Supporting information

Coordination Versatility of the *p*-Hydroquinone-functionalyzed Dibenzobarrelene-based PC(sp^3)P Pincer Ligands

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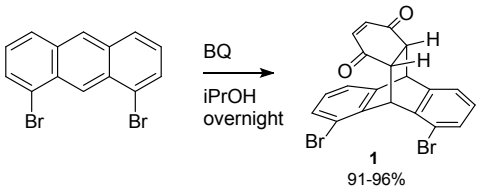
General Considerations. All manipulations were performed using standard Schlenk techniques under dry N_2 or Ar. All reagents were purchased from the usual suppliers and used without further purification**.** All reagents were weighed and handled in air. ^{1}H-, ^{13}C- and ^{31}P-NMR spectra were recorded on a Bruker 400 or 500 MHz instruments with chemical shifts reported in ppm relative to the residual deuterated solvent or the internal standard tetramethylsilane. Diffraction data were collected with a Bruker APEX CCD instrument (MoKα radiation (λ = 0.71073Å)). Crystals were mounted onto glass fibers using epoxy. Single crystal reflection data were collected on a Bruker APEX CCD X-ray diffraction system controlled by a Pentium-based PC running the SMART software package.[2] The integration of data frames and refinement of cell structure were done by the SAINT+ program package.[3] Refinement of the structure **8** on F^2 was carried out by the SHELXTL software package.[4] Electrochemical measurements were conducted with a three-electrode system using a CHI bipotentiostat (model 750, CH Instruments, Austin, TX).

Experimental Details:

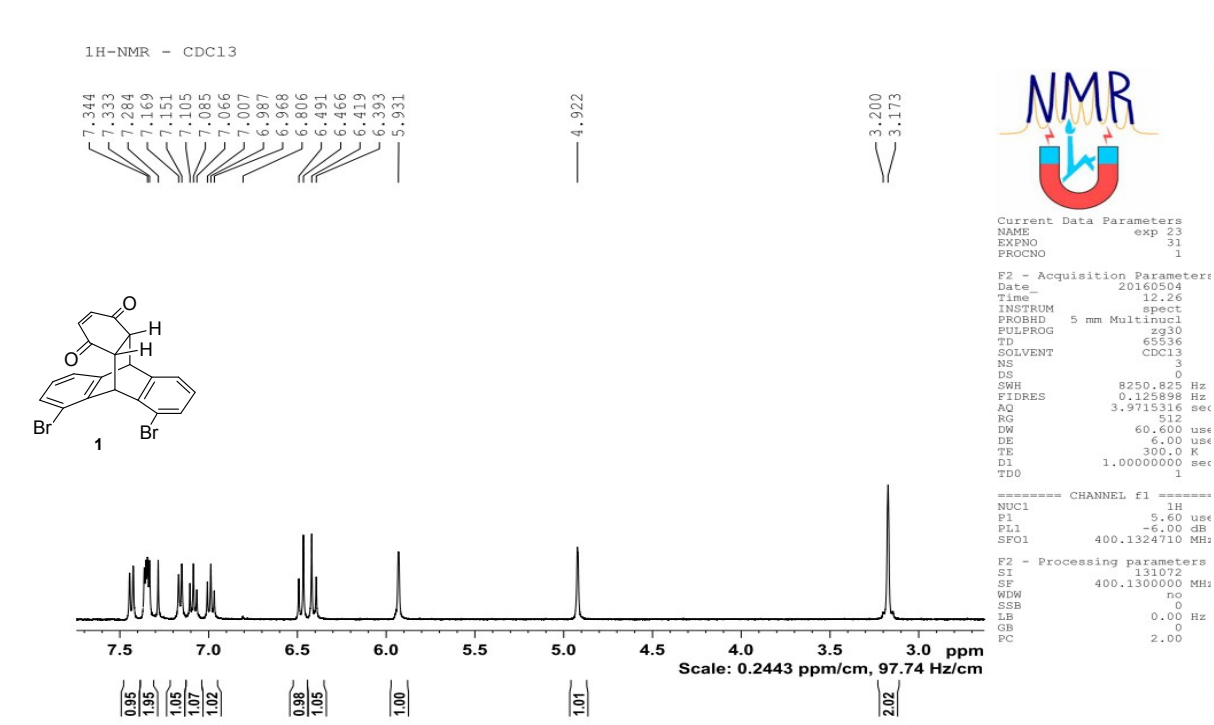


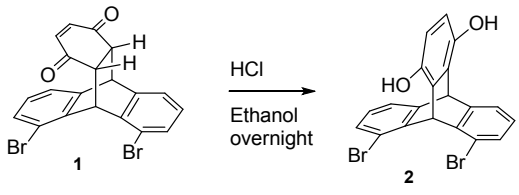
1
91-96%

1,8-dibromoanthracene (3 gr, 8.92 mmol) and *p*-benzoquinone (3.86 gr, 34 mmol) in 50 ml of isopropanol was heated under reflux overnight. The mixture was allowed to cool, then filtered. The brown solid was then transferred to a vessel with 15-20 ml of diethyl ether, stirred for 5-10 minutes in

order to dissolve any *p*-benzoquinone excess left, then filtered. The process was repeated several times, until the filtrate became clear, affording compound **1** as an off-white solid in 91-96% yield (3.58 gr).

^{1}H-NMR ($CDCl_3$) δ: 3.17 (s, 2H), 7.91 (s, 1H), 5.92 (s, 1H), 6.40 (d, 1H, J= 10.19 Hz), 6.47 (d, 1H, J= 10.19 Hz), 6.98 (t, 1H, J= 7.55 Hz), 7.07 (t, 1H, J= 7.55 Hz), 7.14 (d, 1H, J= 7.21 Hz), 7.32 (d, 1H, J= 8.05 Hz), 7.33 (d, 1H, J= 7.24 Hz), 7.42 (d, 1H, J= 8.05 Hz).

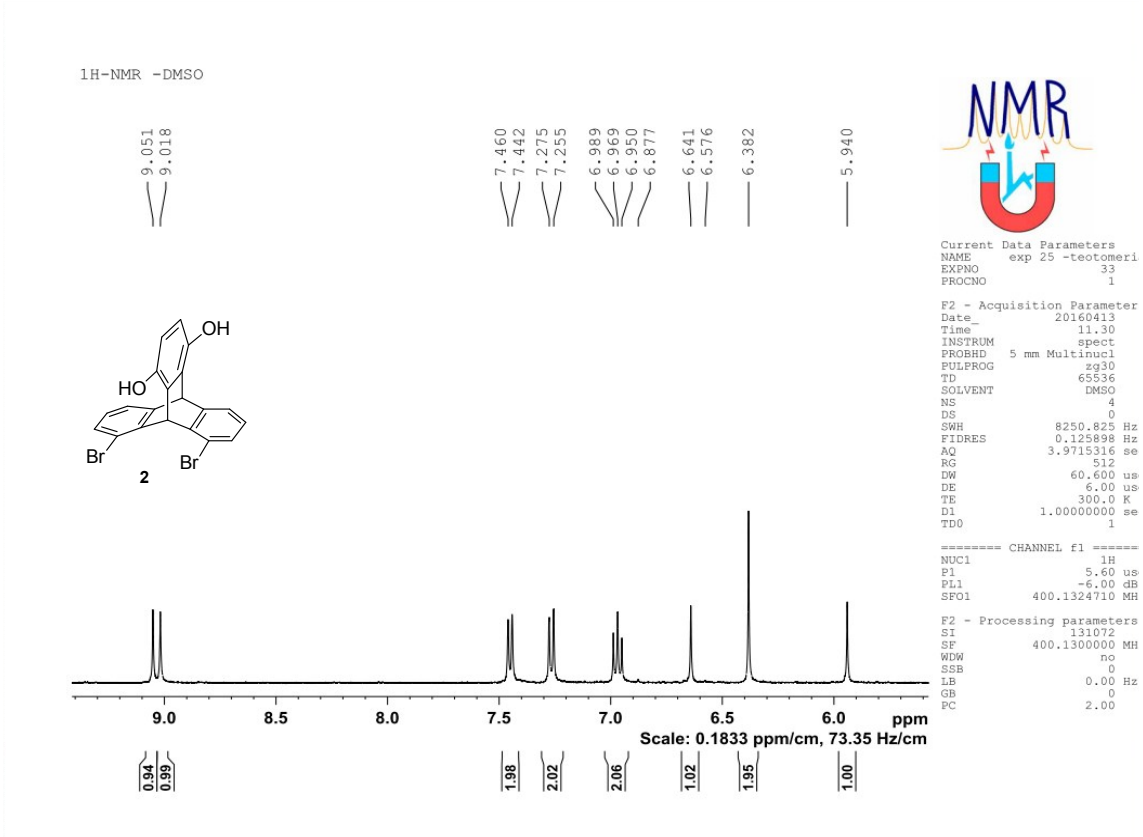


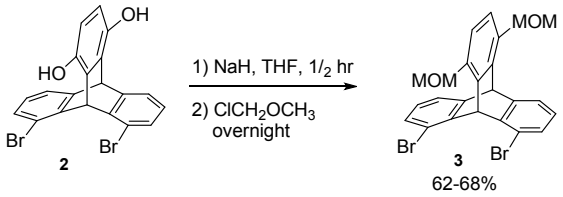


93-95%

HCl 37% (1 mL) was added to the solution of **1** (3.37 gr, 7,58 mmol) in ethanol (50 mL) and heated under reflux overnight. The mixture was allowed to cool, then dissolved with a minimal amount of THF and extracted upon addition of EtOAc and $NaHCO_3$ solution. The organic layer were separated, drayed over Na_2SO_4, filtered and concentrated under reduced pressure, affording compound **2** in 93-95% (3.15 gr).

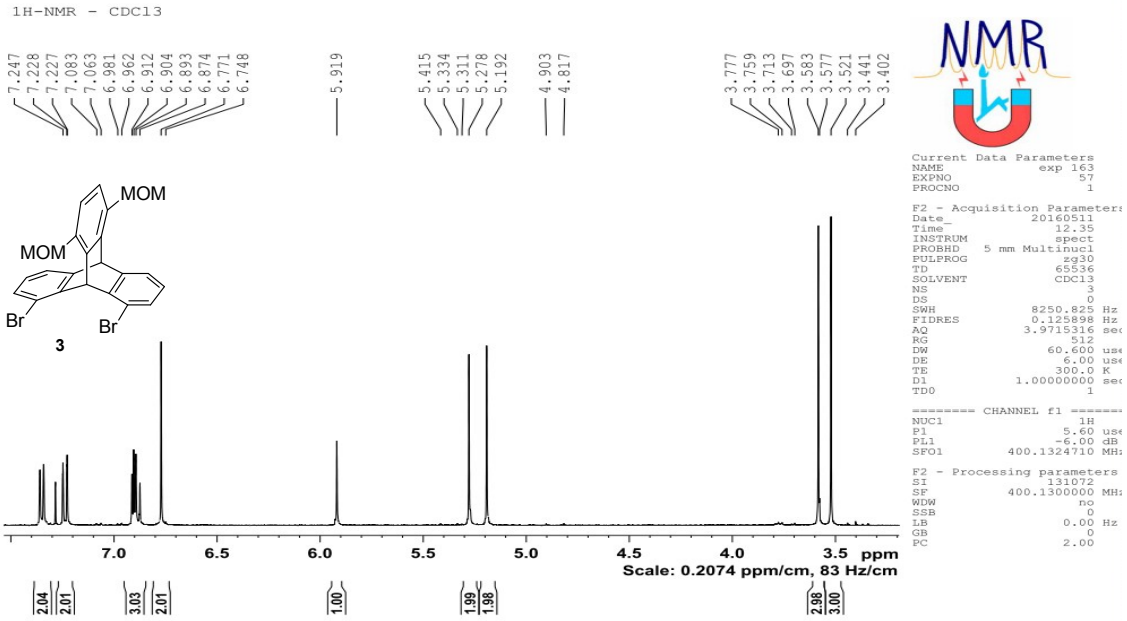
^{1}H-NMR (DMSO-d_6) δ: 5.94 (s, 1H), 6.38 (s, 2H), 6.64 (s, 1H), 6.97 (t, 2H,J = 7.74 Hz), 7.26 (d, 2H, J = 8.25 Hz), 7.44 (d, 2H, J = 7.17 Hz), 8.98 (s, 1H), 9.01 (s, 1H).

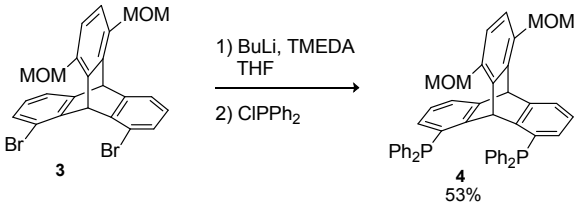




A flame-dried round bottom flask equipped with a dropping funnel was cooled to room temprature under the nitrogen flow. The system was charged with NaH (60% in mineral oil, 0.72 gr, 18 mmol). **2** (2 gr, 4.5 mmol), dissolved in anhydrous THF (50 mL) in a closed flask, was introduced dropwise to NaH whitin 15 minutes observing a rapid color change from brown to green. After 20 minutes, MOMCl (1.4 mL, 18.43 mmol) was added and the mixture was refluxed overnight. The yellow solution was allowed to cool, excess of NaH was neutralized slow addition of MeOH. The mixture was extracted with DCM, the organic layer was separated, drayed over Na_2SO_4, filtered and concentrated under reduced pressure. The product was washed with cold diethyl ether (10-15 mL) and filtered providing **3** in 62.6% yield (1.5 gr).

^{1}H-NMR ($CDCl_3$) δ: 3.52 (s, 3H), 3.58 (s, 3H), 5.19 (s, 2H), 5.23 (s, 2H), 5.92 (s, 1H), 6.77 (s, 2H), 6.89 (t, 2H, J = 8 Hz), 6.90 (s, 1H), 7.07 (d, 2H, J = 8 Hz), 7.23 (d, 2H, J = 8 Hz).

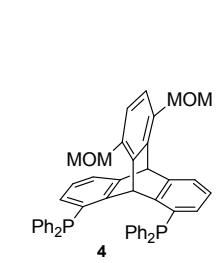




A dried Schlenk flask was charged with **3** (2 gr, 3.75 mmol), anhydrous THF (50 mL), TMEDA (4 mL, 26 mmol) under nitrogen. The mixture was cooled to -78°C (acetone/dry ice). *n*-Butyllithium (1.6M solution in hexane, 7.5 mL, 12 mmol) was added dropwise, and the reaction was allowed to stir for 1/2 h. Subsequently, $ClPPh_2$ (2 mL, 11 mmol) was added and the mixture was stirred for another 1/2h at room temprature. Subsequently the reaction mixture was extracted with $NaHCO_{3(aq)}$\DCM. The organic layer were separated, drayed over Na_2SO_4, filtered and concentrated under reduced pressure, providing a brown oily residue. MeOH was added under nitrogen, and the solution was reflux for 1/2hr, then cooled, generating a white solid. Further filteration provide **4** in 53% (1.5gr).

^{1}H-NMR ($CDCl_3$) δ: 3.12 (s, 3H), 3.56 (s, 3H), 4.53 (s, 2H), 5.2 (s, 2H), 5.94 (s, 1H), 6.57 (d, 1H, J = 8.91 Hz), 6.63 (d, 2H, J = 8.23 Hz), 6.67 (d, 1H, J = 8.23 Hz),6.92 (t, 2H, J = 7.43 Hz), 7.1-7.18 (m, 8H), 7.2-7.26 (m, 11H), 7.4 (d, 2H, J = 7.25 Hz), 7.79 (t, 1H, J = 4.66 Hz.^{31}P-NMR ($CDCl_3$) δ: -18.53(s).

