,-2.5260600633,-0.3017419889\H,-0.8260161323,-4.0803
944359,0.4209171092\H,-2.8248438923,-5.465396433,0.5330440857\C,-0.977
3212947,-0.0003758898,-0.5642765502\N,0.2699508385,0.6150972965,-0.604
950432\C,-4.6756535638,0.238680215,-1.0150062671\C,-5.6681788224,-1.98
```

39861295,-0.557793455\O,-4.8454891856,1.414828692,-1.3217795004\O,-6.6  
754498162,-2.67847755,-0.4674934457\N,-5.7638914664,-0.6344157741,-0.9  
16351079\C,-7.108310772,-0.0825910439,-1.1766520149\H,-6.9966484292,0.  
6719437261,-1.9566792089\H,-7.7182689697,-0.9024499372,-1.5572034966\C  
, -7.7470831892,0.5295594958,0.0750139963\H,-7.0929140367,1.3226004178,  
0.4589956279\H,-7.815969367,-0.2390531804,0.855835714\C,-9.1405302984,  
1.1030161989,-0.2115535948\H,-9.0676823352,1.8506671356,-1.0141112551\  
H,-9.7926067765,0.3040487342,-0.5917779053\C,-9.7841180159,1.743046329  
,1.0218291159\H,-9.1728778547,2.5701820833,1.4044809377\H,-10.77797077  
56,2.1438503856,0.7888423836\H,-9.9019078839,1.0139282477,1.8335616637  
\C,2.0363747804,-4.5006244903,3.7354130074\H,2.4961455452,-3.674925043  
1,4.2924929808\H,1.0102862293,-4.6210217599,4.1055293799\H,2.588353835  
7,-5.4157945013,3.9805334473\H,1.6299959482,-5.0903458309,1.6944188903  
\C,-1.8662888599,-2.2485050328,-0.1155266117\C1,3.2015952557,-0.468622  
2111,-2.6954589694\S,5.611622595,0.4354623146,-0.4411752717\O,6.383482  
663,0.8080547575,0.7926930911\C,5.9108750796,1.6850118874,-1.719423917  
2\H,5.4192143187,1.3748316327,-2.6441414106\H,5.4803288535,2.623097567  
2,-1.360046399\H,6.9911435813,1.7886850994,-1.855628065\C,6.3989336075  
, -1.0081129753,-1.2023998589\H,5.8780279566,-1.2541279574,-2.130188230  
4\H,7.451783002,-0.7735198956,-1.3834639438\H,6.3106094645,-1.83305903  
18,-0.4907594608\Pt,3.2049557644,0.0331043194,-0.3431365453\C1,3.17896  
69219,0.5205381452,1.9867162091\\Version=EM64L-G09RevD.01\State=1-A\HF  
=-3031.4474564\RMSD=1.389e-09\RMSF=1.791e-06\Dipole=-0.1361664,-1.1437  
033,-1.0916096\Quadrupole=-11.8453465,22.388094,-10.5427474,-11.060831  
6,-22.8257992,-7.3239081\PG=C01 [X(C31H37C12N3O3Pt1S1)]\@

**cis:**

1\1\GINC-WN03\FOpt\RB3LYP\GenECP\C31H37C12N3O3Pt1S1\NVASILEV\07-Feb-20

17\0\#\#p b3lyp/genecp opt=tight freq test SCRF(SMD,Solvent=TetraHydroF  
uran)\Title Card Required\0,1\C,1.4122644377,-0.2143715532,-0.083617  
6731\C,-0.5647482918,-1.3058455342,-0.0387404302\N,0.8111501405,-1.412  
2271025,0.171867273\C,1.5564414212,-2.604889841,0.6187350065\H,2.60177  
69917,-2.42313152,0.3602690336\H,1.2175169455,-3.4545961328,0.02023507  
18\C,1.4321488642,-2.8659010868,2.1236484528\H,1.8368179305,-1.9983627  
677,2.6572212575\H,0.3764431275,-2.9526005667,2.4095721068\C,2.1862753  
483,-4.1359027795,2.5394841658\H,3.2399537249,-4.0464609359,2.24054900  
31\C,-0.0077570015,3.0768926709,0.0698409806\C,-0.8401252868,4.0619336  
105,-0.4703940457\C,0.2372105748,3.0861959779,1.4510982561\C,-1.417255  
3082,5.0358114246,0.3491680873\H,-1.040862736,4.0719976336,-1.53942769  
44\C,-0.3456477002,4.0555619824,2.2639386645\H,0.8884046184,2.33428094  
1,1.8901858749\C,-1.1823707444,5.0495956286,1.7288921633\H,-2.06376702  
15,5.7906617056,-0.0923004201\H,-0.1446729215,4.0450672982,3.333114005  
6\C,0.651830424,2.0601290249,-0.841168198\H,1.7350985865,2.2049585797,  
-0.8564705051\H,0.2818386317,2.1655237545,-1.8653892408\C,-1.797116719  
,6.1020688724,2.6202803373\H,-2.3161787608,5.650032986,3.4743367763\H,  
-1.0309779353,6.7727952737,3.0312704684\H,-2.5191950634,6.7175877771,2  
.0739208186\C,-2.0590678026,0.5126515865,-0.7563916709\C,-3.1259178612  
, -0.3610003777,-0.6886178317\C,-2.9448420299,-1.7198124251,-0.29203534  
03\H,-2.2188892203,1.5409896723,-1.0543865699\C,-1.5492503928,-3.60405  
86809,0.4156784139\C,-2.6672242857,-4.4156892626,0.4591022324\C,-3.934  
5152608,-3.9048269512,0.1380589467\H,-4.8152155829,-4.5363739883,0.174  
9421424\C,-4.0738180973,-2.5771917736,-0.2328578207\H,-0.5916794262,-4  
.031427173,0.6758053467\H,-2.5626553114,-5.4569214595,0.7479773761\C,-  
0.7908674155,0.0171789103,-0.4256695066\N,0.4421258926,0.6604981301,-0  
.4308043634\C,-4.4699255496,0.155301085,-1.04622929\C,-5.4319002511,-2  
.0752217804,-0.5644108459\O,-4.6517846517,1.3175470894,-1.3961396564\O  
, -6.4267681973,-2.7896711758,-0.494811287\N,-5.5411107832,-0.740958149  
6,-0.9725388797\C,-6.8831157673,-0.2337754669,-1.3209818708\H,-6.74831  
79806,0.5004920041,-2.1165476886\H,-7.449783578,-1.0808307012,-1.70904  
58392\C,-7.6074864643,0.3961099367,-0.1261681693\H,-6.9985918591,1.219

1152076,0.2689762277\H,-7.6996793666,-0.3511118962,0.6727397213\C,-8.9  
976449973,0.9189217881,-0.5099322683\H,-8.8983493296,1.6482834494,-1.3  
263379601\H,-9.6009728478,0.0907045202,-0.9077039292\C,-9.7344358068,1  
.5689232213,0.6647917009\H,-9.1723248857,2.4240016534,1.0611454387\H,-  
10.7233931396,1.9327887645,0.360958792\H,-9.8801168514,0.8569352324,1.  
