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Supporting Information for

Mixed Phosphine/*N*-Heterocyclic Carbene Palladium Complexes: Synthesis, Characterization and Catalytic use in Aqueous Suzuki-Miyaura Reactions

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General Procedures

All reactions were performed under an inert atmosphere of argon or nitrogen using standard Schlenk line and glovebox techniques. Solvents were purchased and used as received. Flash column chromatography was performed on silica gel 60 (230-400 mesh). ^{1}H, ^{13}C-{^{1}H} and ^{31}P-{^{1}H} Nuclear Magnetic Resonance (NMR) spectra were recorded on a Bruker AC300 or on a Bruker Advance 400 Ultrashield spectrometer between 298 K and 373 K, Gas chromatography (GC) analyses were performed on an Agilent 7890A apparatus equipped with a flame ionization detector and a (5%-phenyl)-methylpolysiloxane column (30 m, 320 μm, film: 0.25 μm). All Reagents were purchased and used as received. HRMS samples were submitted to EPSRC National Mass Spectrometry Service Centre (http://www.swan.ac.uk/nmssc/index.html). Elemental analyses were performed by the London Metropolitan University Service.

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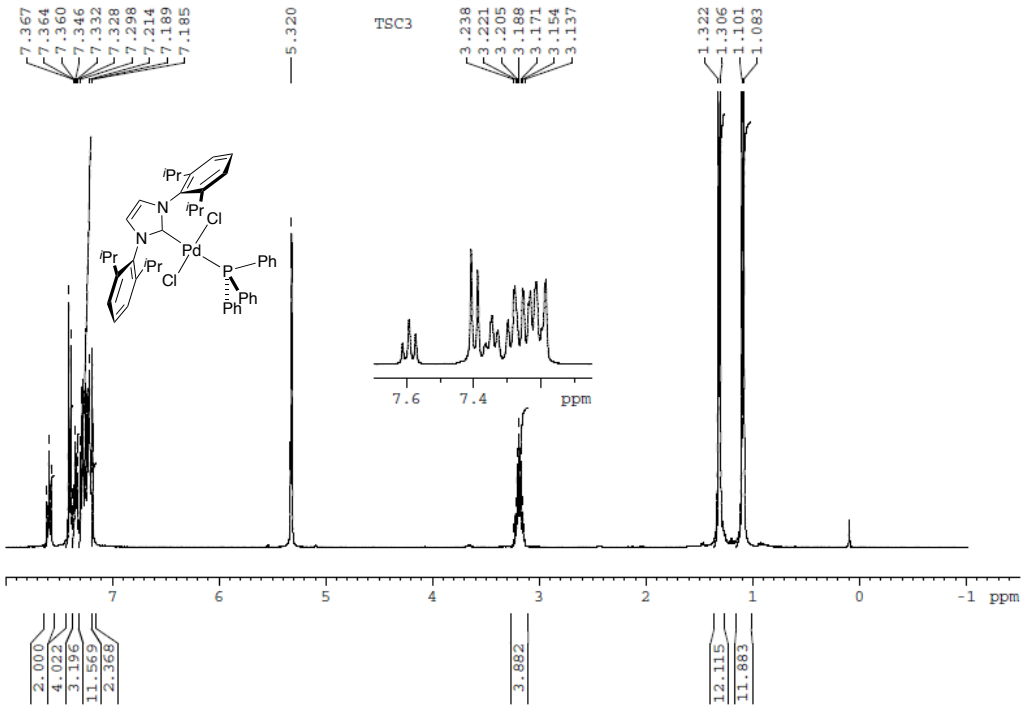
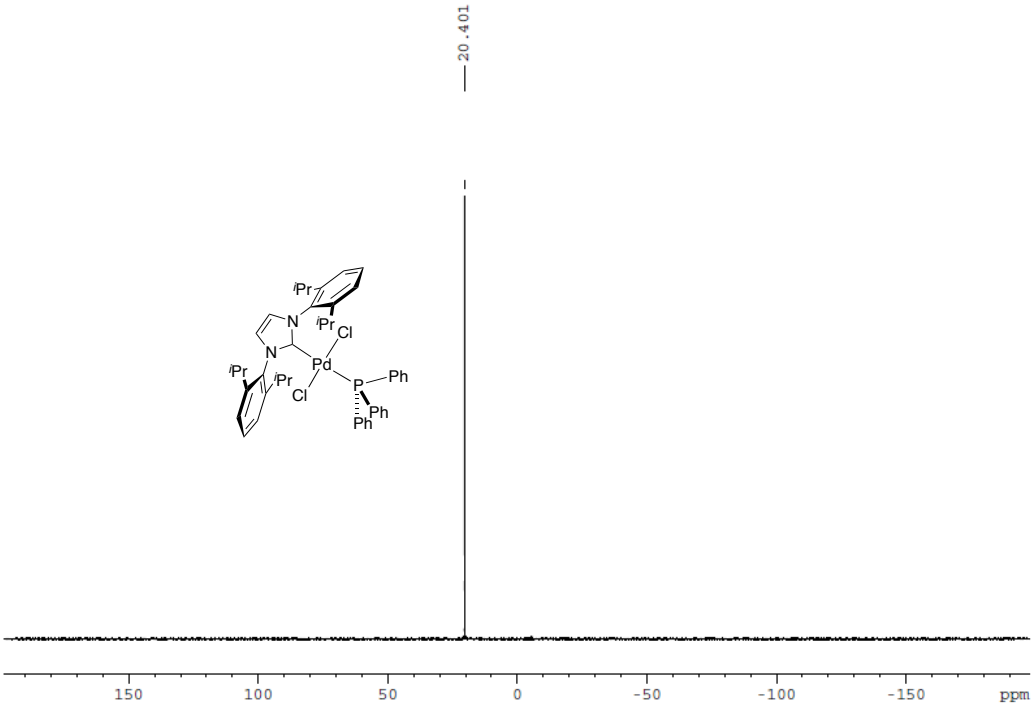
NMR spectra of the complexes