31P-NMR - CDCl3



4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AQ                    0.5063156 sec
RG                       9195.2
DW                         7.725 usec
DE                         6.00 usec
TE                       298.0 K
D1                  2.00000000 sec
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DELTA               1.89999998 sec
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F2 - Processing parameters
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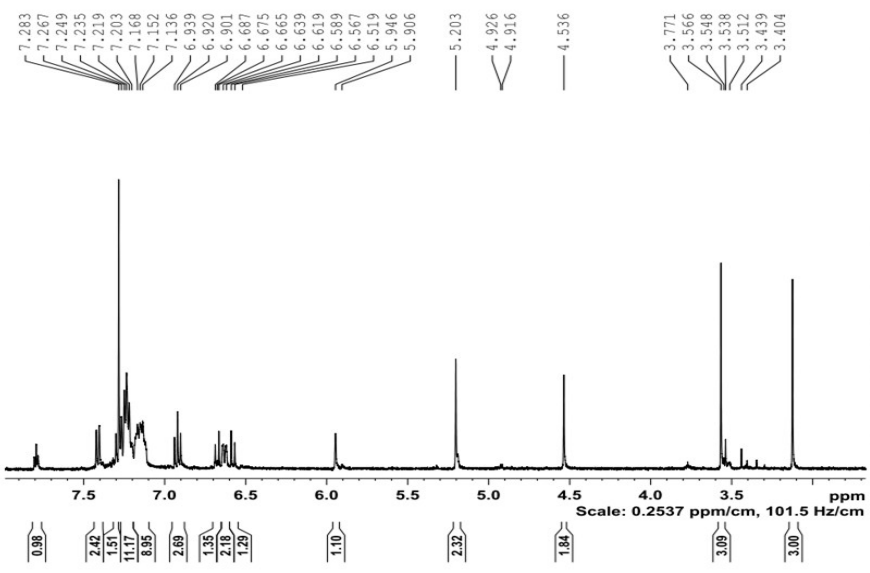
1H-NMR - CDCl3

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D1                  1.00000000 sec
TD0                         1

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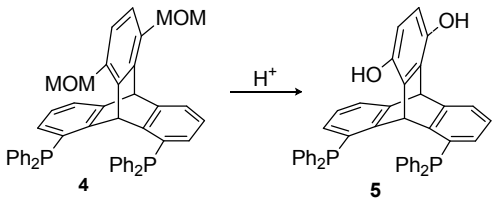
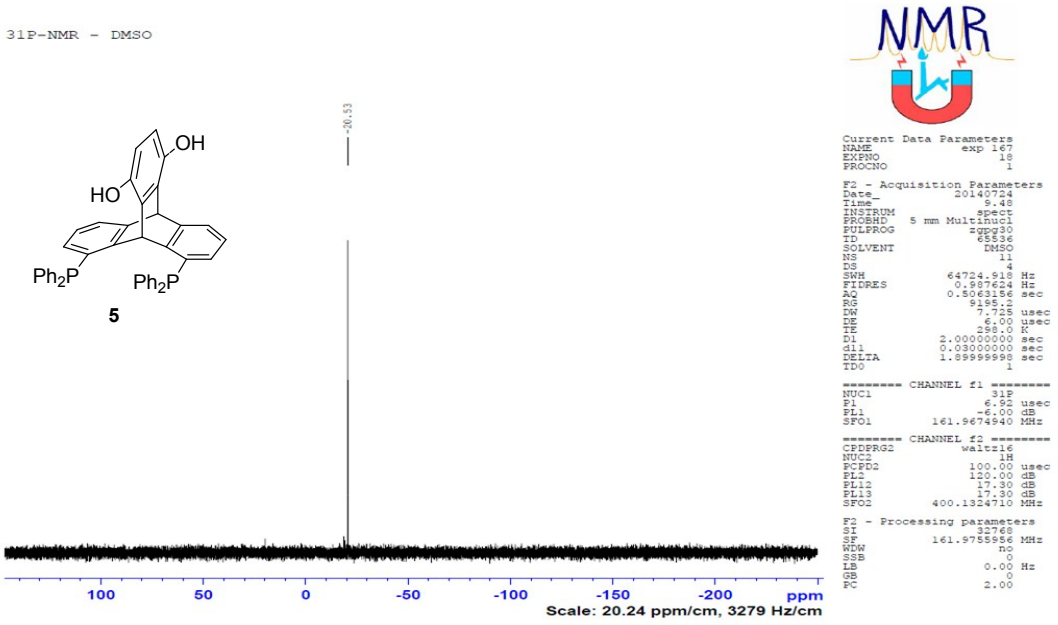


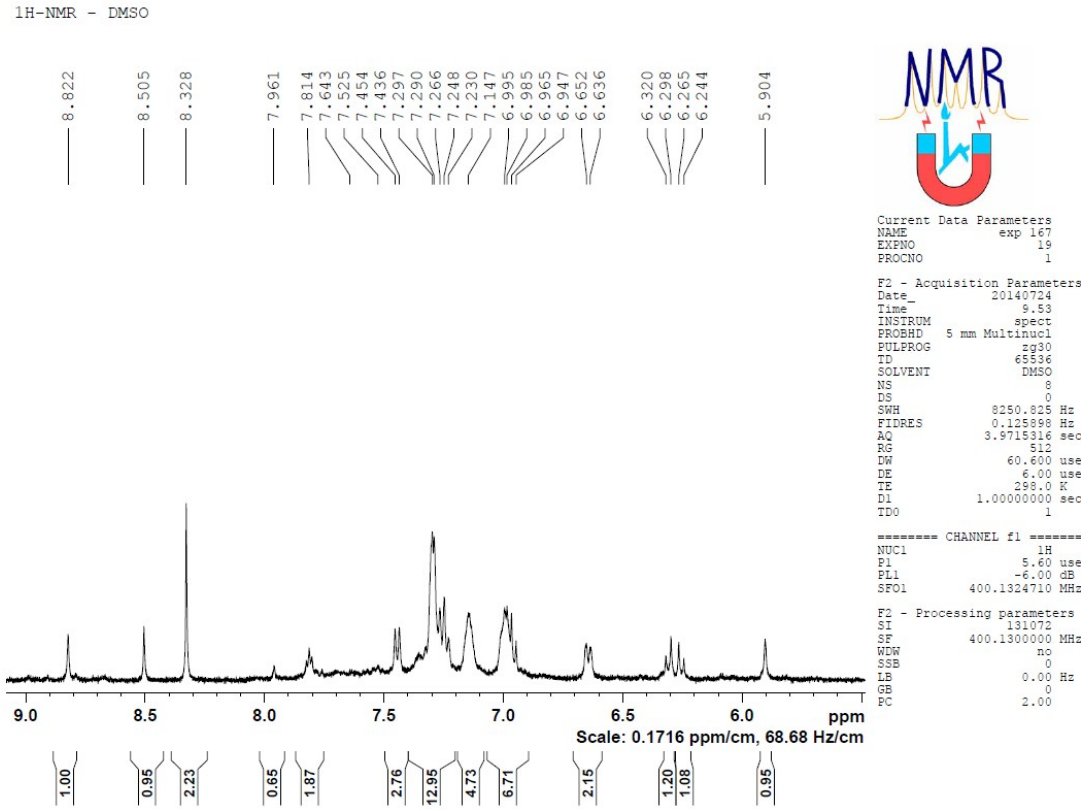
4 → 5

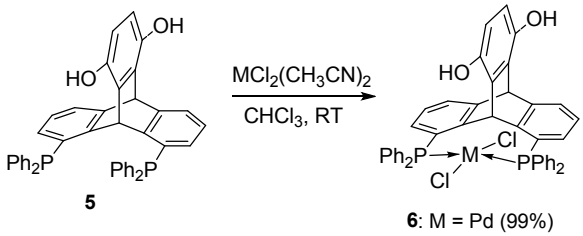
83-87%

HCl 37% (5 mL) was added to the solution of **4** (1.36 gr, 1.8 mmol) in ethanol (50 mL) and refluxed under nitrogen for 1 hr. The reaction mixture was allowed to cool, then transferred to an erlenmeyer flask and $NaHCO_3$ solution was added slowly in order to remove the acidity, until the solution became light green. The mixture was then extracted with EtOAc\HCl (1 M). The organic layer were separated, drayed over Na_2SO_4, filtered and concentrated under reduced pressure, affording compound **5**. Further purification of the solid was achieved by dissolving the solid with a minimal amount of Chloroform (1-2 mL), followed by the addition of Hexane (20-30 mL). The white solid was filtered, providing **5** in 83% yield (1 gr).

^{1}H-NMR (DMSO-d_6) δ: 5.9 (s, 1H), 6.25 (d, 1H, J = 8.53 Hz), 6.30 (d, 1H, J = 8.53 Hz), 6.64 (d, 2H, J = 8.10 Hz), 6.92-6.99 (m, 6H), 7.14 (m, 4H), 7.22-7.38 (m, 12H), 7.44 (d, 2H, J = 7.29 Hz), 7.8 (t, 1H, J = 4.7 Hz), 8.5 (s, 1H), 8.82 (s, 1H), ^{31}P-NMR (DMSO-d_6) δ: -20.53 (s).







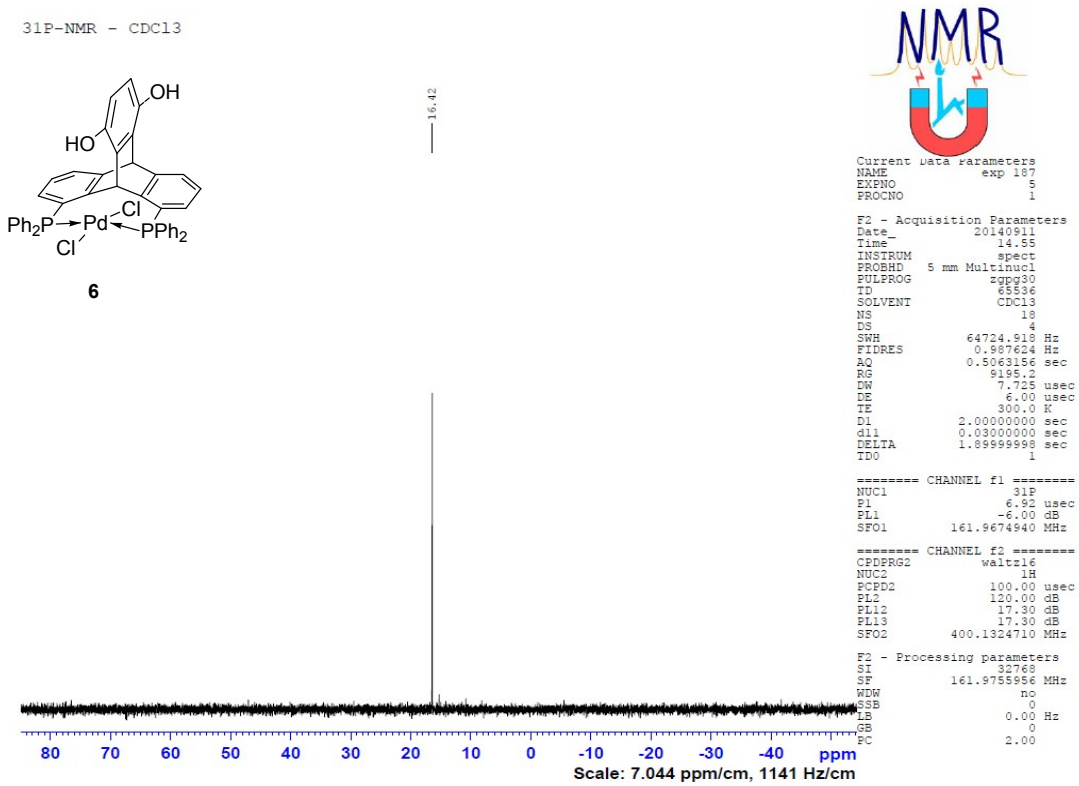
5

6: M = Pd (99%)
8: M = Pt (74%)

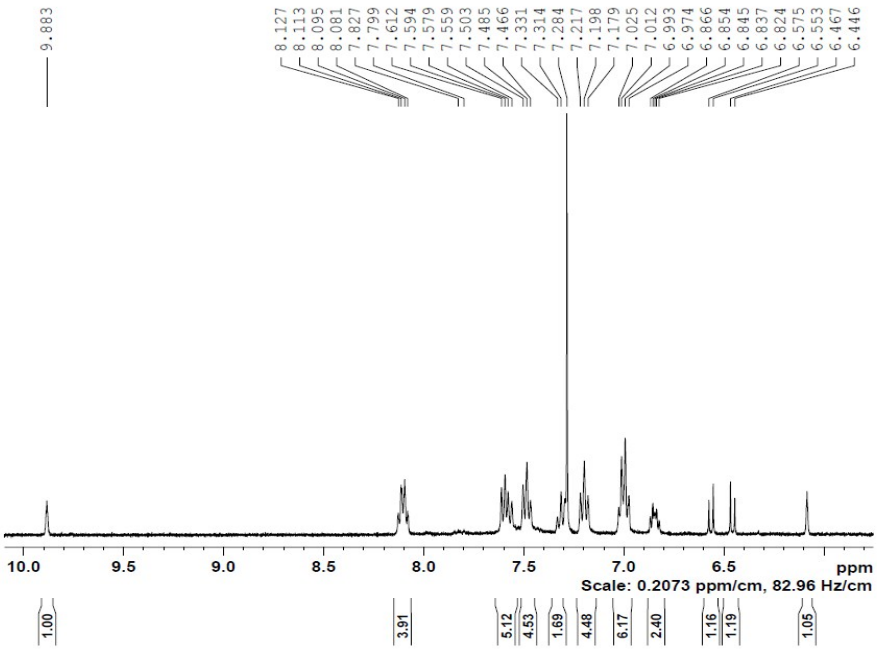
A 5 ml round bottom flask under nitrogen atmosphere was charged with **5** (0.15 mmol), $MCl_2(CH_3CN)_2$ (0.15 mmol) (M = Pd or Pt). $CDCl_3$ (0.5 mL) was added and the mixture was allowed to stir for 1/2 h (overnight for Pt complex). A rapid color change to robust orange for Pd complex observed. Subsequently, the solvent was removed at reduced pressure providing compounds **6** (orange) or **8** (off-white) in 99% and 74% yield, respectively.

6: ^{1}H-NMR ($CDCl_3$) δ: 6.083 (s, 1H), 6.45 (d, 1H, J = 8.56 Hz), 6.56 (d, 1H, J = 8.56 Hz), 6.84 (m, 2H), 7.0 (m, 6H), 7.19 (t, 4H, J = 7.55 Hz), 7.31 (t, 2H, J =7.48 Hz), 7.48 (t, 5H, J = 7.31 Hz), 7.58 (m, 5H), 8.10 (m, 4H), 9.88 (s, 1H),^{31}P-NMR ($CDCl_3$) δ: 16.42 (s).

8: ^{1}H-NMR (DMSO-d_6) δ: 5.85 (s, 1H), 6.28 (d, 1H, J = 8.63 Hz), 6.37 (d, 1H, J = 8.63 Hz), 6.41 (t, 1H, J = 8.0 Hz), 6.89 (t, 2H, J = 7.94 Hz), 7.38-7.4(m, 8H), 7.46-7.55 (m, 10H), 8.17 (m, 4H), 8.81 (s/m, 1H), 8.86 (s, 1H), 8.91 (s, 1H), ^{31}P-NMR (DMSO-d_6) δ: -7.07 (s, satelites at -18.71ppm, 4.53ppm, J = 1885.33 Hz).



1H-NMR - CDCl3

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RG                       512
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TE                    300.0 K
D1                 1.00000000 sec
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F2 - Processing parameters
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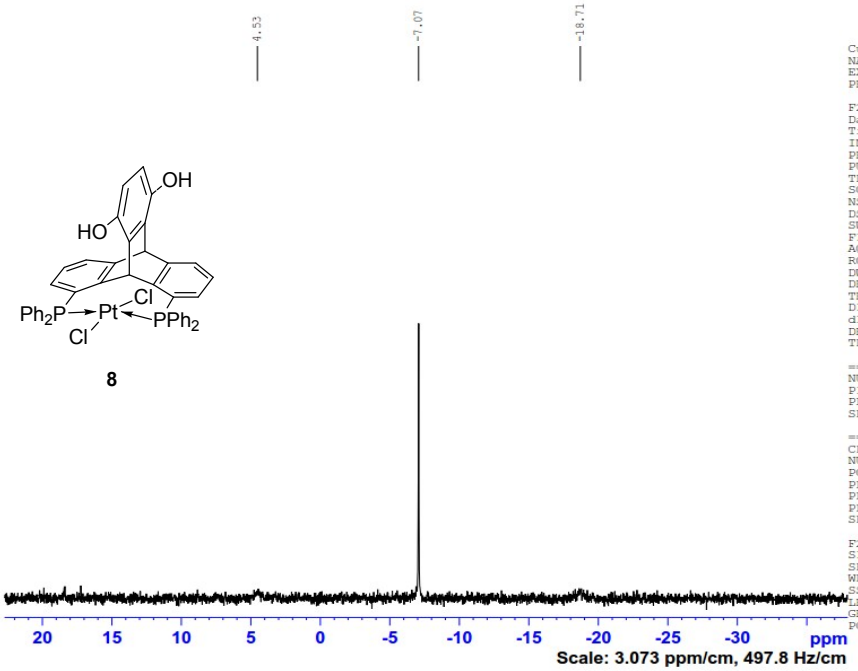
31P-NMR - DMSO