4871225868\C,2.1052629665,-4.3998847126,4.0455080786\H,2.5407267555,-3  
.5705510444,4.6163449432\H,1.06515702,-4.5202644337,4.374247191\H,2.64  
83283924,-5.3127819822,4.3175125321\H,1.7818626233,-5.0001249047,1.993  
0611928\C,-1.6470866946,-2.2387669061,0.0443328615\C1,5.7800782396,0.6  
094040358,0.0511667413\Pt,3.3761998941,0.1618314106,-0.0251332815\C1,3  
.1934215232,0.5651773071,2.3269446822\s,3.5425644349,-0.1953920037,-2.  
3151939107\O,2.2743234793,-0.5315452704,-3.0433864404\C,4.7812149012,-  
1.4727590543,-2.6414657672\H,5.7141619038,-1.1874999778,-2.1509761187\  
H,4.4003201822,-2.4075457228,-2.2235745308\H,4.9016103685,-1.556773350  
7,-3.7254479209\C,4.3080290644,1.2497024683,-3.0886396841\H,5.25470760  
08,1.4576618404,-2.5860853524\H,4.4523922987,1.0275475607,-4.149969425  
4\H,3.6178128704,2.0868084293,-2.9613655247\\Version=EM64L-G09RevD.01\  
State=1-A\HF=-3031.451776\RMSD=5.590e-09\RMSF=1.357e-06\Dipole=-1.3098  
357,-1.6618907,-2.7440592\Quadrupole=-35.2670531,27.1856112,8.081442,-  
18.3817541,-34.6897503,-6.1708571\PG=C01 [X(C31H37C12N3O3Pt1S1)]\@

Archive Entries of complex **3** in CDCl<sub>3</sub>:

*trans*:

```
1\1\GINC-WN03\FOpt\RB3LYP\GenECP\C47H46C12N3O2P1Pt1\NVASILEV\06-Feb-20
17\0\#p b3lyp/genecp opt=tight freq test SCRF(SMD,Solvent=Chloroform)
\\Title Card Required\\0,1\C,-0.1756424112,-0.4495021359,-0.2788357195
\C,-2.2136641491,-1.429484451,-0.1620095078\N,-0.8399018523,-1.6078566
694,0.0069413028\C,-0.1415384387,-2.8265967528,0.4530677308\H,0.899957
06,-2.6994777078,0.1518770778\H,-0.538791401,-3.6729108124,-0.11360270
56\C,-0.2267562288,-3.0483894808,1.9668916769\H,0.2210647476,-2.181555
8403,2.4667417065\H,-1.2753917482,-3.0941307006,2.2870222833\C,0.50075
53089,-4.329859201,2.3949352128\H,1.551080218,-4.2718381138,2.07717304
57\C,-1.3789055708,2.9224782903,-0.1385251808\C,-2.1841423239,3.941071
1838,-0.6572682744\C,-1.0574917063,2.9505119385,1.2270765455\C,-2.6586
290143,4.966010281,0.1661912753\H,-2.4426322747,3.9394928234,-1.714155
021\C,-1.5374379027,3.9714951129,2.0438925765\H,-0.4236532664,2.174830
4208,1.6497282945\C,-2.3465514376,4.9988068131,1.5300047555\H,-3.28449
85697,5.7467765745,-0.2598135314\H,-1.2756255142,3.9756410469,3.099998
5772\C,-0.8284662106,1.8476187598,-1.0557942115\H,0.2598096791,1.91343
34514,-1.1298259149\H,-1.2359914408,1.960732775,-2.0650539471\C,-2.861
8552246,6.0965998504,2.4299281097\H,-3.5390960947,5.6987871276,3.19689
07293\H,-2.0412967703,6.5982484708,2.9582059032\H,-3.4099774523,6.8559
686983,1.8628400825\C,-3.6263127219,0.465174327,-0.8454098207\C,-4.738
6494234,-0.3463972604,-0.7358634938\C,-4.6206806194,-1.7116826231,-0.3
391088133\H,-3.7397184406,1.5003417281,-1.1414879244\C,-3.310222891,-3
.6671838832,0.3373535494\C,-4.4694481916,-4.4163641141,0.4166717241\C,
-5.7159710901,-3.8382657587,0.1293749222\H,-6.6297575087,-4.418650213,
0.1948130771\C,-5.7925332243,-2.5061081488,-0.2435733758\H,-2.36953660
89,-4.1446899426,0.5725619\H,-4.4135112179,-5.4606715828,0.7082946862\C,
-2.3774201247,-0.0983311579,-0.5561481712\N,-1.1096503602,0.47154574
85,-0.609832497\C,-6.0621298128,0.2456711643,-1.0419982304\C,-7.129757
```



5589,-1.9291985865,-0.5323399731\O,-6.1930442595,1.4189172887,-1.37993  
14021\O,-8.1610318642,-2.5870067666,-0.4302437582\N,-7.1786577124,-0.5  
901602434,-0.9344308169\C,-8.5022940217,-0.0058666451,-1.2281478911\H,  
-8.3555571993,0.7279387957,-2.0220208146\H,-9.1290005794,-0.8164640177  
, -1.6016876289\C,-9.1437765902,0.6511242882,-0.0008825561\H,-8.4747925  
65,1.4357096973,0.3749463768\H,-9.2449041293,-0.0976820919,0.795607592  
\C,-10.5173619778,1.2532109602,-0.3233377088\H,-10.4132039259,1.978281  
5755,-1.1429912222\H,-11.1837133344,0.4616564406,-0.6939945296\C,-11.1  
633815955,1.9399297118,0.8835032142\H,-10.538958877,2.7631030936,1.253  
1325796\H,-12.1446370427,2.3564370496,0.6260861964\H,-11.3084949108,1.  