8

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RG                    9195.2
DW                    7.725 usec
DE                     6.00 usec
TE                    298.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
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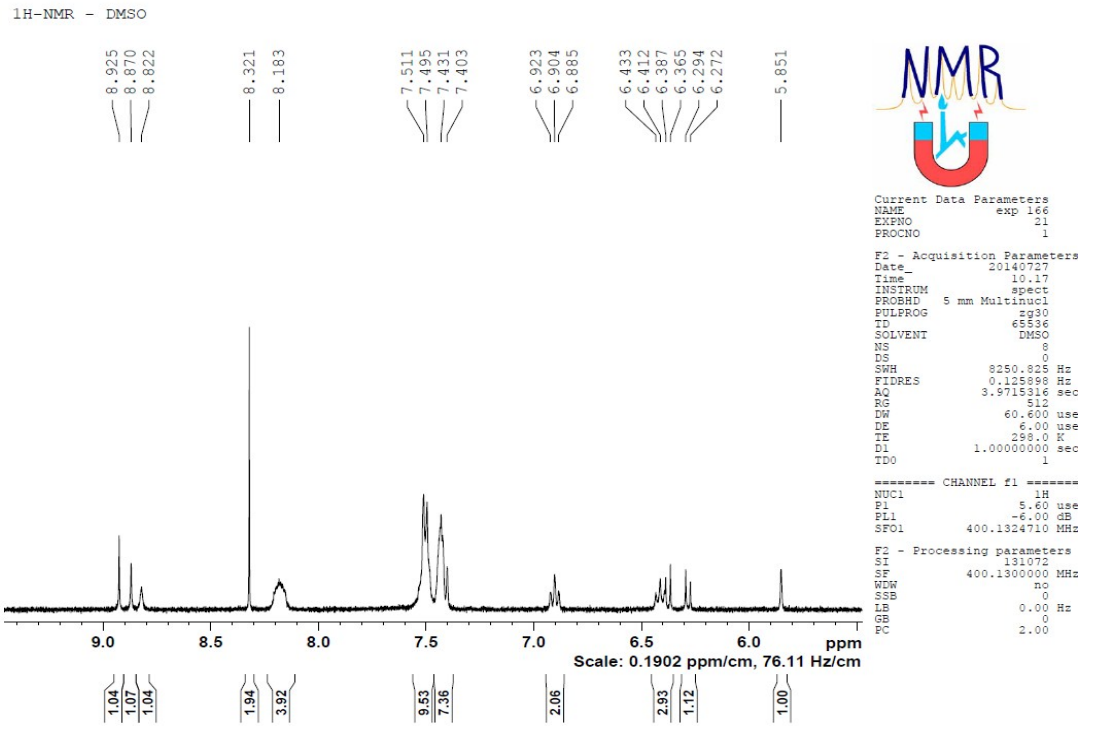
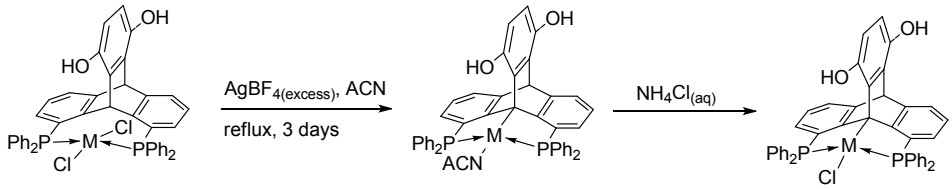




6: M = Pd
8: M = Pt

7: M = Pd (87%)
9: M = Pt (63%)

10: M = Pd (97%)
11 M = Pt (72%)

Complex **6** or **8** (0.12 mmol) was dissolved in acetonitrile (10 mL) while heating for ½ hr. $AgBF_4$ solution in nitromethane (0.96 mmol) was added and the reaction was refluxed for 3 days, then allowed to cool. The solution was filtered, and evaporated affording complex **7** or **9** in 87% or 63% yield respectively.

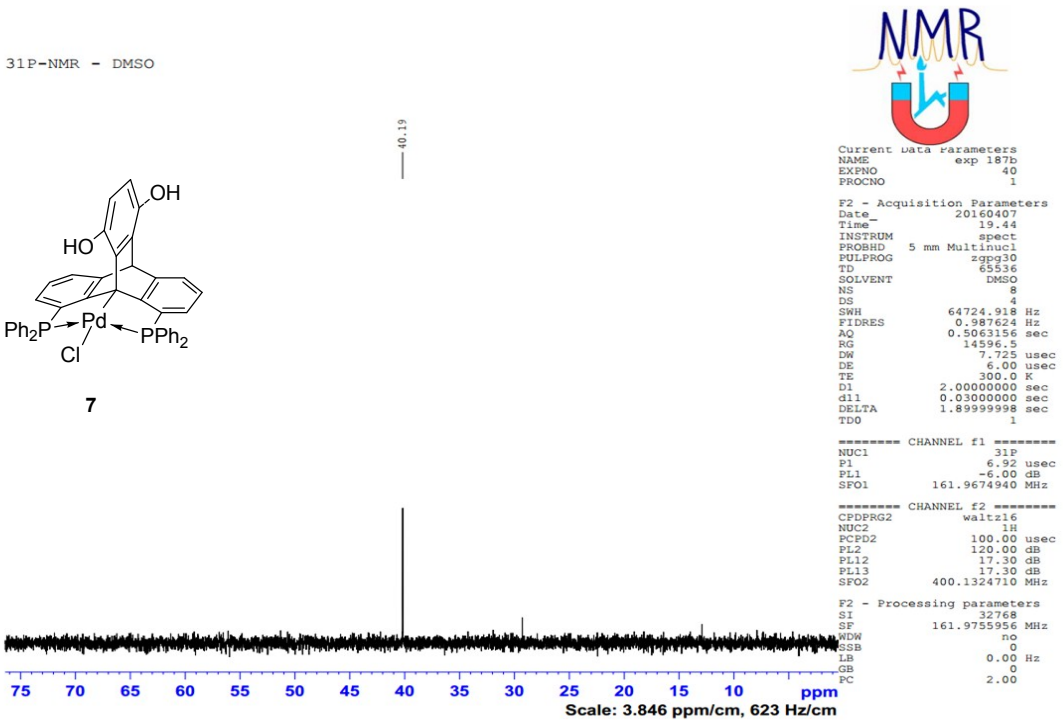
7: ^{1}H-NMR ($CDCl_3$) δ: 2.19 (s, 3H), 5.96 (s, 1H), 6.06 (d, 1H, J = 8 Hz), 6.32 (d, 1H, J = 8 Hz), 7.1-7.17 (m, 1H), 7.31-7.33 (m, 4H), 7.40-7.44 (m, 10H), 7.53-7.54 (m, 4H), 7.79-7.84 (m, 4H), ^{31}P-NMR ($CDCl_3$) δ: 46.45 (s).

9: ^{1}H-NMR ($CDCl_3$) δ: 2.62 (s, 3H), 6.03 (s, 1H), 6.05 (d, 1H, J = 8.8 Hz), 6.17 (d, 1H, J = 8.8 Hz), 7.13-7.16 (m, 4H), 7.38-7.51 (m, 15H), 7.57-7.59 (m, 2H), 7.69-7.78 (m, 5H), ^{31}P-NMR ($CDCl_3$) δ: 45.59 (s, satelliltes at 54.88 ppm, 36.31 ppm, J = 1484 Hz).

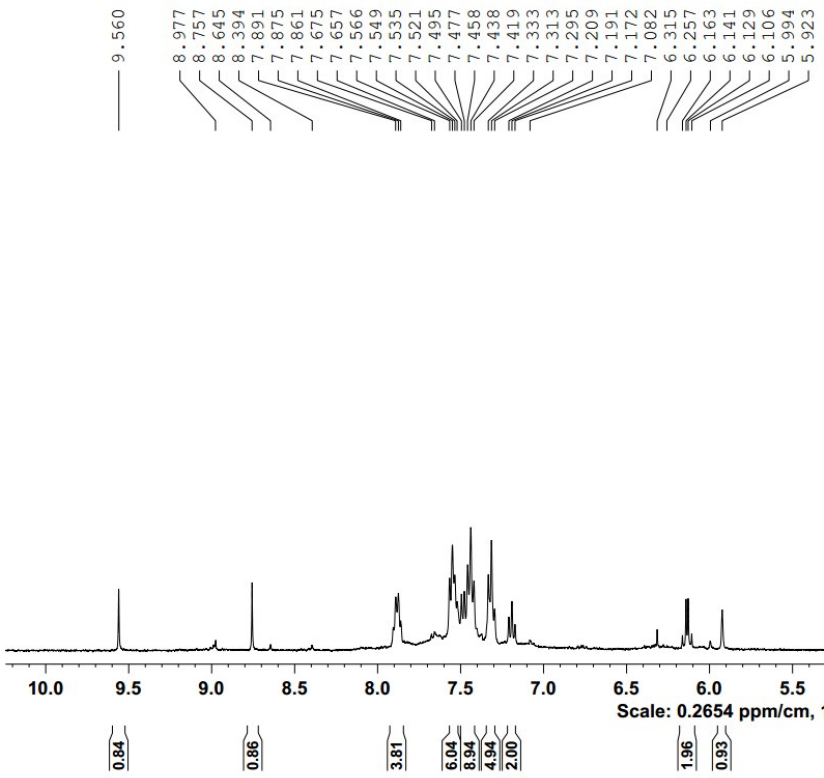
The cooled solution of **7** or **9** in EtOAc was washed twice with aqueous NH_4Cl and with water. The organic layer was separeted, dried over Na_2SO_4, filtered through cilite and evporated under reduced pressure affording compounds **10** or **11** in 97% or 72% yield respectively.

10: ^{1}H-NMR (DMSO-d_6) δ:5.92 (s, 1H), 6.12 (d, 1H, J = 8.51 Hz), 6.15 (d, 1H, J = 8.51 Hz), 7.19 (t, 2H, J = 7.63 Hz), 7.29-7.33 (m, 5H), 7.4-7.5 (m, 9H), 7.5-7.56 (m, 6H), 7.88 (m, 4H), 8.75 (s, 1H), 9.55 (s, 1H), ^{31}P-NMR (DMSO-d_6) δ: 40.19 (s).

11: ^{1}H-NMR (DMSO-d_6) δ: 5.96 (s, 1H), 5.98 (d, 1H, J = 8.74 Hz), 6.09 (d, 1H,J = 8.74 Hz), 7.18 (t, 2H, J = 7.38 Hz), 7.29 (m, 2H), 7.34-7.39 (m, 4H), 7.44-7.56 (m, 14H), 7.86 (m, 4H), 8.55 (s, 1H), 8.70 (s, 1H), ^{31}P-NMR (DMSO-d_6) δ: 42.57 (s, satelites at 32.45 ppm, 52.68 ppm, J = 1639 Hz).



1H-NMR - DMSO

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TE                    300.0 K
D1                 1.00000000 s
TD0                        1

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F2 - Processing parameter
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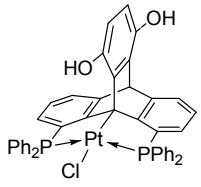
31P-NMR - DMSO



9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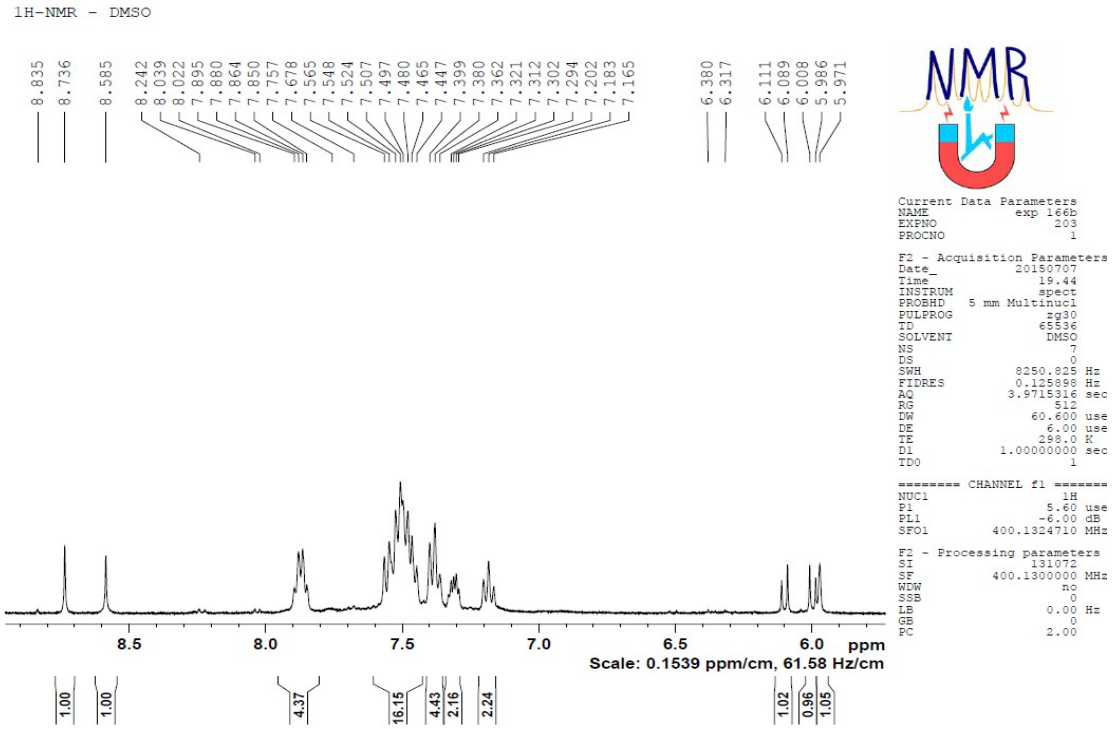
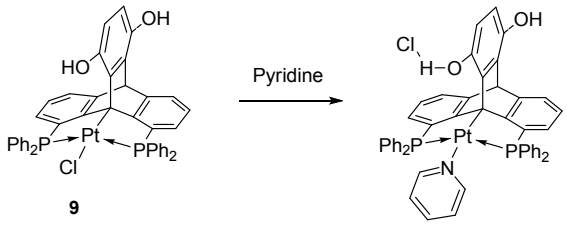
FIDRES              0.987624 Hz
AQ                0.5063156 sec
RG                     9195.2
DW                    7.725 usec
DE                     6.00 usec
TE                    298.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     31P
P1                     6.92 usec
PL1                   -6.00 dB
SFO1          161.9674940 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                100.00 usec
PL2                   120.00 dB
PL12                   17.30 dB
PL13                   17.30 dB
SFO2          400.1324710 MHz