2354592683,1.7123926247\C,0.438573133,-4.5648914887,3.9068295685\H,0.8  
98832624,-3.7341207197,4.45556134\H,-0.5983748488,-4.6583973171,4.2537  
948813\H,0.967285754,-5.4836668923,4.1873929925\H,0.0665032583,-5.1939  
265457,1.8714991383\C,-3.3432001924,-2.3001231735,-0.0398923707\C1,1.7  
715272197,0.3676081802,2.0492168123\P,4.2263513633,0.1857933242,-0.270  
0783947\C,4.7258050242,1.9432608325,-0.0306311196\C,3.7925409537,2.888  
0119815,0.4222966044\C,6.0387958313,2.3611388008,-0.313528854\C,4.1659  
368675,4.2234666225,0.5925828681\H,2.7786687466,2.5782147582,0.6497816  
265\C,6.408861453,3.6945549515,-0.136654648\H,6.771549543,1.6474820379  
, -0.6776631616\C,5.4721810944,4.6287953126,0.3143970487\H,3.4318345972  
,4.9446321226,0.9414942857\H,7.4270562453,4.0035459361,-0.3577156387\H  
,5.7601672569,5.6686136432,0.4451441477\C,5.000978593,-0.7781222086,1.  
0937371792\C,5.9379337128,-0.2318811969,1.9810717723\C,4.6165871714,-2  
.1215941548,1.2463702152\C,6.4855547417,-1.0177614165,2.9986158407\H,6  
.2375512612,0.8068135139,1.8909030798\C,5.1739421368,-2.9063443107,2.2  
557784596\H,3.8772185037,-2.5520592278,0.5762036318\C,6.1088695051,-2.  
3544486405,3.1362050105\H,7.2055913925,-0.5799451021,3.6848235177\H,4.  
8713590224,-3.9448954132,2.3598482584\H,6.5362883884,-2.9629709913,3.9  
287152967\C,5.1680304705,-0.2919461156,-1.7840031949\C,4.9479377637,0.  
4385820907,-2.9647738515\C,6.0853036118,-1.3516391109,-1.8008814692\C,  
5.6395113614,0.119263785,-4.1321573289\H,4.2384279792,1.2602755338,-2.  
9727509189\C,6.7723460897,-1.6729033475,-2.9755258147\H,6.2758787426,-

1.9270932184,-0.9013553956\C,6.5521451562,-0.9397231691,-4.141558944\H  
,5.4597197047,0.6939077619,-5.0368195511\H,7.4831103478,-2.4951471466,  
-2.9718174236\H,7.0884329746,-1.1892784108,-5.0533505598\Pt,1.84473442  
11,-0.1697405171,-0.2949989931\C1,1.7727793929,-0.7741542083,-2.613337  
6293\\Version=EM64L-G09RevD.01\State=1-A\HF=-3514.5754928\RMSD=1.429e-  
09\RMSF=1.105e-06\Dipole=1.6200538,-0.3215557,0.9139398\Quadrupole=-1.  