F2 - Processing parameters
SI                     32768
SF            161.9755956 MHz
WDW                       no
SSB                        0
LB                      0.00 Hz
GB                         0
PC                      2.00
```

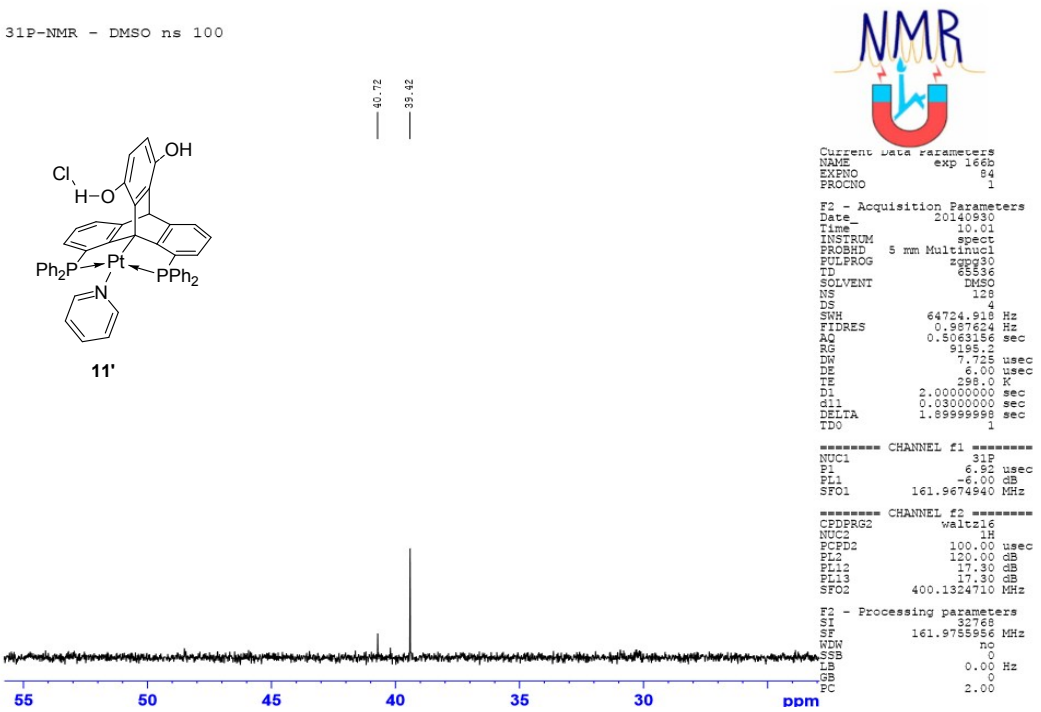


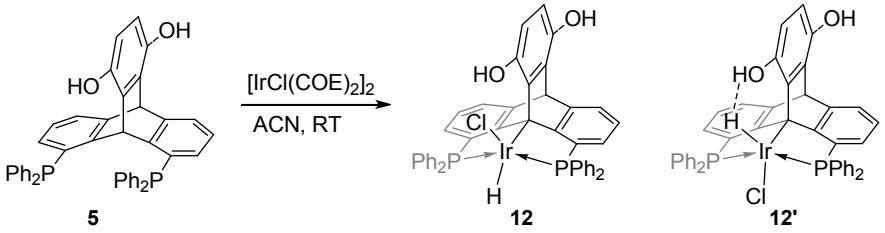


9 **11'**

Compound **9** was dissolved in a minimal amount of pyridine. Crystals suitable for X-Ray analysis were obtained after few weeks, revealing compound **11'**, that contains pyridine as the auxilary ligand and an additional halogen - hydrogen bonding in the outher spher.

11': ^{31}P-NMR (DMSO) δ: 39.42 (s)

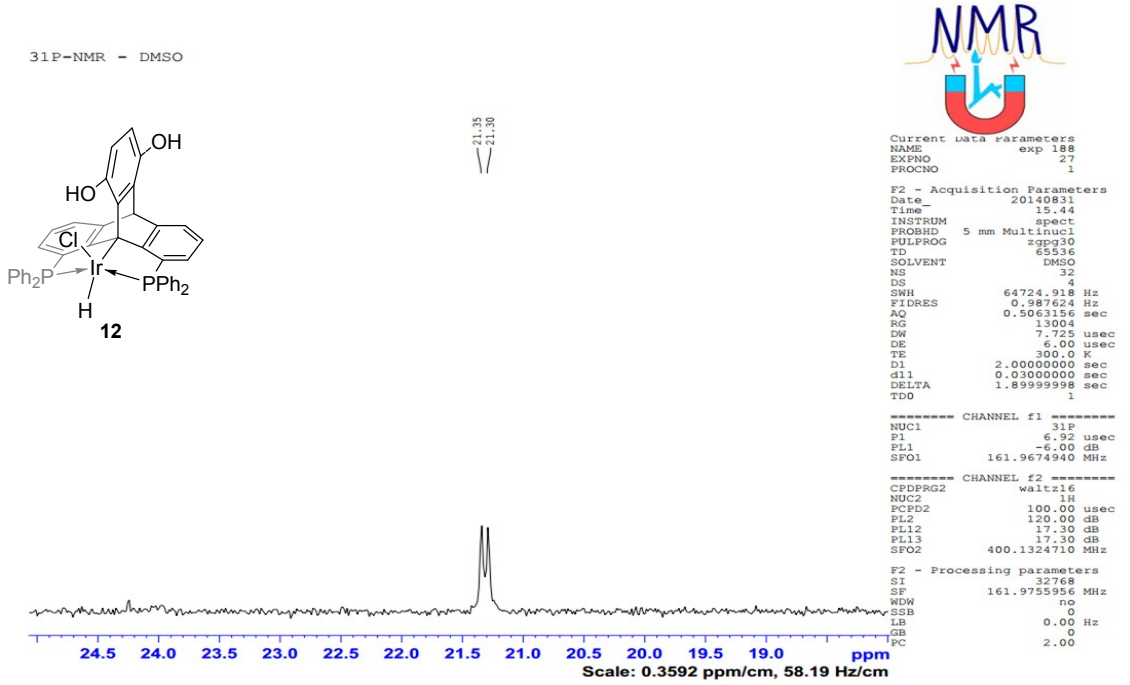


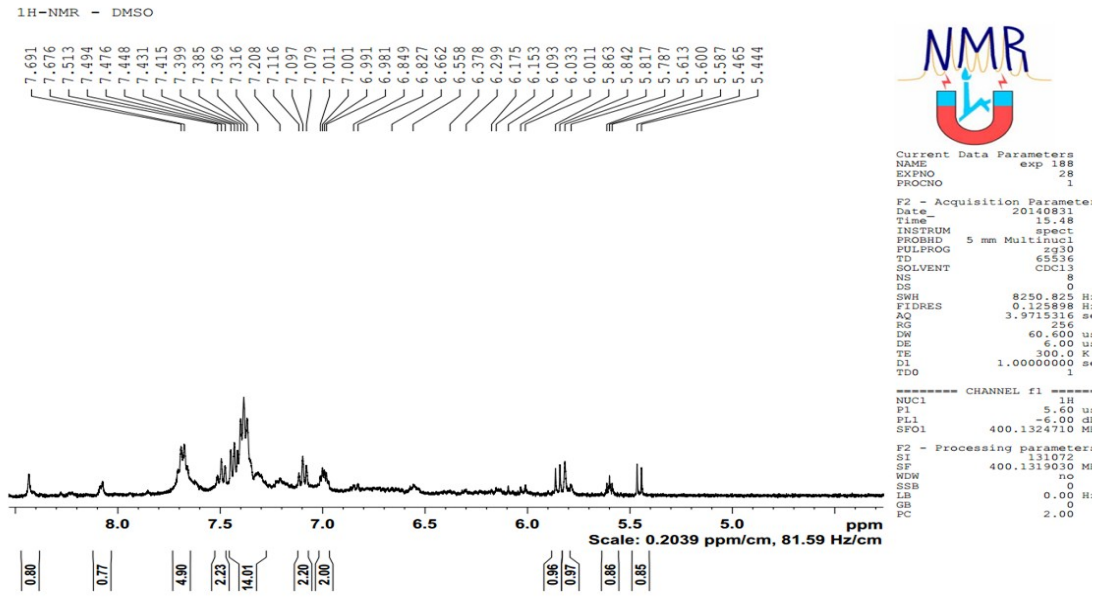


10 mL round bottom Schlenk flask was charged with **5** (0.25 mmol), $[IrCl(COE)_2]_2$ (0.127 mmol) and acetonitrile (5 mL) under nitrogen atmosphere. The orange suspension was allowed to stir for 3 days at room temprature. The solvent was evaporated affording a brown solid. The solid was purified by filtration with 3 portions of 10 mL pentane, providing a mixture of **12** and **12'** as a brown solid in 52% yield.

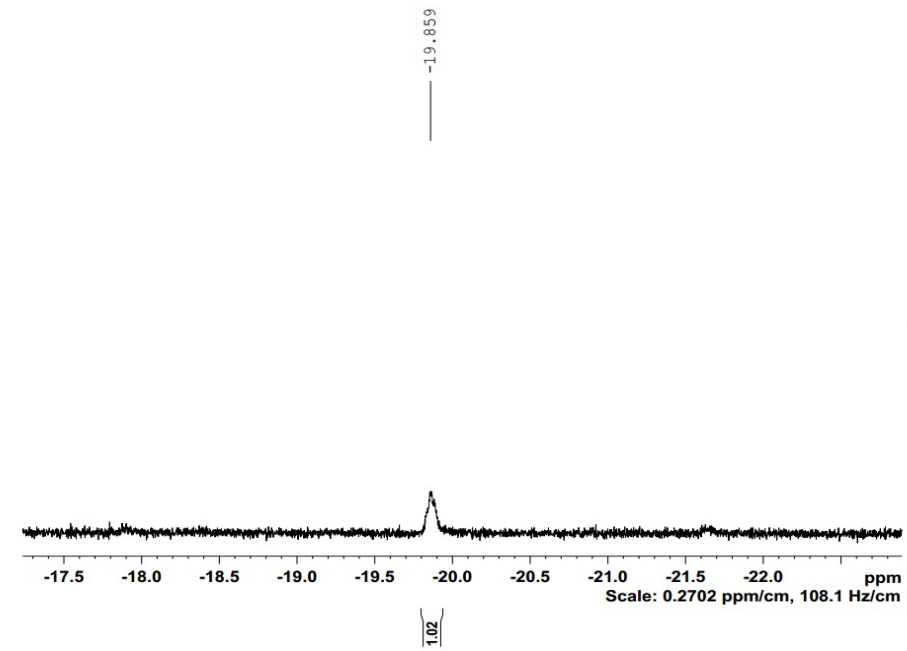
12: ^{1}H-NMR (DMSO-d_6) δ: -19.85 (m, 1H; t, J = 9.58 Hz), 5.45 (d, 1H, J = 8.47 Hz), 5.59 (t, 1H, J = 4.21 Hz), 5.81 (s, 1H), 5.85 (d, 1H, J = 8.47 Hz), 6.99 (m, 2H), 7.09 (t, 2H, J = 8.43 Hz), 7.20-7.44 (m, 14H), 7.49 (t, 2H, J = 7.72 Hz), 7.68 (m, 5H), 8.08 (m, 1H), 8.43 (s, 1H), ^{31}P-NMR (DMSO-d_6) δ: 21.31 (d, J = 7.57 Hz).

12': ^{1}H-NMR (DMSO-d_6) δ: -21.611 (m, 1H; + CD_3OD, t, J = 11.39 Hz), 5.53 (d, 1H, J = 8.09 Hz), 5.79 (s, 1H), 5.81 (s, 1H), 5.91 (d, 1H, J = 8.09 Hz), 7.08 (t, 2H, J = 7.08 Hz), 7.22 (m, 2H), 7.29-7.5 (m, 18H), 7.70 (m, 4H), 8.41 (s, 1H), 8.73 (m, 1H), ^{31}P-NMR (DMSO-d_6) δ: 24.24 (s).





1H-NMR - DMSO

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PROCNO                      1

F2 - Acquisition Paramete
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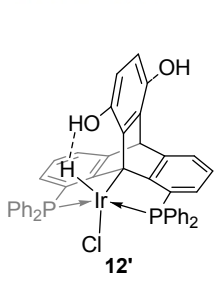
Time                    15.11
INSTRUM                 spect
PROBHD    5 mm Multinucl
PULPROG                  zg30
TD                      65536
SOLVENT                  DMSO
NS                         87
DS                          0
SWH                 40000.000 H
FIDRES                0.610352 H
AQ                    0.8192500 s
RG                          256
DW                     12.500 u
DE                      6.00 u
TE                     298.0 K
D1                  1.00000000 s
TD0                         1

======== CHANNEL f1 =====
NUC1                       1H
P1                      5.60 u
PL1                    -6.00 d
SFO1               400.1324710 M

F2 - Processing parameter
SI                      131072
SF                 400.1300000 M
WDW                        no
SSB                         0
LB                       0.00 H
GB                          0
PC                       2.00
```

1H-NMR - DMSO

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EXPNO                      31
PROCNO                      1

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Time                    12.43
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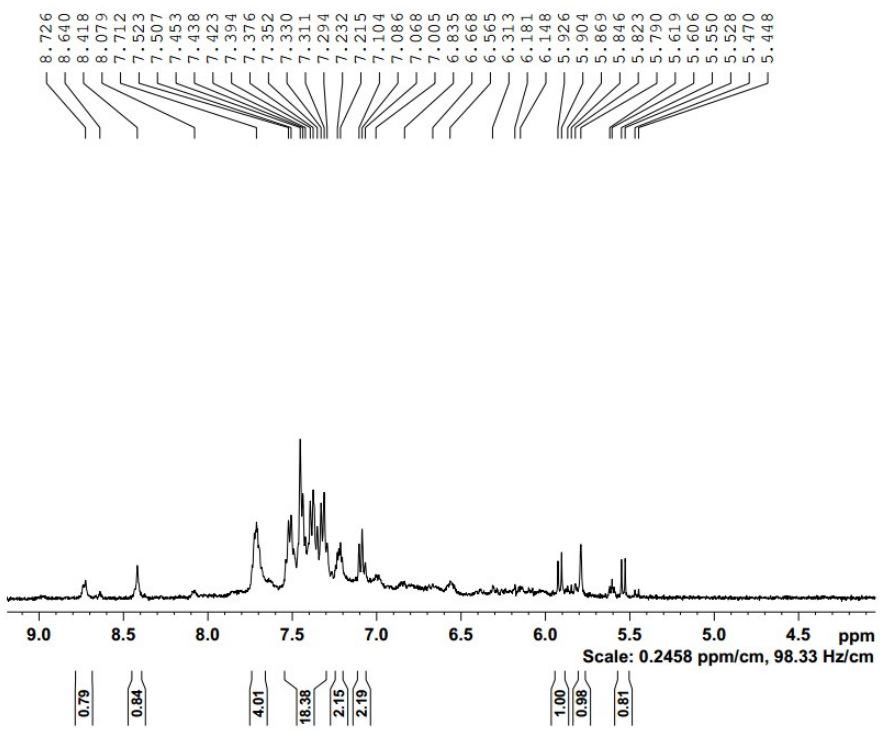
PULPROG              zgpg30
TD                      65536
SOLVENT                  DMSO
NS                         28
DS                          4
SWH                64724.918 Hz
FIDRES             0.987624 Hz
AQ                 0.5063156 sec
RG                    9195.2
DW                     7.725 usec
DE                      6.00 usec
TE                     300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      31P
P1                     6.92 usec
PL1                   -6.00 dB
SFO1              161.9674940 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                       1H
PCPD2                100.00 usec
PL2                   120.00 dB
PL12                   17.30 dB
PL13                   17.30 dB
SFO2              400.1324710 MHz

F2 - Processing parameters
SI                      32768
SF                161.9755956 MHz
WDW                        no
SSB                         0
LB                       0.00 Hz
GB                          0
PC                       2.00
```

1H-NMR - DMSO

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Current Data Parameters
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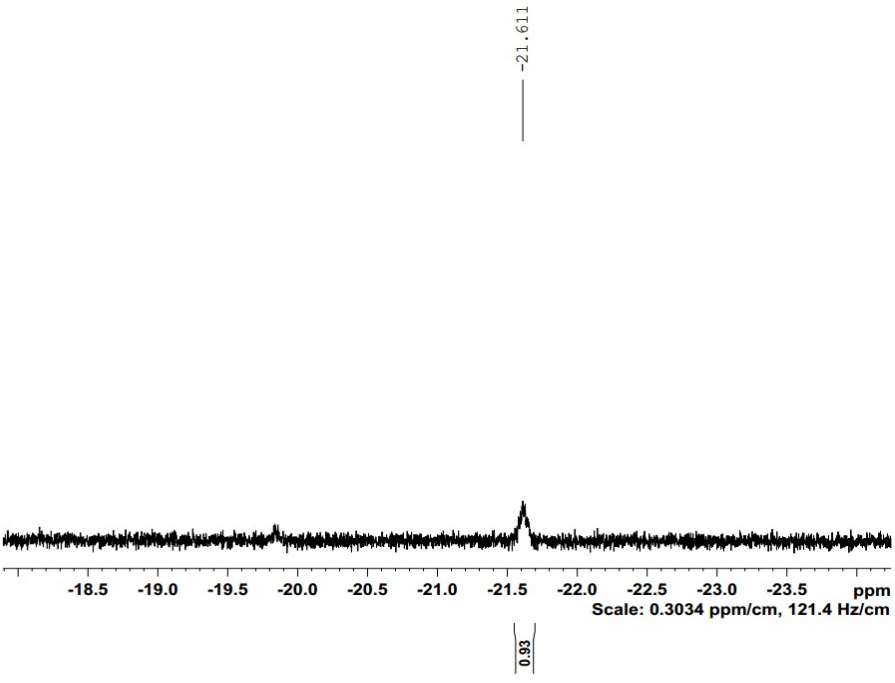
EXPNO                      40
PROCNO                      1

F2 - Acquisition Parameter
Date_                20140909
Time                    12.51
INSTRUM                 spect
PROBHD    5 mm Multinucl
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                          8
DS                          0
SWH                 40000.000 Hz
FIDRES              0.610352 Hz
AQ                  0.8192500 se
RG                        512
DW                     12.500 us
DE                      6.00 us
TE                     300.0 K
D1                 1.00000000 se
TD0                         1

======== CHANNEL f1 ======
NUC1                       1H
P1                       5.60 us
PL1                     -6.00 dB
SFO1              400.1324710 MH

F2 - Processing parameters
SI                     131072
SF                400.1300000 MH
WDW                        no
SSB                         0
LB                       0.00 Hz
GB                          0
PC                       2.00
```

1H-NMR - DMSO

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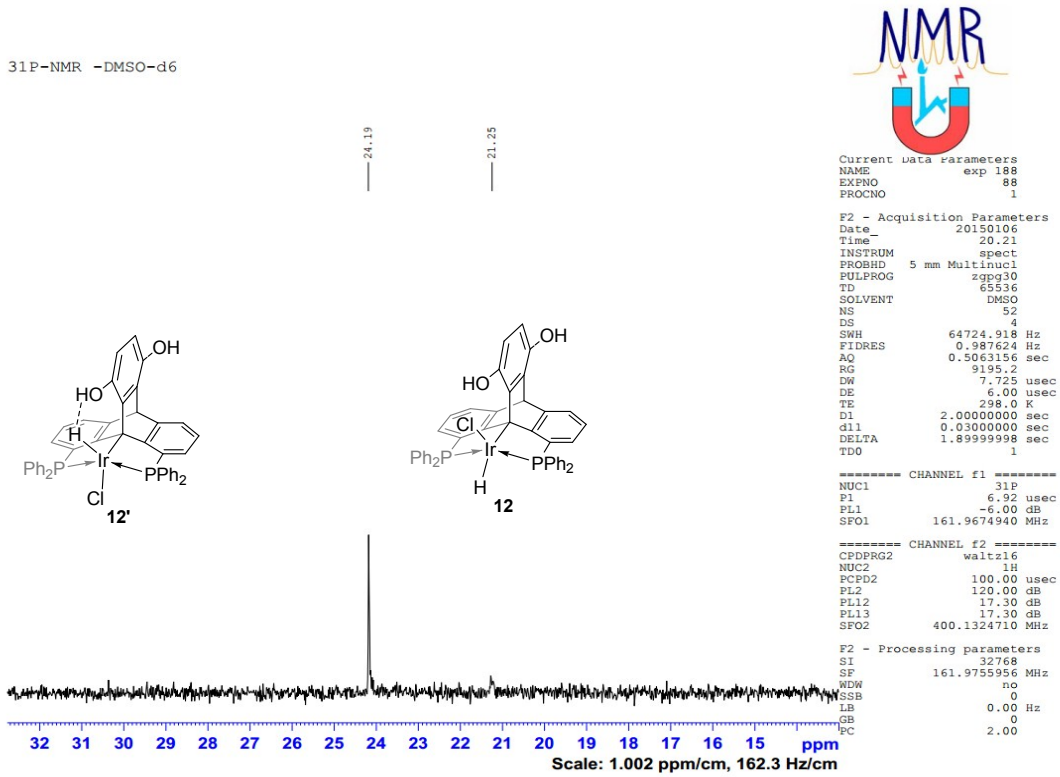
Current Data Parameters
NAME                  exp 188
EXPNO                      40
PROCNO                      1