5814098,19.1482427,-17.5668329,-1.7557107,-1.9673999,-7.3913718\PG=C01  
[X(C47H46C12N3O2P1Pt1)]\@

**cis:**

1\1\GINC-WN29\FOpt\RB3LYP\GenECP\C47H46C12N3O2P1Pt1\NVASILEV\05-Feb-20  
17\0\#p b3lyp/genecp opt=tight freq test SCRF(SMD,Solvent=Chloroform)  
\Title Card Required\0,1\C,0.5263983258,0.0007281808,0.6570931932\C,  
-1.3871490261,-1.1971166888,0.4803890741\N,-0.0496869476,-1.2193921005  
,0.8777587169\C,0.6816250214,-2.3377653118,1.4992163277\H,1.7404009935  
, -2.0975841302,1.3872769944\H,0.4888147818,-3.2378925231,0.9099513838\  
C,0.349728701,-2.5300738658,2.9828739232\H,0.6023112506,-1.6051533286,  
3.5138209738\H,-0.7278492588,-2.6904670352,3.1139735432\C,1.1264850273  
, -3.709322131,3.5836888956\H,2.2034822491,-3.5415267283,3.4440235446\C  
, -1.1034088937,3.2230430992,0.3554929561\C,-1.8726220487,4.096141165,-  
0.4203629496\C,-1.1322233792,3.3603776472,1.7514118334\C,-2.6566969625  
,5.0841445705,0.1813866759\H,-1.8604100669,4.0090595528,-1.5048789981\  
C,-1.9196935054,4.3438377404,2.3450427212\H,-0.5314322491,2.7000951968  
,2.3719780706\C,-2.6970064681,5.2237021844,1.573148928\H,-3.2482694637  
,5.7505478853,-0.4420386498\H,-1.9279834888,4.4347082628,3.429203959\C  
, -0.222935756,2.1913950191,-0.3216799852\H,0.8355055803,2.3984194573,-  
0.1424291976\H,-0.389486474,2.2094371833,-1.4037538788\C,-3.5471207532  
,6.2830872336,2.2330328522\H,-4.3014773805,5.836223136,2.8933040963\H,  
-2.9388944844,6.9543915287,2.8525508791\H,-4.0719554965,6.8941750905,1  
.491521211\C,-2.8570521456,0.5077285956,-0.5118797275\C,-3.8752410706,

-0.4239040794,-0.562924512\C,-3.6810904682,-1.7569653873,-0.094938662\  
H,-3.0308423438,1.5164873184,-0.8639601081\C,-2.3056458648,-3.53475980  
12,0.8770338145\C,-3.3740742538,-4.4077237118,0.7913051433\C,-4.606722  
9385,-3.9815143605,0.2719442263\H,-5.4500569799,-4.6603943959,0.206719  
2635\C,-4.759277607,-2.6765079036,-0.1670941944\H,-1.374335829,-3.8993  
483383,1.286209741\H,-3.2579950021,-5.431778366,1.1326395434\C,-1.6237  
128252,0.0982241034,0.0108041048\N,-0.433373641,0.8066113725,0.1402669  
959\C,-5.1773506093,0.0038029787,-1.1272643068\C,-6.0769441361,-2.2645  
34168,-0.7135519145\O,-5.369502386,1.1446557517,-1.538472186\O,-7.0320  
826748,-3.0335479654,-0.7653697887\N,-6.1957253479,-0.9530940038,-1.18  
5617742\C,-7.495496848,-0.5391224857,-1.7509443457\H,-7.2822524027,0.1  
96073429,-2.5282715453\H,-7.9368797254,-1.4253079515,-2.2089597381\C,-  
8.439090397,0.0501241203,-0.6966535075\H,-7.9582999726,0.9210494084,-0  
.2331104857\H,-8.5987262986,-0.6921881918,0.0959859801\C,-9.7886581619  
,0.4628668185,-1.2984688874\H,-9.6211072943,1.1942395442,-2.1016862459  
\H,-10.2594033159,-0.4115945638,-1.7697680872\C,-10.7448125188,1.05798  
77086,-0.26057228\H,-10.3177679272,1.9546296105,0.2062717256\H,-11.699  
7824103,1.3441613742,-0.7174353956\H,-10.9612589464,0.338745421,0.5395  
280517\C,0.8329984148,-3.9099359985,5.0731575743\H,1.0997839623,-3.017  
3246959,5.6519255111\H,-0.2314702298,-4.1128566298,5.2464046168\H,1.40  
32213454,-4.7540023484,5.4788615338\H,0.8835130102,-4.6308007382,3.034  
3477186\C,-2.4193853167,-2.1885219472,0.4437383376\C1,4.6254205088,1.3  
213968951,1.7134458514\C1,1.5816250737,1.1398909391,3.2937506157\Pt,2.  
4048990032,0.537275599,1.0706255245\P,3.2402738987,-0.0834339601,-0.99  
84098619\C,3.5965331095,1.335712063,-2.1152007842\C,3.9005317165,2.591  
4304675,-1.5649540892\C,3.5986638866,1.1815074532,-3.5134154808\C,4.20  
1406639,3.6706491876,-2.3981712278\H,3.9165553378,2.7186831036,-0.4879  
907853\C,3.902187793,2.2642687213,-4.3403853533\H,3.3595809037,0.22290  
63799,-3.9622584678\C,4.2021017959,3.5105295988,-3.7850493578\H,4.4345  
114526,4.6360903004,-1.9578088034\H,3.9002343732,2.1318408175,-5.41884  
91517\H,4.4344443748,4.3527667308,-4.4312247881\C,4.7905963979,-1.0665  
930839,-0.8735496372\C,5.7348612065,-1.0710014114,-1.9111969163\C,5.00

66757009,-1.8729652528,0.2550845713\C,6.8704753283,-1.8784124753,-1.82  
35428611\H,5.5960998298,-0.4425619475,-2.7845715914\C,6.1392436898,-2.  
6842942768,0.3347547053\H,4.2989102252,-1.8513386678,1.0775410629\C,7.  
072604825,-2.6885912919,-0.7044267874\H,7.5991245232,-1.8678340249,-2.  
6296286591\H,6.2977619766,-3.3006470144,1.2153525763\H,7.9590444436,-3.  
.313697778,-0.6378855309\C,2.100454364,-1.1615292306,-1.9723132394\C,0.  
.9867020546,-0.6014249208,-2.6228105423\C,2.296748594,-2.5494277052,-2.  
.0360363452\C,0.0962495143,-1.4132954845,-3.32583493\H,0.8182155713,0.  
4714896738,-2.5974157312\C,1.3980077059,-3.359981631,-2.7350127365\H,3.  
.1522019042,-3.0043822069,-1.5479945695\C,0.2979985027,-2.795357867,-3.  
.3816945098\H,-0.7548875082,-0.964547691,-3.8306986349\H,1.5674197806,  
-4.4324548184,-2.7783298074\H,-0.3968131683,-3.425854004,-3.9296960423  
\Version=EM64L-G09RevD.01\State=1-A\HF=-3514.5831551\RMSD=2.042e-09\R  
MSF=2.905e-06\Dipole=-1.0307597,-2.9198054,-4.466783\Quadrupole=-23.38  
48672,25.891839,-2.5069718,-24.5859904,-34.0556819,-16.308852\PG=C01 [X  
(C47H46Cl2N3O2P1Pt1)]\@

## Archive Entries of complex 4 in Pyridine:

### *trans:*

```
1\1\GINC-WN10\FOpt\RB3LYP\GenECP\C34H36Cl2N4O2Pt1\NVASILEV\04-Feb-2017
\0\#p b3lyp/genecp opt=tight freq test SCRF(SMD,Solvent=Pyridine)\Title
Card Required\0,1\C,1.1587546844,-0.333062069,-0.3449866794\C,-0.
8529429888,-1.3642683992,-0.2250318752\N,0.5262690349,-1.5160230632,-0
.0815672965\C,1.260679619,-2.7329817671,0.3105409513\H,2.2902008947,-2
.5809530319,-0.0194388191\H,0.8593369797,-3.5712491534,-0.2638472879\C
,1.2301428107,-2.9945885858,1.8200362158\H,1.6805361295,-2.1332407272,
2.3282043154\H,0.193594999,-3.0664844099,2.1728655766\C,1.9917943105,-
4.2754128363,2.1854346098\H,3.0212452927,-4.2047636345,1.8073819712\C,
-0.1580073249,3.0033173615,-0.1014312513\C,-0.9704615837,4.0218038453,
-0.6099724493\C,0.1240439384,2.99356979,1.2729860318\C,-1.4898390719,5
.0091328855,0.2320528785\H,-1.2010075288,4.0466190711,-1.6728106141\C,
-0.4014201205,3.9765217305,2.1090032772\H,0.7599508276,2.2161255227,1.
6891492077\C,-1.2167351803,5.0039339137,1.6049646146\H,-2.1211818244,5
.7897962754,-0.1859855494\H,-0.1722386446,3.9506447652,3.1723675905\C,
0.4370907824,1.9721460718,-1.0410569787\H,1.5234803244,2.0777297741,-1
.0992033847\H,0.0340124755,2.1008599888,-2.0499817882\C,-1.768583334,6
.0702221992,2.5206900585\H,-2.2816043983,5.6301289347,3.3846607323\H,-
0.96780594,6.70860427,2.9169714244\H,-2.4813386232,6.7162872053,1.9979
111819\C,-2.3193848047,0.5119101283,-0.8434570594\C,-3.4110694027,-0.3
277688604,-0.7353384929\C,-3.2554741389,-1.6979251096,-0.3695062686\H,
-2.4585763292,1.5493567737,-1.1197761639\C,-1.888243584,-3.6365146396,
0.2424290164\C,-3.0282928723,-4.4138971952,0.3256356371\C,-4.292475945
5,-3.85889342,0.0721015067\H,-5.1897362594,-4.4639030579,0.1412253149\
C,-4.4072238232,-2.521273953,-0.2709430058\H,-0.9334142703,-4.09760293
29,0.4507598792\H,-2.9434013569,-5.4624342297,0.5938731598\C,-1.053953
9434,-0.0279690545,-0.582464451\N,0.1977323418,0.5760438696,-0.6356735
462\C,-4.7528324346,0.2390488746,-1.0093333064\C,-5.7625028905,-1.9699
```

165162,-0.5243236974\O,-4.9156940902,1.4140793875,-1.3260905367\O,-6.7  
761122085,-2.6543356553,-0.4218716772\N,-5.8486333394,-0.6230525726,-0  
.8944583792\C,-7.1891092986,-0.0617454419,-1.153112023\H,-7.0755390902  
,0.6821311401,-1.94302452\H,-7.8092257415,-0.8801480511,-1.5200694201\  
C,-7.8149676326,0.5719542305,0.0943381982\H,-7.1505654988,1.3624081872  
,0.465935679\H,-7.8881931679,-0.1862708048,0.8849313697\C,-9.203440654  
1,1.1570873927,-0.1925507694\H,-9.1266284127,1.8928640792,-1.005675558  
5\H,-9.8663263942,0.3603816701,-0.5585489635\C,-9.8331712726,1.8209532  
709,1.0351746974\H,-9.2110264627,2.6466780223,1.4032236502\H,-10.82401  
11889,2.229362064,0.8022123077\H,-9.9543632627,1.1045309288,1.85772818  
55\C,2.0195777348,-4.5362632938,3.6940785763\H,2.5085017162,-3.7130296  
931,4.2301048118\H,1.0051255249,-4.6406986484,4.099597349\H,2.56751959  
48,-5.4571840426,3.9268484162\H,1.5332892075,-5.1328544562,1.672815699  
5\C,-1.9600473066,-2.263143847,-0.1047434081\C1,3.1436182701,0.5340749  
431,1.9589839473\Pt,3.1250149452,-0.0220817914,-0.372807038\C1,3.18362  
46461,-0.5876484047,-2.7042958155\N,5.2286659949,0.3204705383,-0.43186  
07413\C,5.7319821946,1.3506676117,-1.1397973593\H,5.0131238003,1.97001  
51587,-1.6633811641\C,6.074695336,-0.4875428025,0.2367313001\H,5.62200  
96829,-1.2975342206,0.7965769787\C,7.0968998753,1.609331133,-1.2004065  
829\H,7.455334443,2.4537201447,-1.7796004472\C,7.4517682838,-0.2959444  
445,0.2163220901\H,8.0941130955,-0.9754701754,0.7663577581\C,7.9750077  
618,0.7716524642,-0.5129624309\H,9.0460510883,0.9481593744,-0.54432536  
63\\Version=EM64L-G09RevD.01\State=1-A\HF=-2726.5656355\RMSD=7.134e-09  
\RMSF=1.472e-06\Dipole=1.8439814,-0.51829,0.663707\Quadrupole=14.43807  
11,11.0354143,-25.4734854,-1.7115093,-1.8094824,-10.0581741\PG=C01 [X(  
C34H36C12N4O2Pt1)]\@

**cis:**

1\1\GINC-WN11\FOpt\RB3LYP\GenECP\C34H36C12N4O2Pt1\NVASILEV\04-Feb-2017  
\0\#p b3lyp/genecp opt=tight freq test SCRF(SMD,Solvent=Pyridine)\Ti

tle Card Required\0,1\C,-1.4196139856,-0.1797175684,-0.0407765014\C,0  
.5721036202,-1.2555608382,-0.0505180607\N,-0.7946778372,-1.3671897676,  
-0.3075914185\C,-1.5138579747,-2.5493670689,-0.819187947\H,-2.56939134  
14,-2.3733117414,-0.6015180718\H,-1.1971103026,-3.4163470991,-0.233293  
895\C,-1.325767907,-2.7697245825,-2.3239783487\H,-1.7191884472,-1.8931  
279583,-2.851192502\H,-0.2586558105,-2.8394923687,-2.5696500506\C,-2.0  
495262743,-4.0373091713,-2.7970990775\H,-3.1146151541,-3.9656763667,-2  
.5357409896\C,-0.0585032606,3.1152578974,-0.1234756381\C,0.762054644,4  
.1127570972,0.4122730396\C,-0.3114533686,3.1219461687,-1.5034589806\C,  
1.3190788793,5.0962819086,-0.4101168691\H,0.9687943512,4.1248952463,1.  