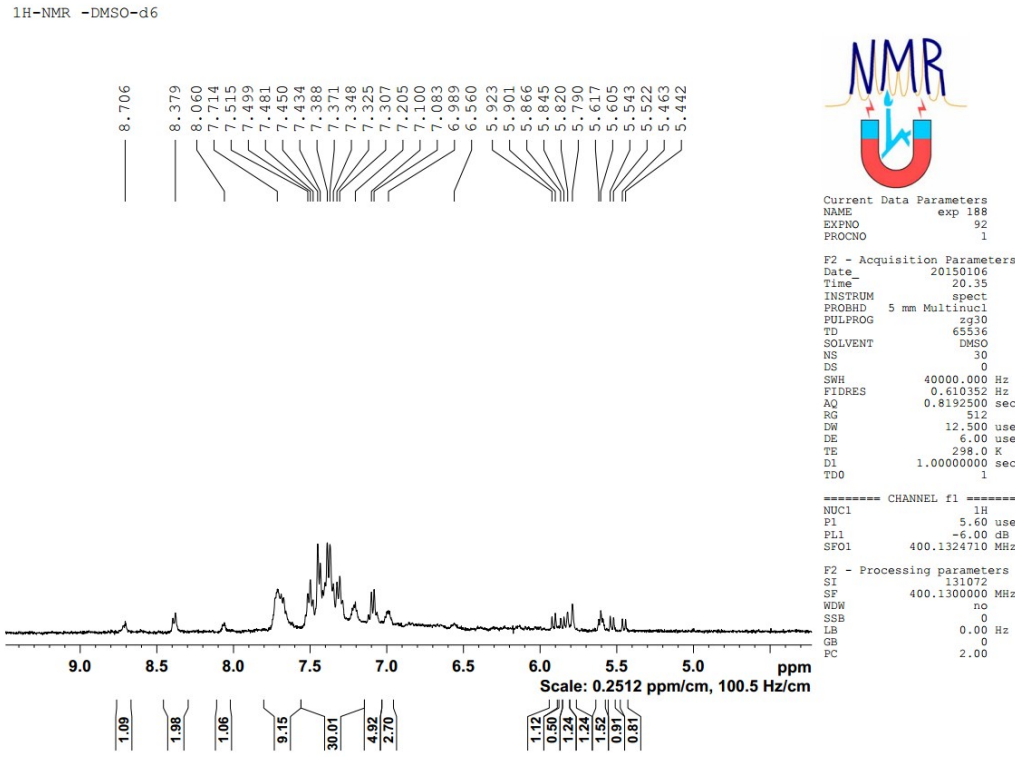
F2 - Acquisition Parameter
Date_                20140909
Time                    12.51
INSTRUM                 spect
PROBHD    5 mm Multinucl
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                          8
DS                          0
SWH                 40000.000 Hz
FIDRES              0.610352 Hz
AQ                  0.8192500 se
RG                        512
DW                     12.500 us
DE                      6.00 us
TE                     300.0 K
D1                 1.00000000 se
TD0                         1

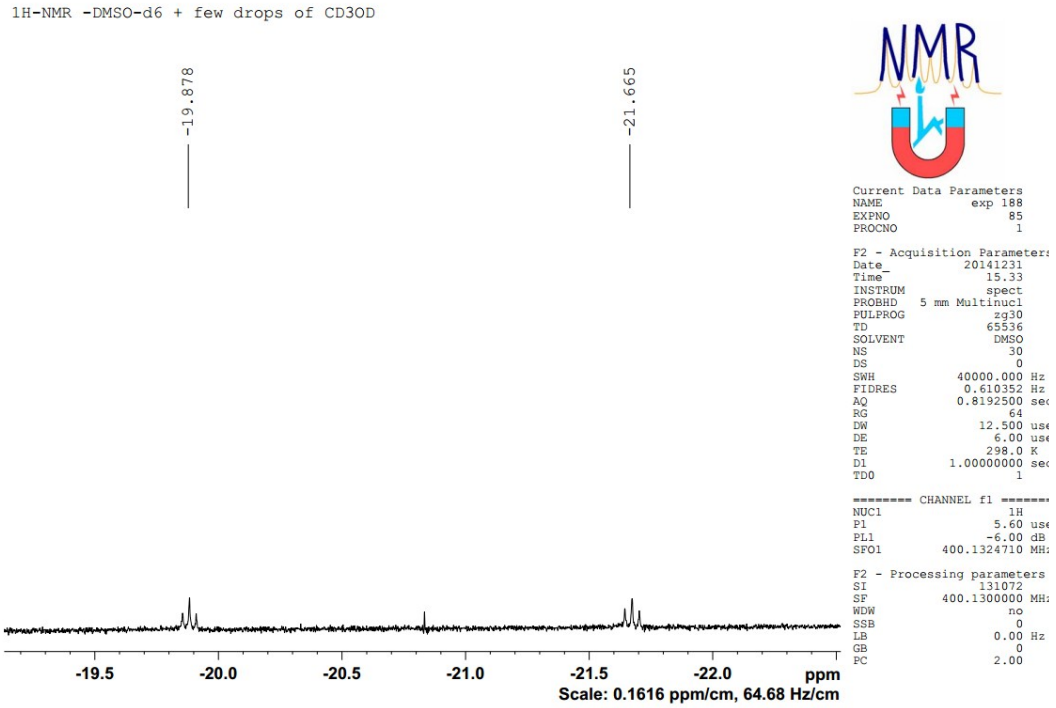
======== CHANNEL f1 ======
NUC1                       1H
P1                       5.60 us
PL1                     -6.00 dB
SFO1              400.1324710 MH