4801293229\C,0.2511213434,4.1011483775,-2.3191994319\H,-0.9535224978,2  
.3602434928,-1.939309174\C,1.0761353043,5.1074418722,-1.7886203555\H,1  
.9565174433,5.8608658198,0.0278478969\H,0.0441485803,4.0882071651,-3.3  
872788788\C,-0.6924792244,2.0830562865,0.7895952625\H,-1.7775693669,2.  
2068530502,0.8238196988\H,-0.3077168922,2.1883662126,1.8083287144\C,1.  
6710457081,6.168578172,-2.6832952964\H,2.203776051,5.7233601918,-3.532  
6555508\H,0.8921966908,6.8194342337,-3.102186009\H,2.3766677804,6.8031  
24611,-2.1371653432\C,2.027610833,0.5537934806,0.7623242453\C,3.103504  
0388,-0.3109288291,0.7100850929\C,2.9446860539,-1.6618081653,0.2795216  
285\H,2.1682396366,1.5760045746,1.0901599537\C,1.5862194654,-3.5359703  
889,-0.5222126136\C,2.709443246,-4.3413858656,-0.5427134074\C,3.960929  
4699,-3.8324927698,-0.1616816224\H,4.8455521125,-4.4594786409,-0.17948  
63886\C,4.0792899777,-2.5130386461,0.2441876348\H,0.6406948477,-3.9614  
229551,-0.8255291202\H,2.6213461823,-5.3761344733,-0.858980448\C,0.774  
8424315,0.058684689,0.3778021611\N,-0.4640826104,0.6907979914,0.365133  
8998\C,4.4314102749,0.2054699798,1.1216067475\C,5.4198067554,-2.013615  
0657,0.6415666054\O,4.5957387492,1.3636176832,1.4942727819\O,6.4194986  
63,-2.7243944103,0.6037987117\N,5.5086638514,-0.6855603117,1.073104078  
\C,6.8357545185,-0.1821196803,1.47876539\H,6.6685287059,0.5603412589,2  
.2601245509\H,7.3794830341,-1.0280302001,1.9010939075\C,7.6193716439,0  
.431068339,0.3129166748\H,7.0379263166,1.2568151953,-0.1168466208\H,7.  
7402881503,-0.323658092,-0.4749206108\C,8.9965903973,0.942216234,0.754

8947791\H, 8.8686371771, 1.6890250664, 1.551221483\H, 9.5660665137, 0.11314  
70107, 1.1982470283\C, 9.8007941565, 1.5566323733, -0.3944906609\H, 9.27322  
18159, 2.4120028672, -0.8354649725\H, 10.7796091211, 1.9115172437, -0.04963  
52761\H, 9.974704387, 0.8253939971, -1.1941944274\C, -1.9093761263, -4.2688  
613117, -4.3039548979\H, -2.3342816503, -3.4336672038, -4.8744499831\H, -0.  
8563146988, -4.3697746636, -4.5959939934\H, -2.4300341326, -5.1828776037, -  
4.6137399955\H, -1.6559862233, -4.9085133454, -2.2539587386\C, 1.663145175  
, -2.1791532897, -0.1167250434\C1, -3.1885456851, 0.6197060622, -2.48298263  
93\Pt, -3.3779845577, 0.1693419701, -0.1420279429\C1, -5.7994634277, 0.5663  
014549, -0.1998240846\N, -3.5762988987, -0.1778760972, 1.8860677394\C, -3.3  
812134407, -1.4075845141, 2.4069111009\H, -3.0868015715, -2.1850842944, 1.7  
134855094\C, -3.947275995, 0.8316737868, 2.7026146644\H, -4.102690456, 1.79  
55747342, 2.2359049353\C, -3.551657982, -1.6666431757, 3.7615391591\H, -3.3  
886360147, -2.6726389943, 4.13312828\C, -4.1284265608, 0.6416456003, 4.0671  
606517\H, -4.4243278163, 1.483499757, 4.6838243698\C, -3.929921783, -0.6271  
791039, 4.6104672852\H, -4.068224822, -0.8027135299, 5.6729348931\\Version  
=EM64L-G09RevD.01\State=1-A\HF=-2726.5621609\RMSD=5.093e-09\RMSF=1.764  
e-06\Dipole=3.1071335, -2.3304674, 4.5204047\Quadrupole=-60.6662217, 33.0  
998174, 27.5664042, 18.4556537, -39.432165, 3.0721977\PG=C01 [X(C34H36C12N  
4O2Pt1)]\@



Archive Entries of complex **5** in CDCl<sub>3</sub>:

*trans*:

1\1\GINC-WN21\SP\RB3LYP\GenECP\C36H41C12N5O2Pt1\NVASILEV\07-Feb-2017\0  
\\#p rb3lyp/genecp nmr test SCRF(SMD,Solvent=Chloroform) POP=NBOREAD\  
Title Card Required\\0,1\C,0,0.57089,-0.383037,-0.293856\C,0,-1.474958  
, -1.355158,-0.237142\N,0,-0.10419,-1.552849,-0.073696\C,0,0.585395,-2.  
79963,0.303082\H,0,1.626148,-2.667933,0.000791\H,0,0.175448,-3.611673,  
-0.302936\C,0,0.51065,-3.098876,1.804118\H,0,0.972095,-2.263609,2.3443  
57\H,0,-0.535636,-3.150295,2.131329\C,0,1.228564,-4.408603,2.156514\H,  
0,2.271937,-4.351562,1.816538\C,0,-0.641066,2.983588,0.022984\C,0,-1.4  
47812,4.01932,-0.458124\C,0,-0.343396,2.945953,1.393754\C,0,-1.949185,  
4.995555,0.407544\H,0,-1.687586,4.068691,-1.518267\C,0,-0.850444,3.918  
043,2.252547\H,0,0.293585,2.157623,1.78732\C,0,-1.66246,4.961357,1.776  
703\H,0,-2.576618,5.790295,0.010666\H,0,-0.607484,3.871507,3.312162\C,  
0,-0.065116,1.960644,-0.936896\H,0,1.0252,2.028184,-0.974062\H,0,-0.44  
4273,2.130932,-1.949268\C,0,-2.202078,6.00899,2.721164\H,0,-2.81399,5.  
556442,3.511825\H,0,-1.389615,6.55359,3.219406\H,0,-2.822898,6.74151,2  
.195162\C,0,-2.872802,0.580483,-0.827909\C,0,-3.990715,-0.229456,-0.76  
824\C,0,-3.882891,-1.613422,-0.440689\H,0,-2.978913,1.629984,-1.071177  
\C,0,-2.587589,-3.607297,0.147328\C,0,-3.751296,-4.352787,0.182872\C,0  
, -4.992738,-3.754374,-0.08442\H,0,-5.91007,-4.332048,-0.053524\C,0,-5.  
059637,-2.405114,-0.391841\H,0,-1.651407,-4.100916,0.366425\H,0,-3.702  
963,-5.410186,0.42443\C,0,-1.628865,-0.003445,-0.560288\N,0,-0.358325,  
0.561981,-0.575909\C,0,-5.308337,0.384543,-1.05346\C,0,-6.391635,-1.80  
6989,-0.660162\O,0,-5.431294,1.573902,-1.333468\O,0,-7.42734,-2.463064  
, -0.597779\N,0,-6.430305,-0.449489,-0.995504\C,0,-7.748452,0.156097,-1  
.269592\H,0,-7.591778,0.927559,-2.024935\H,0,-8.376597,-0.63142,-1.687  
498\C,0,-8.395998,0.755151,-0.016141\H,0,-7.725828,1.516441,0.402981\H  
,0,-8.507137,-0.031568,0.741527\C,0,-9.763906,1.380054,-0.318687\H,0,-  
9.649591,2.144211,-1.100622\H,0,-10.431418,0.611524,-0.733153\C,0,-10.

415886,2.00983,0.915706\H,0,-9.790133,2.810231,1.330345\H,0,-11.392917  
,2.444008,0.671727\H,0,-10.571189,1.266075,1.707606\C,0,1.197221,-4.71  
3643,3.656834\H,0,1.681524,-3.915857,4.233407\H,0,0.167218,-4.809454,4  
.023351\H,0,1.718944,-5.651556,3.881551\H,0,0.769558,-5.241083,1.60389  
7\C,0,-2.610311,-2.22339,-0.164018\C1,0,2.539516,0.344926,2.060652\Pt,  
0,2.546095,-0.134626,-0.288863\C1,0,2.587797,-0.617396,-2.638739\N,0,4  
.656494,0.125698,-0.318183\C,0,5.250797,0.975908,-1.183917\H,0,4.58964  
3,1.51169,-1.854625\C,0,5.46264,-0.559448,0.522298\H,0,4.96691,-1.2252  
93,1.219\C,0,6.615622,1.170765,-1.245403\H,0,7.002833,1.878358,-1.9669  
66\C,0,6.83748,-0.438622,0.527956\H,0,7.404043,-1.029229,1.236282\C,0,  
7.477686,0.448158,-0.378275\N,0,8.829847,0.595185,-0.414616\C,0,9.4405  
75,1.539775,-1.344169\H,0,10.524935,1.487518,-1.242543\H,0,9.184609,1.  