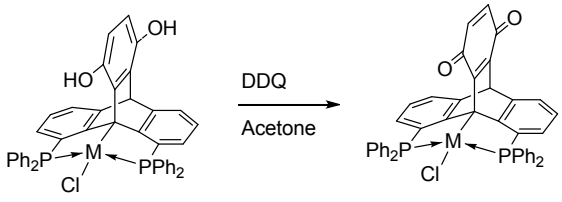
F2 - Processing parameters
SI                     131072
SF                400.1300000 MH
WDW                        no
SSB                         0
LB                       0.00 Hz
GB                          0
PC                       2.00
```

The mixture (12 +12’):









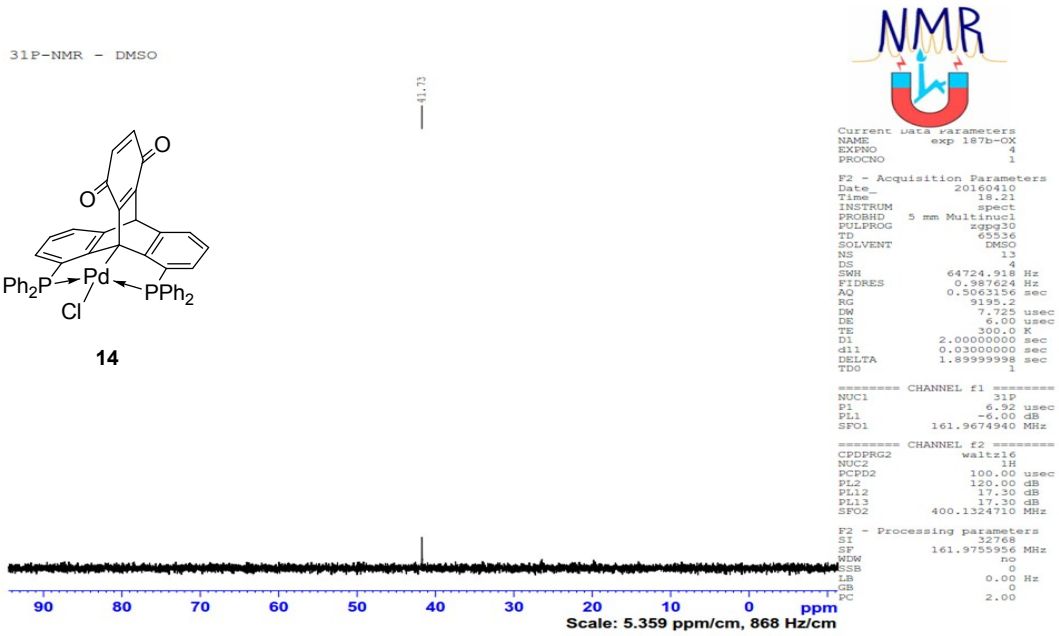
7: M = Pd
9: M = Pt

14: M = Pd (100%)
15: M = Pt (100%)

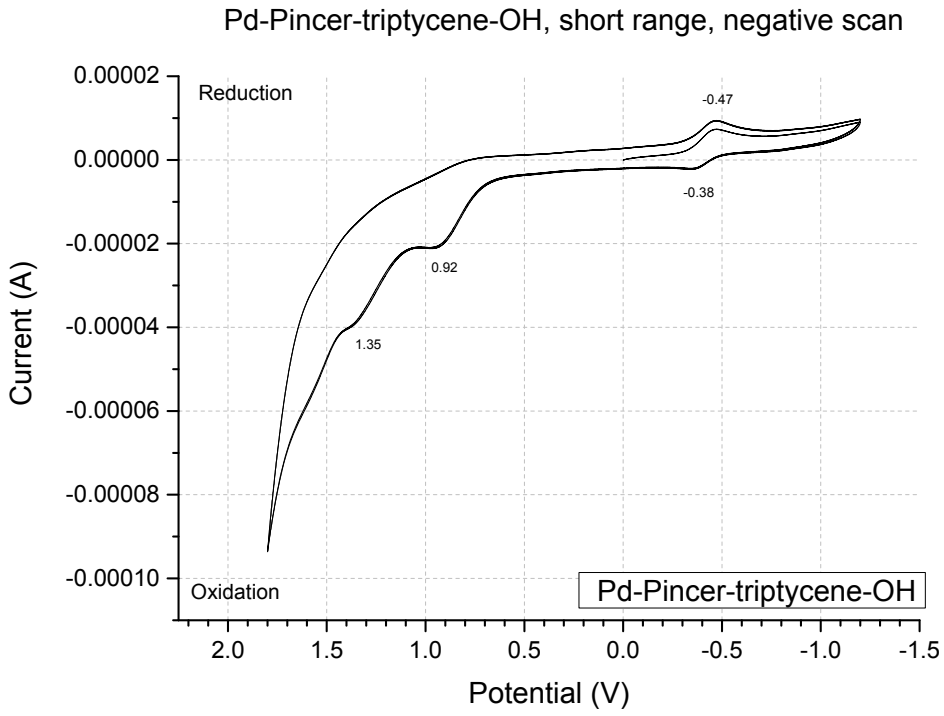
10ml round bottom flask, was charged with pincers **7** or **9** (1equiv), DDQ (1equiv) and acetone (5 mL) under nitrogen atmosphere. A gray suspension was formed rapidly. The mixture was allowed to stir for 30 minutes. The solid was filtered off and the filtrate was extracted with EtOAc\water. The organic layer were drayed over Na_2SO_4, filttered and evaporated till dryness, providing **14** or **15** as a brown solid in 100% yield.

14: ^{1}H-NMR (DMSO-d_6) δ: 6.02 (s, 1H), 6.47 (d, 1H, J = 10.44 Hz), 6.55 (d, 1H, J = 10.44 Hz), 7.29 (t, 2H, J = 5.8 Hz), 7.37 (m, 4H), 7.49 (m, 12H), 7.72 (m, 7H), ^{31}P-NMR (DMSO-d_6) δ: 41.73 (s).

15: ^{1}H-NMR (DMSO-d_6) δ: 6.04 (s, 1H), 6.37 (d, 1H, J = 10.32 Hz), 6.51 (d, 1H, J = 10.32 Hz), 7.25 (t, 2H, J = 7.39 Hz), 7.34-7.43 (m, 6H), 7.45-7.54 (m, 12H), 7.68 (d, 2H, J = 7.06 Hz), 7.76 (m, 3H), ^{31}P-NMR (DMSO-d_6) δ: 42.47 (s, satelites at: 32.3ppm, 52.61, J = 1637 Hz).



Electrochemical measurements were carried out in regular three-electrode electrochemical cell with disc glassy carbon electrode (3 mm diameter), Ag wire electrode, and Ag/AgBr as as a working, counter and reference electrodes, respectively. The data was collcted in DMF medium with 0.1 M TBATFB as an electrolyte under oxygen-free atmosphere (Ar). Glassy carbon electrode was polished with alumina slurry (1 and 0.05 μm, Buehler, IL, USA) followed by sonication in ethanol and water (10 min each) before every experiment. Calibration of the Ag/AgBr electrode was routinely performed with ferrocene couple prior to all measurements. The analyte concentration (complexes **10** and **11**) was 3 mM; Scan rate of 0.1 V sec^{-1}.



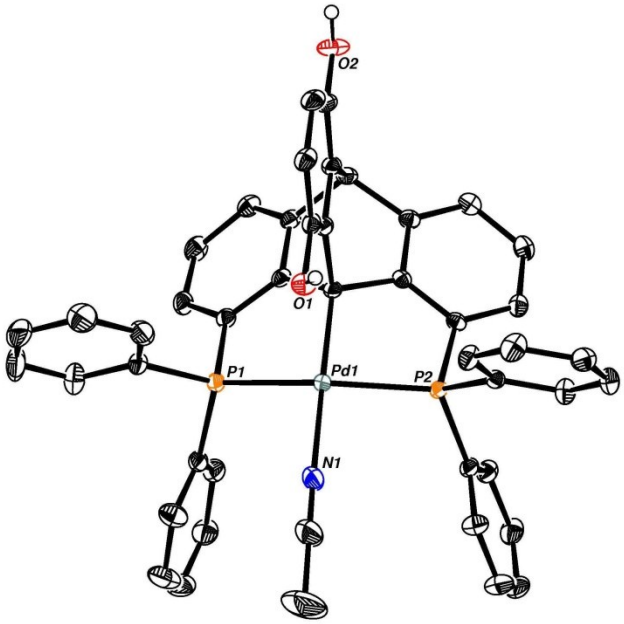


Table 1. Crystal data and structure refinement for **7**

Identification code	7	
Empirical formula	C48 H38 B Cl4 F4 N O2 P2 Pd	
Formula weight	1057.74	
Temperature	173(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 17.8139(9) Å	α= 90°.
	b = 11.4514(6) Å	β= 95.349(1)°.
	c = 23.023(1) Å	γ = 90°.
Volume	4676.1(4) $Å^3$	
Z	4	
Density (calculated)	1.502 Mg/m^3	
Absorption coefficient	0.750 mm^{-1}	
F(000)	2136	
Crystal size	0.35 x 0.25 x 0.14 mm^3	
Theta range for data collection	1.99 to 27.00°.	
Index ranges	-22<=h<=22, -14<=k<=14, -29<=l<=29	
Reflections collected	50892	

Independent reflections	10209 [R(int) = 0.0292]
Completeness to theta = 27.00°	99.9 %
Absorption correction	None
Max. and min. transmission	0.9023 and 0.7793
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10209 / 0 / 571
Goodness-of-fit on F^2	1.090
Final R indices [I>2sigma(I)]	R1 = 0.0424, wR2 = 0.1048
R indices (all data)	R1 = 0.0464, wR2 = 0.1069
Largest diff. peak and hole	1.632 and -1.055 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	4814(2)	2345(3)	6678(1)	28(1)
C(1)	7668(1)	2982(2)	5058(1)	17(1)
C(2)	7432(1)	1721(2)	4100(1)	21(1)
C(3)	8360(1)	2335(2)	4879(1)	18(1)
C(4)	9043(1)	2276(2)	5218(1)	20(1)
C(5)	9645(2)	1667(2)	5012(1)	26(1)
C(6)	9553(2)	1132(3)	4472(1)	30(1)
C(7)	8851(2)	1130(2)	4145(1)	26(1)
C(8)	8252(1)	1710(2)	4356(1)	21(1)
C(9)	7342(1)	3656(2)	4519(1)	17(1)
C(10)	7113(1)	4811(2)	4526(1)	18(1)
C(11)	6788(2)	5334(2)	4010(1)	23(1)
C(12)	6703(2)	4691(3)	3501(1)	26(1)
C(13)	6913(2)	3509(3)	3497(1)	24(1)
C(14)	7224(1)	2998(2)	4006(1)	20(1)
C(15)	7089(1)	1991(2)	5110(1)	19(1)
C(16)	6691(1)	1726(2)	5581(1)	21(1)
C(17)	6184(2)	789(2)	5538(1)	25(1)
C(18)	6077(2)	138(2)	5035(1)	28(1)
C(19)	6472(2)	398(2)	4555(1)	25(1)
C(20)	6976(1)	1322(2)	4596(1)	20(1)
C(21)	9118(2)	1757(2)	6463(1)	25(1)
C(22)	9829(2)	1293(3)	6641(2)	39(1)
C(23)	9896(2)	405(3)	7049(2)	51(1)
C(24)	9264(2)	-25(3)	7287(2)	49(1)
C(25)	8565(2)	428(3)	7113(2)	47(1)
C(26)	8489(2)	1320(3)	6699(1)	35(1)
C(27)	9819(2)	3840(2)	6091(1)	24(1)
C(28)	10000(2)	4220(3)	6660(1)	34(1)
C(29)	10594(2)	4990(3)	6789(2)	44(1)
C(30)	11006(2)	5391(3)	6348(2)	42(1)
C(31)	10828(2)	5018(3)	5782(2)	36(1)

C(32)	10239(2)	4245(3)	5651(1)	29(1)
C(33)	6240(1)	5772(2)	5421(1)	19(1)
C(34)	5898(2)	5098(2)	5822(1)	27(1)
C(35)	5161(2)	5350(3)	5941(2)	33(1)
C(36)	4779(2)	6267(3)	5663(1)	30(1)
C(37)	5118(2)	6943(3)	5262(1)	30(1)
C(38)	5850(2)	6704(3)	5145(1)	26(1)
C(39)	7622(1)	6846(2)	5226(1)	21(1)
C(40)	7979(2)	7227(2)	4750(1)	26(1)
C(41)	8283(2)	8352(3)	4749(2)	33(1)
C(42)	8248(2)	9072(3)	5219(2)	36(1)
C(43)	7901(2)	8692(3)	5698(2)	39(1)
C(44)	7587(2)	7590(3)	5702(1)	29(1)
C(45)	8325(3)	5753(4)	6845(2)	59(1)
C(46)	8572(4)	6598(6)	7295(3)	120(3)
C(47)	5866(3)	7803(5)	6758(3)	88(2)
C(48)	7713(2)	3284(4)	1837(2)	55(1)
Cl(1)	5109(1)	8752(2)	6687(1)	98(1)
Cl(2)	6680(1)	8468(2)	7069(1)	102(1)
Cl(3)	7580(1)	4605(1)	2192(1)	63(1)
Cl(4)	6938(1)	2331(1)	1865(1)	67(1)
F(1)	5563(1)	2712(2)	6673(1)	37(1)
F(2)	4522(1)	2122(2)	6108(1)	54(1)
F(3)	4769(2)	1364(2)	7004(1)	62(1)
F(4)	4415(1)	3232(2)	6903(1)	60(1)
N(1)	8146(2)	5114(2)	6492(1)	35(1)
O(1)	6807(1)	2385(2)	6084(1)	25(1)
O(2)	6400(1)	-217(2)	4045(1)	35(1)
P(1)	8995(1)	2930(1)	5930(1)	19(1)
P(2)	7186(1)	5415(1)	5253(1)	16(1)
Pd(1)	7907(1)	4030(1)	5773(1)	17(1)

Table 3. Bond lengths [Å] and angles [°] for 7.

B(1)-F(3)	1.357(4)
B(1)-F(4)	1.370(4)
B(1)-F(2)	1.389(4)
B(1)-F(1)	1.400(4)
C(1)-C(3)	1.529(3)
C(1)-C(9)	1.529(3)
C(1)-C(15)	1.545(3)
C(1)-Pd(1)	2.050(2)
C(2)-C(14)	1.519(4)
C(2)-C(8)	1.523(3)
C(2)-C(20)	1.531(4)
C(2)-H(2)	1.0000
C(3)-C(4)	1.384(4)
C(3)-C(8)	1.400(4)
C(4)-C(5)	1.398(4)
C(4)-P(1)	1.811(3)
C(5)-C(6)	1.382(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.399(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.381(4)
C(7)-H(7)	0.9500
C(9)-C(10)	1.385(4)
C(9)-C(14)	1.401(4)
C(10)-C(11)	1.406(4)
C(10)-P(2)	1.804(3)
C(11)-C(12)	1.380(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.405(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.379(4)
C(13)-H(13)	0.9500
C(15)-C(16)	1.383(4)
C(15)-C(20)	1.409(4)
C(16)-O(1)	1.382(3)

C(16)-C(17)	1.400(4)
C(17)-C(18)	1.377(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.395(4)
C(18)-H(18)	0.9500
C(19)-O(2)	1.366(3)
C(19)-C(20)	1.385(4)
C(21)-C(26)	1.384(4)
C(21)-C(22)	1.400(4)
C(21)-P(1)	1.819(3)
C(22)-C(23)	1.381(5)
C(22)-H(22)	0.9500
C(23)-C(24)	1.388(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.374(6)
C(24)-H(24)	0.9500
C(25)-C(26)	1.394(4)
C(25)-H(25)	0.9500
C(26)-H(26)	0.9500
C(27)-C(28)	1.389(4)
C(27)-C(32)	1.394(4)
C(27)-P(1)	1.811(3)
C(28)-C(29)	1.388(4)
C(28)-H(28)	0.9500
C(29)-C(30)	1.385(5)
C(29)-H(29)	0.9500
C(30)-C(31)	1.379(5)
C(30)-H(30)	0.9500
C(31)-C(32)	1.385(4)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
C(33)-C(34)	1.386(4)
C(33)-C(38)	1.395(4)
C(33)-P(2)	1.812(3)
C(34)-C(35)	1.395(4)
C(34)-H(34)	0.9500
C(35)-C(36)	1.375(4)

C(35)-H(35)	0.9500
C(36)-C(37)	1.385(4)
C(36)-H(36)	0.9500
C(37)-C(38)	1.383(4)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
C(39)-C(40)	1.388(4)
C(39)-C(44)	1.393(4)
C(39)-P(2)	1.816(3)
C(40)-C(41)	1.397(4)
C(40)-H(40)	0.9500
C(41)-C(42)	1.366(5)
C(41)-H(41)	0.9500
C(42)-C(43)	1.383(5)
C(42)-H(42)	0.9500
C(43)-C(44)	1.380(4)
C(43)-H(43)	0.9500
C(44)-H(44)	0.9500
C(45)-N(1)	1.118(4)
C(45)-C(46)	1.457(6)
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-Cl(1)	1.728(6)
C(47)-Cl(2)	1.732(6)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(48)-Cl(3)	1.745(4)
C(48)-Cl(4)	1.765(4)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
F(1)-H(1)	1.9044
N(1)-Pd(1)	2.080(3)
O(1)-H(1)	0.8400
O(2)-H(2A)	0.8400
P(1)-Pd(1)	2.3110(7)
P(2)-Pd(1)	2.3053(7)

F(3)-B(1)-F(4)	110.2(3)
F(3)-B(1)-F(2)	109.5(3)
F(4)-B(1)-F(2)	109.4(3)
F(3)-B(1)-F(1)	111.0(3)
F(4)-B(1)-F(1)	108.0(3)
F(2)-B(1)-F(1)	108.8(3)
C(3)-C(1)-C(9)	106.3(2)
C(3)-C(1)-C(15)	103.07(19)
C(9)-C(1)-C(15)	103.19(19)
C(3)-C(1)-Pd(1)	112.78(16)
C(9)-C(1)-Pd(1)	113.04(16)
C(15)-C(1)-Pd(1)	117.30(17)
C(14)-C(2)-C(8)	106.0(2)
C(14)-C(2)-C(20)	104.7(2)
C(8)-C(2)-C(20)	105.5(2)
C(14)-C(2)-H(2)	113.3
C(8)-C(2)-H(2)	113.3
C(20)-C(2)-H(2)	113.3
C(4)-C(3)-C(8)	120.3(2)
C(4)-C(3)-C(1)	124.1(2)
C(8)-C(3)-C(1)	115.5(2)
C(3)-C(4)-C(5)	119.6(2)
C(3)-C(4)-P(1)	112.11(19)
C(5)-C(4)-P(1)	128.0(2)
C(6)-C(5)-C(4)	119.8(3)
C(6)-C(5)-H(5)	120.1
C(4)-C(5)-H(5)	120.1
C(5)-C(6)-C(7)	120.6(3)
C(5)-C(6)-H(6)	119.7
C(7)-C(6)-H(6)	119.7
C(8)-C(7)-C(6)	119.5(3)
C(8)-C(7)-H(7)	120.3
C(6)-C(7)-H(7)	120.3
C(7)-C(8)-C(3)	119.9(2)
C(7)-C(8)-C(2)	127.8(2)
C(3)-C(8)-C(2)	112.2(2)

C(10)-C(9)-C(14)	120.2(2)
C(10)-C(9)-C(1)	124.2(2)
C(14)-C(9)-C(1)	115.4(2)
C(9)-C(10)-C(11)	119.7(2)
C(9)-C(10)-P(2)	112.36(19)
C(11)-C(10)-P(2)	127.6(2)
C(12)-C(11)-C(10)	119.6(2)
C(12)-C(11)-H(11)	120.2
C(10)-C(11)-H(11)	120.2
C(11)-C(12)-C(13)	120.8(2)
C(11)-C(12)-H(12)	119.6
C(13)-C(12)-H(12)	119.6
C(14)-C(13)-C(12)	119.3(3)
C(14)-C(13)-H(13)	120.4
C(12)-C(13)-H(13)	120.4
C(13)-C(14)-C(9)	120.3(2)
C(13)-C(14)-C(2)	127.1(2)
C(9)-C(14)-C(2)	112.5(2)
C(16)-C(15)-C(20)	119.6(2)
C(16)-C(15)-C(1)	128.1(2)
C(20)-C(15)-C(1)	112.3(2)
O(1)-C(16)-C(15)	119.3(2)
O(1)-C(16)-C(17)	121.5(2)
C(15)-C(16)-C(17)	119.2(2)
C(18)-C(17)-C(16)	120.8(3)
C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(17)-C(18)-C(19)	120.6(2)
C(17)-C(18)-H(18)	119.7
C(19)-C(18)-H(18)	119.7
O(2)-C(19)-C(20)	117.4(3)
O(2)-C(19)-C(18)	123.8(2)
C(20)-C(19)-C(18)	118.8(3)
C(19)-C(20)-C(15)	120.9(2)
C(19)-C(20)-C(2)	124.3(2)
C(15)-C(20)-C(2)	114.8(2)
C(26)-C(21)-C(22)	119.5(3)

C(26)-C(21)-P(1)	118.7(2)
C(22)-C(21)-P(1)	121.8(2)
C(23)-C(22)-C(21)	119.8(3)
C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1
C(22)-C(23)-C(24)	120.5(3)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
C(25)-C(24)-C(23)	119.8(3)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	120.3(4)
C(24)-C(25)-H(25)	119.8
C(26)-C(25)-H(25)	119.8
C(21)-C(26)-C(25)	120.1(3)
C(21)-C(26)-H(26)	119.9
C(25)-C(26)-H(26)	119.9
C(28)-C(27)-C(32)	119.2(3)
C(28)-C(27)-P(1)	119.1(2)
C(32)-C(27)-P(1)	121.5(2)
C(29)-C(28)-C(27)	120.4(3)
C(29)-C(28)-H(28)	119.8
C(27)-C(28)-H(28)	119.8