299644,-2.383547\H,0,9.126852,2.571811,-1.138846\C,0,9.674897,-0.15034  
7,0.512608\H,0,10.719857,0.083689,0.307534\H,0,9.46296,0.113729,1.5570  
14\H,0,9.539368,-1.232617,0.394739\\Version=EM64L-G09RevA.02\State=1-A  
\HF=-2860.5424807\RMSD=4.839e-09\Dipole=3.5919187,-0.3515107,0.670874\  
Quadrupole=41.7865693,-5.0543137,-36.7322556,2.3537215,-4.0802416,-9.4  
966865\PG=C01 [X(C36H41C12N5O2Pt1)]\@

**cis:**

1\1\GINC-WN19\FOpt\RB3LYP\GenECP\C36H41C12N5O2Pt1\NVASILEV\04-Feb-2017  
\0\#p b3lyp/genecp opt=tight freq test SCRF(SMD,Solvent=Chloroform)\  
Title Card Required\\0,1\C,1.1143347419,0.2418276583,0.5534061921\C,-0

.8444405905,-0.8277622079,0.9571411855\N,0.4668629642,-0.6293217851,1.3906250668\C,1.1067432561,-1.1957811383,2.5929656774\H,2.1808879191,-1.0653013727,2.4468930085\H,0.9054667411,-2.2704354855,2.6096321083\C,0.6754475613,-0.5059496159,3.8919689017\H,0.9401111857,0.554486123,3.8173972348\H,-0.4142982263,-0.5590416352,4.0093962528\C,1.3608233093,-1.1305997216,5.1148442877\H,2.4503947298,-1.0709767814,4.9873990433\C,-0.2780287648,2.8262041219,-1.4653649182\C,-1.085280284,3.2158545413,-2.5382947105\C,-0.1607221172,3.6877171815,-0.3640783332\C,-1.7629768675,4.438161804,-2.5149460818\H,-1.1852919896,2.5644642635,-3.4042253453\C,-0.8420338844,4.9021052012,-0.3443567979\H,0.4721120434,3.4106181627,0.4755486392\C,-1.6555724771,5.3008406948,-1.4184512534\H,-2.3854894891,4.7202718416,-3.3609919322\H,-0.7354673667,5.557489589,0.5175703147\C,0.4946118829,1.5224444309,-1.5239022162\H,1.5710850297,1.7062769826,-1.4929191681\H,0.2684157373,0.984108922,-2.4498487281\C,-2.3938338106,6.6176533842,-1.3784850585\H,-3.1640565425,6.6195480062,-0.5959364808\H,-1.714895024,7.4508437503,-1.158958259\H,-2.8889379038,6.8286091118,-2.331950398\C,-2.1796308339,0.0229251841,-0.9248864678\C,-3.2411701978,-0.7530061691,-0.5018162959\C,-3.1352281434,-1.5818630862,0.6541419287\H,-2.2863055984,0.6506641139,-1.8002811601\C,-1.8925721107,-2.5094721564,2.5492000771\C,-2.998064012,-3.2583978529,2.9070080911\C,-4.1852582951,-3.1837272214,2.1614843645\H,-5.0575711933,-3.7645979069,2.440562776\C,-4.2537894462,-2.3602451926,1.0494890283\H,-0.9980390651,-2.5922162276,3.1498767547\H,-2.9468843467,-3.9074749702,3.77579629\C,-0.9937844413,-0.0320837465,-0.1824114037\N,0.2201871904,0.6109876728,-0.3973625925\C,-4.4975921921,-0.696765545,-1.286187338\C,-5.5258816822,-2.3088948803,0.2859508326\O,-4.6158131515,0.0117733874,-2.2820589758\O,-6.5157249817,-2.9529380145,0.6202274822\N,-5.561003429,-1.494040992,-0.8505480218\C,-6.8206401356,-1.4428001942,-1.6195977591\H,-6.5484438995,-1.2562277436,-2.6592662609\H,-7.2788947106,-2.4295888922,-1.5412925582\C,-7.7801648387,-0.361941625,-1.1097905617\H,-7.2818354195,0.6146346585,-1.1628019729\H,-8.006168444,-0.5539620748,-0.0531520655\C,-9.0835334056,-0.3225233269,-1.9180407405\H,-8.8498482005,-0.138348078,-2.

9761282168\H,-9.5675839688,-1.3084875858,-1.8753890417\C,-10.059632484  
3,0.7462540407,-1.4179543481\H,-9.6182504333,1.7488974945,-1.480783198  
5\H,-10.9818505514,0.7518090869,-2.0114232615\H,-10.3385133265,0.57123  
79879,-0.3711284375\C,0.9643627374,-0.4441844721,6.4250119292\H,1.2367  
577332,0.6181022626,6.4117685827\H,-0.1174165283,-0.5081844572,6.59886  
78261\H,1.4677258835,-0.9070688584,7.2821274222\H,1.1137947444,-2.2010  
130303,5.1719255805\C,-1.9211905025,-1.6484925808,1.4218208075\C1,2.45  
75413072,2.4540902395,2.2830833432\C1,5.3829249613,1.4256553873,0.7552  
184563\N,3.5395517209,-0.6136756617,-0.7691485762\C,3.3841515225,-1.94  
07686742,-0.5597816181\H,2.9468974841,-2.2281830447,0.3888886534\C,4.0  
922475105,-0.2299777786,-1.9438651659\H,4.2274869558,0.8350520122,-2.0  
826457114\C,3.7577952064,-2.9014189223,-1.4758137098\H,3.6052408573,-3  
.9416516611,-1.2187164965\C,4.4847741087,-1.1208182091,-2.9200166131\H  
,4.9199873937,-0.7238525827,-3.8277814699\C,4.3308860265,-2.5191562116  
, -2.7189741208\Pt,3.0230320869,0.7921397439,0.6592030486\C,5.323118852  
5,-2.9909010062,-4.9017776236\H,6.2727459257,-2.4701830172,-4.72292164  
05\H,5.5234988936,-3.8618786449,-5.525895529\H,4.6577243322,-2.3197220  
842,-5.4580458312\C,4.5709192505,-4.8589386075,-3.3804958723\H,3.52608  
98554,-5.1291049488,-3.1835897783\H,4.90666519,-5.4215167836,-4.251763  
182\H,5.178185434,-5.1658853566,-2.5191250405\N,4.7068680415,-3.430760  
2236,-3.652781849\\Version=EM64L-G09RevD.01\State=1-A\HF=-2860.536353\  
RMSD=7.334e-09\RMSF=1.456e-06\Dipole=-1.4692971,-5.5238789,-3.6743006\  
Quadrupole=-41.5399353,16.88435,24.6555853,-52.8449664,-41.759967,-1.4  
797118\PG=C01 [X(C36H41Cl2N5O2Pt1)]\@