C(30)-C(29)-C(28)	119.9(3)
C(30)-C(29)-H(29)	120.1
C(28)-C(29)-H(29)	120.1
C(31)-C(30)-C(29)	120.0(3)
C(31)-C(30)-H(30)	120.0
C(29)-C(30)-H(30)	120.0
C(30)-C(31)-C(32)	120.4(3)
C(30)-C(31)-H(31)	119.8
C(32)-C(31)-H(31)	119.8
C(31)-C(32)-C(27)	120.1(3)
C(31)-C(32)-H(32)	120.0
C(27)-C(32)-H(32)	120.0
C(34)-C(33)-C(38)	119.9(2)
C(34)-C(33)-P(2)	119.5(2)

C(38)-C(33)-P(2)	120.6(2)
C(33)-C(34)-C(35)	119.7(3)
C(33)-C(34)-H(34)	120.2
C(35)-C(34)-H(34)	120.2
C(36)-C(35)-C(34)	120.0(3)
C(36)-C(35)-H(35)	120.0
C(34)-C(35)-H(35)	120.0
C(35)-C(36)-C(37)	120.5(3)
C(35)-C(36)-H(36)	119.7
C(37)-C(36)-H(36)	119.7
C(38)-C(37)-C(36)	119.8(3)
C(38)-C(37)-H(37)	120.1
C(36)-C(37)-H(37)	120.1
C(37)-C(38)-C(33)	120.0(3)
C(37)-C(38)-H(38)	120.0
C(33)-C(38)-H(38)	120.0
C(40)-C(39)-C(44)	119.0(3)
C(40)-C(39)-P(2)	122.6(2)
C(44)-C(39)-P(2)	118.4(2)
C(39)-C(40)-C(41)	119.8(3)
C(39)-C(40)-H(40)	120.1
C(41)-C(40)-H(40)	120.1
C(42)-C(41)-C(40)	120.6(3)
C(42)-C(41)-H(41)	119.7
C(40)-C(41)-H(41)	119.7
C(41)-C(42)-C(43)	119.9(3)
C(41)-C(42)-H(42)	120.1
C(43)-C(42)-H(42)	120.1
C(44)-C(43)-C(42)	120.3(3)
C(44)-C(43)-H(43)	119.9
C(42)-C(43)-H(43)	119.9
C(43)-C(44)-C(39)	120.4(3)
C(43)-C(44)-H(44)	119.8
C(39)-C(44)-H(44)	119.8
N(1)-C(45)-C(46)	178.5(7)
C(45)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46B)	109.5

H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
Cl(1)-C(47)-Cl(2)	112.2(3)
Cl(1)-C(47)-H(47A)	109.2
Cl(2)-C(47)-H(47A)	109.2
Cl(1)-C(47)-H(47B)	109.2
Cl(2)-C(47)-H(47B)	109.2
H(47A)-C(47)-H(47B)	107.9
Cl(3)-C(48)-Cl(4)	112.2(2)
Cl(3)-C(48)-H(48A)	109.2
Cl(4)-C(48)-H(48A)	109.2
Cl(3)-C(48)-H(48B)	109.2
Cl(4)-C(48)-H(48B)	109.2
H(48A)-C(48)-H(48B)	107.9
B(1)-F(1)-H(1)	138.4
C(45)-N(1)-Pd(1)	172.9(4)
C(16)-O(1)-H(1)	109.5
C(19)-O(2)-H(2A)	109.5
C(27)-P(1)-C(4)	108.48(13)
C(27)-P(1)-C(21)	104.04(13)
C(4)-P(1)-C(21)	107.03(12)
C(27)-P(1)-Pd(1)	111.72(9)
C(4)-P(1)-Pd(1)	101.18(9)
C(21)-P(1)-Pd(1)	123.67(10)
C(10)-P(2)-C(33)	107.24(11)
C(10)-P(2)-C(39)	107.99(12)
C(33)-P(2)-C(39)	102.32(12)
C(10)-P(2)-Pd(1)	101.98(9)
C(33)-P(2)-Pd(1)	121.88(9)
C(39)-P(2)-Pd(1)	114.75(9)
C(1)-Pd(1)-N(1)	179.20(10)
C(1)-Pd(1)-P(2)	85.47(7)
N(1)-Pd(1)-P(2)	93.77(7)
C(1)-Pd(1)-P(1)	85.12(7)
N(1)-Pd(1)-P(1)	95.43(7)

P(2)-Pd(1)-P(1)	150.99(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 7. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	31(2)	26(2)	26(2)	4(1)	1(1)	-6(1)
C(1)	15(1)	15(1)	20(1)	-1(1)	1(1)	-2(1)
C(2)	19(1)	20(1)	24(1)	-7(1)	1(1)	-1(1)
C(3)	17(1)	14(1)	24(1)	1(1)	5(1)	-1(1)
C(4)	19(1)	17(1)	25(1)	2(1)	2(1)	-2(1)
C(5)	18(1)	25(1)	36(2)	1(1)	1(1)	4(1)
C(6)	24(1)	27(2)	40(2)	-1(1)	10(1)	6(1)
C(7)	28(1)	21(1)	29(1)	-2(1)	8(1)	2(1)
C(8)	20(1)	17(1)	26(1)	0(1)	4(1)	-1(1)
C(9)	12(1)	19(1)	19(1)	1(1)	2(1)	-3(1)
C(10)	13(1)	22(1)	20(1)	-1(1)	2(1)	-2(1)
C(11)	20(1)	22(1)	26(1)	4(1)	3(1)	2(1)
C(12)	23(1)	32(2)	22(1)	4(1)	2(1)	2(1)
C(13)	21(1)	30(1)	21(1)	-2(1)	4(1)	-1(1)
C(14)	17(1)	22(1)	22(1)	-3(1)	3(1)	-2(1)
C(15)	15(1)	16(1)	26(1)	0(1)	1(1)	0(1)
C(16)	17(1)	18(1)	27(1)	3(1)	2(1)	2(1)
C(17)	21(1)	20(1)	34(2)	4(1)	8(1)	-1(1)
C(18)	20(1)	19(1)	44(2)	0(1)	4(1)	-5(1)
C(19)	21(1)	17(1)	36(2)	-5(1)	1(1)	-1(1)
C(20)	17(1)	17(1)	27(1)	-2(1)	1(1)	0(1)
C(21)	30(1)	20(1)	24(1)	3(1)	-2(1)	3(1)
C(22)	38(2)	38(2)	41(2)	8(1)	0(1)	13(1)
C(23)	60(2)	42(2)	48(2)	11(2)	-10(2)	23(2)
C(24)	77(3)	27(2)	40(2)	11(1)	-12(2)	-1(2)
C(25)	56(2)	40(2)	43(2)	17(2)	-2(2)	-17(2)
C(26)	35(2)	33(2)	35(2)	8(1)	-6(1)	-8(1)
C(27)	16(1)	21(1)	33(2)	2(1)	-2(1)	0(1)
C(28)	27(2)	42(2)	34(2)	-5(1)	3(1)	-7(1)
C(29)	33(2)	52(2)	45(2)	-18(2)	-4(1)	-9(2)
C(30)	27(2)	35(2)	62(2)	-7(2)	0(2)	-11(1)
C(31)	28(2)	31(2)	49(2)	6(1)	5(1)	-6(1)

C(32)	27(1)	25(1)	34(2)	3(1)	0(1)	-1(1)
C(33)	17(1)	18(1)	21(1)	-3(1)	1(1)	1(1)
C(34)	23(1)	22(1)	36(2)	6(1)	6(1)	2(1)
C(35)	25(1)	30(2)	47(2)	6(1)	14(1)	-2(1)
C(36)	18(1)	29(2)	42(2)	-6(1)	5(1)	0(1)
C(37)	24(1)	31(2)	35(2)	3(1)	-2(1)	8(1)
C(38)	23(1)	27(1)	29(1)	5(1)	4(1)	4(1)
C(39)	17(1)	15(1)	30(1)	1(1)	0(1)	-1(1)
C(40)	21(1)	22(1)	35(2)	1(1)	4(1)	1(1)
C(41)	26(1)	25(2)	48(2)	10(1)	5(1)	-3(1)
C(42)	30(2)	19(1)	58(2)	3(1)	-5(1)	-7(1)
C(43)	45(2)	26(2)	45(2)	-11(1)	-1(2)	-4(1)
C(44)	33(2)	23(1)	32(2)	-4(1)	3(1)	-6(1)
C(45)	62(3)	52(2)	55(2)	-23(2)	-28(2)	18(2)
C(46)	125(5)	106(5)	116(5)	-76(4)	-61(4)	17(4)
C(47)	91(4)	69(3)	101(4)	-31(3)	-10(3)	10(3)
C(48)	44(2)	59(2)	64(3)	-5(2)	18(2)	-4(2)
Cl(1)	132(1)	89(1)	77(1)	-3(1)	19(1)	49(1)
Cl(2)	118(1)	119(1)	71(1)	-32(1)	13(1)	-48(1)
Cl(3)	97(1)	53(1)	44(1)	2(1)	26(1)	-10(1)
Cl(4)	73(1)	78(1)	54(1)	-13(1)	24(1)	-29(1)
F(1)	27(1)	49(1)	36(1)	-6(1)	6(1)	-7(1)
F(2)	72(2)	54(1)	33(1)	4(1)	-15(1)	-34(1)
F(3)	86(2)	46(1)	52(1)	25(1)	-8(1)	-19(1)
F(4)	43(1)	58(1)	81(2)	-15(1)	10(1)	9(1)
N(1)	39(1)	33(1)	30(1)	-7(1)	-12(1)	10(1)
O(1)	23(1)	26(1)	25(1)	-1(1)	6(1)	-4(1)
O(2)	34(1)	28(1)	45(1)	-17(1)	7(1)	-12(1)
P(1)	17(1)	17(1)	23(1)	2(1)	-1(1)	0(1)
P(2)	16(1)	14(1)	19(1)	0(1)	1(1)	0(1)
Pd(1)	17(1)	16(1)	18(1)	-1(1)	-1(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 7.

	x	y	z	U(eq)
H(2)	7339	1237	3739	25
H(5)	10115	1621	5242	32
H(6)	9971	761	4322	36
H(7)	8786	734	3782	31
H(11)	6628	6126	4011	27
H(12)	6501	5052	3149	31
H(13)	6841	3066	3147	29
H(17)	5910	600	5860	30
H(18)	5731	-495	5013	33
H(22)	10265	1587	6482	47
H(23)	10379	87	7168	61
H(24)	9314	-631	7570	59
H(25)	8132	132	7274	56
H(26)	8004	1629	6580	42
H(28)	9716	3951	6962	41
H(29)	10718	5243	7179	53
H(30)	11410	5922	6435	50
H(31)	11112	5294	5480	43
H(32)	10121	3990	5260	34
H(34)	6163	4468	6014	32
H(35)	4923	4889	6213	40
H(36)	4279	6438	5747	36
H(37)	4849	7569	5069	36
H(38)	6087	7175	4875	32
H(40)	8017	6725	4426	31
H(41)	8517	8618	4419	40
H(42)	8461	9832	5217	43
H(43)	7878	9192	6025	47
H(44)	7347	7338	6031	35
H(46A)	8836	6192	7629	181
H(46B)	8133	7009	7422	181

H(46C)	8914	7163	7139	181
H(47A)	5958	7499	6368	106
H(47B)	5742	7132	7003	106
H(48A)	8173	2900	2021	65
H(48B)	7791	3442	1424	65
H(1)	6416	2371	6262	37
H(2A)	6064	-728	4060	53

Table 6. Hydrogen bonds for 7 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2A)...F(2)#1	0.84	1.93	2.733(3)	160.7
O(1)-H(1)...F(1)	0.84	1.90	2.730(3)	167.1

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

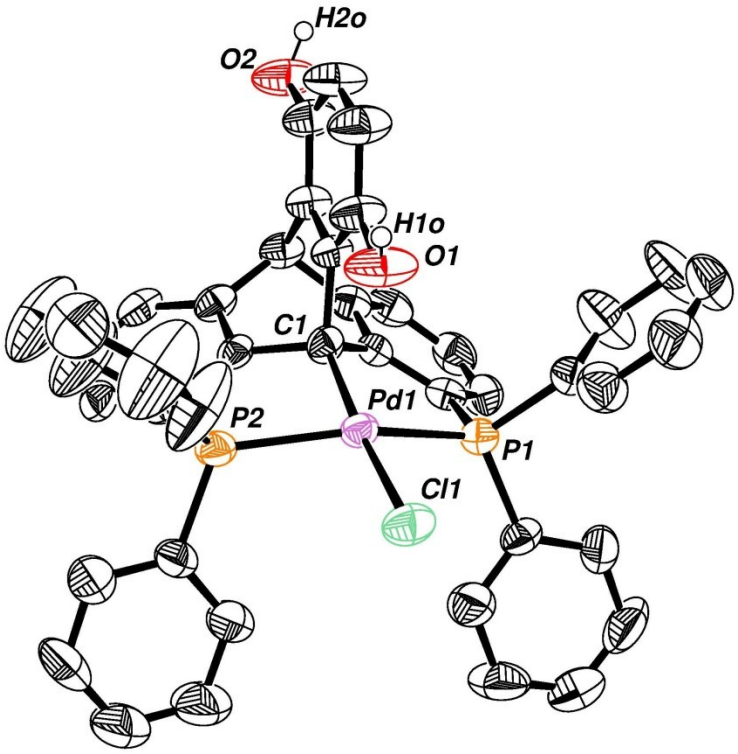


Table 1. Crystal data and structure refinement for 10.

Identification code	10	
Empirical formula	C50 H43 Cl O4 P2 Pd	
Formula weight	911.63	
Temperature	295(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.279(2) Å	α= 107.224(3)°.
	b = 11.916(2) Å	β= 96.427(3)°.

	c = 17.261(2) Å γ = 95.698(3)°.
Volume	2180.4(5) $Å^3$
Z	2
Density (calculated)	1.389 Mg/m^3
Absorption coefficient	0.604 mm^{-1}
F(000)	936
Crystal size	0.16 x 0.15 x 0.04 mm^3
Theta range for data collection	2.06 to 27.00°.
Index ranges	-14<=h<=14, -15<=k<=15, -22<=l<=22
Reflections collected	24380
Independent reflections	9420 [R(int) = 0.0919]
Completeness to theta = 27.00°	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9762 and 0.9095
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9420 / 1 / 531
Goodness-of-fit on F^2	1.011
Final R indices [I>2sigma(I)]	R1 = 0.0821, wR2 = 0.1476
R indices (all data)	R1 = 0.1356, wR2 = 0.1659
Largest diff. peak and hole	0.608 and -0.495 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 10. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9194(5)	8072(5)	7783(3)	38(1)
C(2)	9537(5)	9277(5)	7648(3)	36(1)
C(3)	8750(5)	9734(5)	7170(3)	41(1)
C(4)	9117(6)	10827(5)	7081(4)	51(2)
C(5)	10240(6)	11424(6)	7424(4)	58(2)
C(6)	11059(6)	10931(5)	7850(4)	52(2)
C(7)	10704(5)	9834(5)	7941(4)	43(1)
C(8)	11459(5)	9094(5)	8314(4)	44(2)
C(9)	10838(5)	8833(5)	8980(4)	44(2)
C(10)	11304(6)	9048(5)	9796(4)	52(2)
C(11)	10616(6)	8657(6)	10299(4)	55(2)
C(12)	9483(6)	8031(5)	10011(4)	50(2)
C(13)	8989(5)	7820(5)	9193(4)	41(1)
C(14)	9656(5)	8269(5)	8700(3)	36(1)
C(15)	10128(5)	7344(5)	7357(3)	41(1)
C(16)	9885(5)	6243(5)	6760(4)	54(2)
C(17)	10841(6)	5701(6)	6445(4)	71(2)
C(18)	12004(6)	6244(6)	6725(4)	64(2)
C(19)	12259(5)	7324(6)	7320(4)	58(2)
C(20)	11328(5)	7894(5)	7636(4)	45(2)
C(21)	7552(6)	8126(6)	5600(4)	50(2)
C(22)	8437(7)	8582(8)	5249(5)	91(3)
C(23)	8495(9)	8052(10)	4415(5)	115(4)
C(24)	7696(9)	7143(9)	3959(5)	88(3)
C(25)	6812(8)	6689(7)	4293(5)	80(2)
C(26)	6743(6)	7186(6)	5129(4)	67(2)
C(27)	6189(5)	9585(5)	6702(4)	43(2)
C(28)	5522(6)	9746(6)	7337(5)	68(2)
C(29)	4596(7)	10435(7)	7395(6)	81(2)
C(30)	4325(6)	10959(7)	6814(6)	73(2)
C(31)	4960(8)	10830(7)	6191(5)	86(3)
C(32)	5879(7)	10136(6)	6126(4)	68(2)

C(33)	7682(5)	5412(5)	8589(4)	46(2)
C(34)	6951(8)	4553(7)	7990(6)	114(4)
C(35)	6948(10)	3356(7)	7906(7)	135(5)
C(36)	7710(9)	3038(7)	8424(6)	84(2)
C(37)	8460(9)	3850(8)	8998(7)	122(4)
C(38)	8447(8)	5047(7)	9089(6)	107(3)
C(39)	6449(5)	7360(5)	9300(4)	48(2)
C(40)	5674(6)	8108(6)	9138(4)	61(2)
C(41)	4815(7)	8448(7)	9638(6)	89(3)
C(42)	4713(8)	8062(9)	10286(6)	101(3)
C(43)	5494(9)	7363(10)	10469(6)	114(4)
C(44)	6363(8)	6991(7)	9979(5)	88(3)
C(1AC)	7911(16)	1690(11)	4553(8)	224(8)
C(2AC)	7771(12)	2842(11)	5137(7)	131(4)
C(3AC)	6611(11)	3257(17)	5103(10)	241(10)
C(4AC)	8375(18)	4540(17)	1352(11)	298(13)
C(5AC)	7511(11)	5322(10)	1501(6)	105(3)
C(6AC)	6329(13)	4875(14)	1607(11)	232(8)
Cl(1)	5379(1)	6445(2)	6903(1)	57(1)
O(1)	8702(4)	5735(4)	6513(3)	73(2)
O(2)	13414(4)	7900(5)	7631(4)	78(2)
O(1AC)	8566(7)	3377(6)	5632(5)	174(4)
O(2AC)	7724(8)	6291(7)	1597(6)	194(5)
P(1)	7412(1)	8704(1)	6683(1)	42(1)
P(2)	7592(1)	6938(1)	8638(1)	41(1)
Pd(1)	7412(1)	7410(1)	7438(1)	36(1)

Table 3. Bond lengths [Å] and angles [°] for 10.

C(1)-C(2)	1.541(7)
C(1)-C(15)	1.543(7)
C(1)-C(14)	1.551(7)
C(1)-Pd(1)	2.039(5)
C(2)-C(7)	1.380(7)
C(2)-C(3)	1.400(7)
C(3)-C(4)	1.386(8)
C(3)-P(1)	1.796(6)
C(4)-C(5)	1.365(8)
C(4)-H(4)	0.9300
C(5)-C(6)	1.398(8)
C(5)-H(5)	0.9300
C(6)-C(7)	1.388(8)
C(6)-H(6)	0.9300
C(7)-C(8)	1.510(8)
C(8)-C(9)	1.502(8)
C(8)-C(20)	1.537(8)
C(8)-H(8)	0.9800
C(9)-C(10)	1.386(8)
C(9)-C(14)	1.396(7)
C(10)-C(11)	1.376(9)
C(10)-H(10)	0.9300
C(11)-C(12)	1.373(8)
C(11)-H(11)	0.9300
C(12)-C(13)	1.398(8)
C(12)-H(12)	0.9300
C(13)-C(14)	1.381(8)
C(13)-P(2)	1.801(6)
C(15)-C(16)	1.387(8)
C(15)-C(20)	1.409(7)
C(16)-O(1)	1.373(7)
C(16)-C(17)	1.392(8)
C(17)-C(18)	1.371(8)
C(17)-H(17)	0.9300
C(18)-C(19)	1.368(8)

C(18)-H(18)	0.9300
C(19)-O(2)	1.380(7)
C(19)-C(20)	1.382(8)
C(21)-C(26)	1.357(9)
C(21)-C(22)	1.372(9)
C(21)-P(1)	1.821(6)
C(22)-C(23)	1.402(10)
C(22)-H(22)	0.9300
C(23)-C(24)	1.322(11)
C(23)-H(23)	0.9300
C(24)-C(25)	1.351(11)
C(24)-H(24)	0.9300
C(25)-C(26)	1.402(9)
C(25)-H(25)	0.9300
C(26)-H(26)	0.9300
C(27)-C(28)	1.375(8)
C(27)-C(32)	1.379(8)
C(27)-P(1)	1.812(6)
C(28)-C(29)	1.385(9)
C(28)-H(28)	0.9300
C(29)-C(30)	1.352(10)
C(29)-H(29)	0.9300
C(30)-C(31)	1.337(10)
C(30)-H(30)	0.9300
C(31)-C(32)	1.383(9)
C(31)-H(31)	0.9300
C(32)-H(32)	0.9300
C(33)-C(38)	1.344(9)
C(33)-C(34)	1.347(9)
C(33)-P(2)	1.809(6)
C(34)-C(35)	1.390(10)
C(34)-H(34)	0.9300
C(35)-C(36)	1.332(11)
C(35)-H(35)	0.9300
C(36)-C(37)	1.310(11)
C(36)-H(36)	0.9300
C(37)-C(38)	1.390(10)

C(37)-H(37)	0.9300
C(38)-H(38)	0.9300
C(39)-C(40)	1.374(8)
C(39)-C(44)	1.377(9)
C(39)-P(2)	1.826(6)
C(40)-C(41)	1.381(9)
C(40)-H(40)	0.9300
C(41)-C(42)	1.340(10)
C(41)-H(41)	0.9300
C(42)-C(43)	1.346(11)
C(42)-H(42)	0.9300
C(43)-C(44)	1.387(10)
C(43)-H(43)	0.9300
C(44)-H(44)	0.9300
C(1AC)-C(2AC)	1.478(16)
C(1AC)-H(1A1)	0.9600
C(1AC)-H(1A2)	0.9600
C(1AC)-H(1A3)	0.9600
C(2AC)-O(1AC)	1.155(11)
C(2AC)-C(3AC)	1.445(16)
C(3AC)-H(3A1)	0.9600
C(3AC)-H(3A2)	0.9600
C(3AC)-H(3A3)	0.9600
C(4AC)-C(5AC)	1.406(16)
C(4AC)-H(4A1)	0.9600
C(4AC)-H(4A2)	0.9600
C(4AC)-H(4A3)	0.9600
C(5AC)-O(2AC)	1.114(10)
C(5AC)-C(6AC)	1.438(15)
C(6AC)-H(6A1)	0.9600
C(6AC)-H(6A2)	0.9600
C(6AC)-H(6A3)	0.9600
Cl(1)-Pd(1)	2.4101(15)
O(1)-H(1O)	0.8190
O(2)-H(2O)	0.83(2)
P(1)-Pd(1)	2.2951(16)
P(2)-Pd(1)	2.2948(17)

C(2)-C(1)-C(15)	101.4(4)
C(2)-C(1)-C(14)	105.2(4)
C(15)-C(1)-C(14)	101.7(4)
C(2)-C(1)-Pd(1)	114.1(4)
C(15)-C(1)-Pd(1)	118.6(4)
C(14)-C(1)-Pd(1)	114.0(4)
C(7)-C(2)-C(3)	120.7(5)
C(7)-C(2)-C(1)	117.2(5)
C(3)-C(2)-C(1)	121.7(5)
C(4)-C(3)-C(2)	118.5(5)
C(4)-C(3)-P(1)	129.0(5)
C(2)-C(3)-P(1)	112.3(4)
C(5)-C(4)-C(3)	120.7(6)
C(5)-C(4)-H(4)	119.7
C(3)-C(4)-H(4)	119.7
C(4)-C(5)-C(6)	120.9(6)
C(4)-C(5)-H(5)	119.6
C(6)-C(5)-H(5)	119.6
C(7)-C(6)-C(5)	119.0(6)
C(7)-C(6)-H(6)	120.5
C(5)-C(6)-H(6)	120.5
C(2)-C(7)-C(6)	119.8(6)
C(2)-C(7)-C(8)	112.1(5)
C(6)-C(7)-C(8)	128.0(5)
C(9)-C(8)-C(7)	107.5(5)
C(9)-C(8)-C(20)	105.0(5)
C(7)-C(8)-C(20)	104.5(5)
C(9)-C(8)-H(8)	113.1
C(7)-C(8)-H(8)	113.1
C(20)-C(8)-H(8)	113.1
C(10)-C(9)-C(14)	118.7(6)
C(10)-C(9)-C(8)	128.3(6)
C(14)-C(9)-C(8)	113.0(5)
C(11)-C(10)-C(9)	119.6(6)
C(11)-C(10)-H(10)	120.2
C(9)-C(10)-H(10)	120.2

C(12)-C(11)-C(10)	121.8(6)
C(12)-C(11)-H(11)	119.1
C(10)-C(11)-H(11)	119.1
C(11)-C(12)-C(13)	119.5(6)
C(11)-C(12)-H(12)	120.2
C(13)-C(12)-H(12)	120.2
C(14)-C(13)-C(12)	118.5(6)
C(14)-C(13)-P(2)	112.5(4)
C(12)-C(13)-P(2)	128.8(5)
C(13)-C(14)-C(9)	121.6(5)
C(13)-C(14)-C(1)	122.4(5)
C(9)-C(14)-C(1)	115.7(5)
C(16)-C(15)-C(20)	120.0(5)
C(16)-C(15)-C(1)	126.3(5)
C(20)-C(15)-C(1)	113.7(5)
O(1)-C(16)-C(15)	117.9(5)
O(1)-C(16)-C(17)	123.2(6)
C(15)-C(16)-C(17)	118.9(5)
C(18)-C(17)-C(16)	120.5(6)
C(18)-C(17)-H(17)	119.8
C(16)-C(17)-H(17)	119.8
C(19)-C(18)-C(17)	121.2(6)
C(19)-C(18)-H(18)	119.4
C(17)-C(18)-H(18)	119.4
C(18)-C(19)-O(2)	123.5(6)
C(18)-C(19)-C(20)	119.7(5)
O(2)-C(19)-C(20)	116.8(6)
C(19)-C(20)-C(15)	119.7(5)
C(19)-C(20)-C(8)	126.2(5)
C(15)-C(20)-C(8)	114.0(5)
C(26)-C(21)-C(22)	119.2(6)
C(26)-C(21)-P(1)	117.5(5)
C(22)-C(21)-P(1)	123.3(6)
C(21)-C(22)-C(23)	119.1(8)
C(21)-C(22)-H(22)	120.4
C(23)-C(22)-H(22)	120.4
C(24)-C(23)-C(22)	121.3(8)

C(24)-C(23)-H(23)	119.4
C(22)-C(23)-H(23)	119.4
C(23)-C(24)-C(25)	120.4(8)
C(23)-C(24)-H(24)	119.8
C(25)-C(24)-H(24)	119.8
C(24)-C(25)-C(26)	119.7(8)
C(24)-C(25)-H(25)	120.1
C(26)-C(25)-H(25)	120.1
C(21)-C(26)-C(25)	120.3(7)
C(21)-C(26)-H(26)	119.8
C(25)-C(26)-H(26)	119.8
C(28)-C(27)-C(32)	116.4(6)
C(28)-C(27)-P(1)	119.1(5)
C(32)-C(27)-P(1)	124.5(5)
C(27)-C(28)-C(29)	121.6(7)
C(27)-C(28)-H(28)	119.2
C(29)-C(28)-H(28)	119.2
C(30)-C(29)-C(28)	119.8(7)
C(30)-C(29)-H(29)	120.1
C(28)-C(29)-H(29)	120.1
C(31)-C(30)-C(29)	120.3(7)
C(31)-C(30)-H(30)	119.9
C(29)-C(30)-H(30)	119.9
C(30)-C(31)-C(32)	120.2(7)
C(30)-C(31)-H(31)	119.9
C(32)-C(31)-H(31)	119.9
C(27)-C(32)-C(31)	121.7(7)
C(27)-C(32)-H(32)	119.2
C(31)-C(32)-H(32)	119.2
C(38)-C(33)-C(34)	116.2(6)
C(38)-C(33)-P(2)	125.7(5)
C(34)-C(33)-P(2)	118.1(5)
C(33)-C(34)-C(35)	122.3(8)
C(33)-C(34)-H(34)	118.8
C(35)-C(34)-H(34)	118.8
C(36)-C(35)-C(34)	119.3(8)
C(36)-C(35)-H(35)	120.4

C(34)-C(35)-H(35)	120.4
C(37)-C(36)-C(35)	119.9(8)
C(37)-C(36)-H(36)	120.1
C(35)-C(36)-H(36)	120.1
C(36)-C(37)-C(38)	120.7(8)
C(36)-C(37)-H(37)	119.7
C(38)-C(37)-H(37)	119.7
C(33)-C(38)-C(37)	121.6(8)
C(33)-C(38)-H(38)	119.2
C(37)-C(38)-H(38)	119.2
C(40)-C(39)-C(44)	118.3(6)
C(40)-C(39)-P(2)	119.2(5)
C(44)-C(39)-P(2)	122.4(5)
C(39)-C(40)-C(41)	120.0(7)
C(39)-C(40)-H(40)	120.0
C(41)-C(40)-H(40)	120.0
C(42)-C(41)-C(40)	121.5(8)
C(42)-C(41)-H(41)	119.2
C(40)-C(41)-H(41)	119.2
C(41)-C(42)-C(43)	119.2(8)
C(41)-C(42)-H(42)	120.4
C(43)-C(42)-H(42)	120.4
C(42)-C(43)-C(44)	121.1(8)
C(42)-C(43)-H(43)	119.4
C(44)-C(43)-H(43)	119.4
C(39)-C(44)-C(43)	119.8(7)
C(39)-C(44)-H(44)	120.1
C(43)-C(44)-H(44)	120.1
C(2AC)-C(1AC)-H(1A1)	109.5
C(2AC)-C(1AC)-H(1A2)	109.5
H(1A1)-C(1AC)-H(1A2)	109.5
C(2AC)-C(1AC)-H(1A3)	109.5
H(1A1)-C(1AC)-H(1A3)	109.5
H(1A2)-C(1AC)-H(1A3)	109.5
O(1AC)-C(2AC)-C(3AC)	120.7(14)
O(1AC)-C(2AC)-C(1AC)	120.2(14)
C(3AC)-C(2AC)-C(1AC)	119.0(12)

C(2AC)-C(3AC)-H(3A1)	109.5
C(2AC)-C(3AC)-H(3A2)	109.5
H(3A1)-C(3AC)-H(3A2)	109.5
C(2AC)-C(3AC)-H(3A3)	109.5
H(3A1)-C(3AC)-H(3A3)	109.5
H(3A2)-C(3AC)-H(3A3)	109.5
C(5AC)-C(4AC)-H(4A1)	109.5
C(5AC)-C(4AC)-H(4A2)	109.5
H(4A1)-C(4AC)-H(4A2)	109.5
C(5AC)-C(4AC)-H(4A3)	109.5
H(4A1)-C(4AC)-H(4A3)	109.5
H(4A2)-C(4AC)-H(4A3)	109.5
O(2AC)-C(5AC)-C(4AC)	122.9(14)
O(2AC)-C(5AC)-C(6AC)	118.1(14)
C(4AC)-C(5AC)-C(6AC)	118.7(12)
C(5AC)-C(6AC)-H(6A1)	109.5
C(5AC)-C(6AC)-H(6A2)	109.5
H(6A1)-C(6AC)-H(6A2)	109.5
C(5AC)-C(6AC)-H(6A3)	109.5
H(6A1)-C(6AC)-H(6A3)	109.5
H(6A2)-C(6AC)-H(6A3)	109.5
C(16)-O(1)-H(1O)	107.0
C(19)-O(2)-H(2O)	106(7)
C(3)-P(1)-C(27)	106.2(3)
C(3)-P(1)-C(21)	106.8(3)
C(27)-P(1)-C(21)	104.3(3)
C(3)-P(1)-Pd(1)	102.2(2)
C(27)-P(1)-Pd(1)	118.3(2)
C(21)-P(1)-Pd(1)	117.9(2)
C(13)-P(2)-C(33)	108.1(3)
C(13)-P(2)-C(39)	106.1(3)
C(33)-P(2)-C(39)	103.6(3)
C(13)-P(2)-Pd(1)	102.7(2)
C(33)-P(2)-Pd(1)	118.6(2)
C(39)-P(2)-Pd(1)	116.9(2)
C(1)-Pd(1)-P(2)	84.74(16)
C(1)-Pd(1)-P(1)	84.36(16)

P(2)-Pd(1)-P(1)	153.89(6)
C(1)-Pd(1)-Cl(1)	173.23(16)
P(2)-Pd(1)-Cl(1)	97.59(6)
P(1)-Pd(1)-Cl(1)	95.99(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 10. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	33(3)	40(3)	37(3)	9(3)	-2(2)	2(2)
C(2)	36(3)	39(3)	33(3)	10(3)	11(3)	7(3)
C(3)	37(3)	42(3)	44(4)	11(3)	16(3)	7(3)
C(4)	53(4)	50(4)	58(4)	28(3)	13(3)	7(3)
C(5)	69(5)	50(4)	63(5)	26(4)	26(4)	6(4)
C(6)	49(4)	47(4)	54(4)	6(3)	17(3)	-3(3)
C(7)	39(3)	42(4)	46(4)	9(3)	11(3)	3(3)
C(8)	27(3)	42(3)	55(4)	7(3)	2(3)	-2(3)
C(9)	42(3)	35(3)	53(4)	9(3)	1(3)	11(3)
C(10)	41(4)	48(4)	60(4)	9(3)	-6(3)	17(3)
C(11)	61(4)	52(4)	47(4)	7(3)	-5(3)	25(3)
C(12)	63(4)	49(4)	45(4)	20(3)	11(3)	26(3)
C(13)	47(3)	32(3)	43(4)	12(3)	1(3)	14(3)
C(14)	39(3)	29(3)	40(3)	10(3)	3(3)	13(2)
C(15)	31(3)	43(3)	48(4)	12(3)	7(3)	12(3)
C(16)	32(3)	45(4)	72(5)	1(3)	6(3)	5(3)
C(17)	51(4)	61(5)	81(5)	-11(4)	8(4)	19(4)
C(18)	42(4)	51(4)	86(5)	-5(4)	20(4)	13(3)
C(19)	29(3)	60(4)	78(5)	14(4)	8(3)	5(3)
C(20)	35(3)	43(4)	55(4)	8(3)	9(3)	9(3)
C(21)	56(4)	59(4)	40(4)	17(3)	13(3)	25(3)
C(22)	96(6)	102(7)	58(5)	3(5)	29(5)	-16(5)
C(23)	124(8)	156(10)	58(6)	16(6)	51(6)	-3(7)
C(24)	116(8)	107(7)	43(5)	15(5)	22(5)	39(6)
C(25)	102(7)	65(5)	57(5)	-3(4)	1(5)	17(5)
C(26)	68(5)	68(5)	57(5)	11(4)	10(4)	7(4)
C(27)	40(3)	39(3)	49(4)	10(3)	2(3)	13(3)
C(28)	69(5)	76(5)	80(5)	43(4)	26(4)	29(4)
C(29)	73(5)	76(5)	115(7)	39(5)	49(5)	39(4)
C(30)	55(5)	65(5)	100(7)	24(5)	6(4)	22(4)
C(31)	90(6)	94(6)	83(6)	38(5)	-12(5)	43(5)
C(32)	83(5)	84(5)	47(4)	26(4)	9(4)	37(4)

C(33)	54(4)	36(3)	51(4)	16(3)	8(3)	9(3)
C(34)	131(8)	55(5)	135(8)	30(5)	-69(7)	5(5)
C(35)	157(10)	42(5)	171(11)	23(6)	-67(8)	-13(6)
C(36)	116(7)	45(5)	100(7)	30(5)	28(6)	19(5)
C(37)	153(9)	48(5)	148(9)	27(6)	-46(8)	30(6)
C(38)	120(7)	46(5)	133(8)	18(5)	-50(6)	18(5)
C(39)	51(4)	52(4)	46(4)	16(3)	19(3)	16(3)
C(40)	60(4)	69(5)	65(5)	29(4)	26(4)	21(4)
C(41)	89(6)	95(6)	107(7)	42(6)	50(5)	52(5)
C(42)	103(7)	132(8)	107(7)	57(7)	64(6)	69(6)
C(43)	130(8)	170(10)	100(7)	87(7)	82(6)	70(8)
C(44)	106(7)	111(7)	84(6)	58(5)	47(5)	65(6)
C(1AC)	380(20)	91(9)	149(12)	14(9)	-44(14)	-44(12)
C(2AC)	124(10)	130(10)	109(9)	26(8)	-18(8)	-40(8)
C(3AC)	87(10)	440(30)	249(19)	210(20)	-2(11)	12(13)
C(4AC)	430(30)	340(30)	300(20)	220(20)	250(20)	260(30)
C(5AC)	141(10)	77(7)	93(7)	45(6)	-13(6)	-29(7)
C(6AC)	168(14)	240(18)	320(20)	172(17)	-10(14)	-47(13)
Cl(1)	33(1)	64(1)	68(1)	16(1)	4(1)	4(1)
O(1)	38(3)	53(3)	101(4)	-18(3)	11(2)	1(2)
O(2)	29(3)	76(4)	111(4)	1(3)	17(3)	5(2)
O(1AC)	109(6)	113(6)	209(9)	-65(6)	-44(6)	17(4)
O(2AC)	183(8)	97(6)	267(11)	66(7)	-81(7)	-46(6)
P(1)	41(1)	46(1)	40(1)	13(1)	8(1)	13(1)
P(2)	40(1)	39(1)	47(1)	15(1)	12(1)	14(1)
Pd(1)	29(1)	40(1)	39(1)	11(1)	4(1)	5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for 10.

	x	y	z	U(eq)
H(4)	8594	11158	6784	61
H(5)	10463	12169	7373	69
H(6)	11830	11331	8070	62
H(8)	12299	9462	8504	53
H(10)	12077	9453	10002	62
H(11)	10927	8822	10850	66
H(12)	9047	7749	10358	59
H(17)	10689	4965	6042	85
H(18)	12632	5872	6505	77
H(22)	8992	9234	5560	109
H(23)	9107	8345	4179	138
H(24)	7743	6814	3405	106
H(25)	6252	6049	3970	96
H(26)	6140	6870	5361	80
H(28)	5696	9384	7737	82
H(29)	4162	10537	7832	98
H(30)	3695	11411	6848	88
H(31)	4782	11208	5800	104
H(32)	6298	10039	5681	82
H(34)	6429	4768	7619	137
H(35)	6419	2784	7493	162
H(36)	7710	2240	8377	100
H(37)	9007	3623	9348	146
H(38)	8980	5609	9505	128
H(40)	5726	8385	8691	73
H(41)	4296	8957	9524	107
H(42)	4109	8275	10604	122
H(43)	5450	7125	10933	137
H(44)	6885	6495	10108	105
H(1A1)	8593	1790	4281	336
H(1A2)	7197	1401	4154	336

H(1A3)	8035	1129	4845	336
H(3A1)	6130	2948	5438	362
H(3A2)	6211	2991	4546	362
H(3A3)	6722	4109	5302	362
H(4A1)	8993	4852	1102	447
H(4A2)	7995	3780	991	447
H(4A3)	8726	4455	1861	447
H(6A1)	5861	5517	1750	349
H(6A2)	6396	4516	2037	349
H(6A3)	5941	4294	1105	349
H(1O)	8704	5029	6279	110
H(2O)	13850(80)	7600(90)	7290(50)	170(50)

Table 6. Hydrogen bonds for 10 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1O)...O(1AC)	0.82	1.93	2.750(8)	173.5
O(2)-H(2O)...Cl(1)#1	0.83(2)	2.34(6)	3.098(5)	151(10)

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z