^{1}H, ^{31}P-{^{1}H} and ^{13}C-{^{1}H} NMR spectra of [$PdCl_2$(IPr){PPh_3}] (2a)

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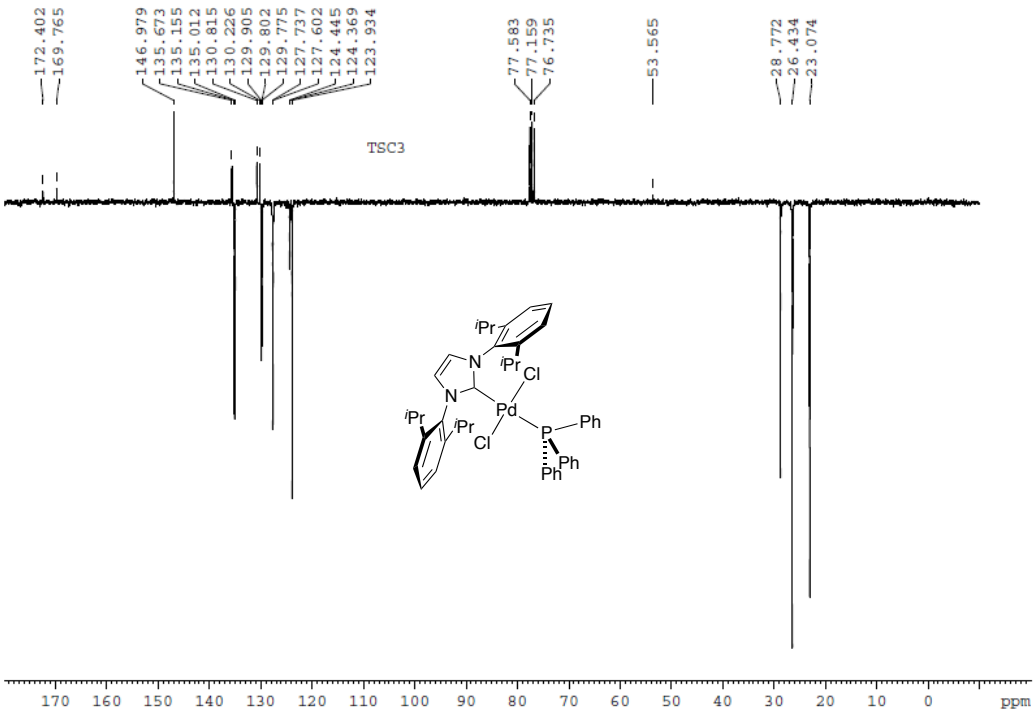
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127.602
124.445
124.369
123.934
77.583
77.159
76.735
53.565
28.772
26.434
23.074
TSC3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
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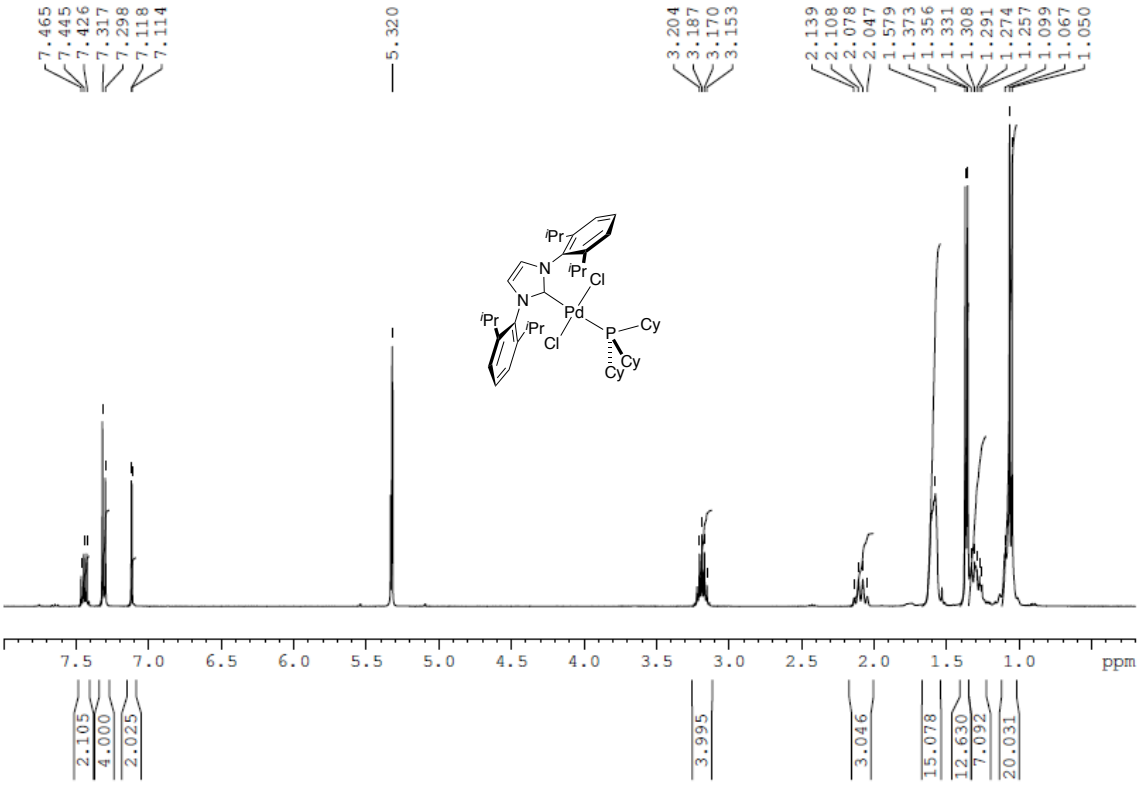
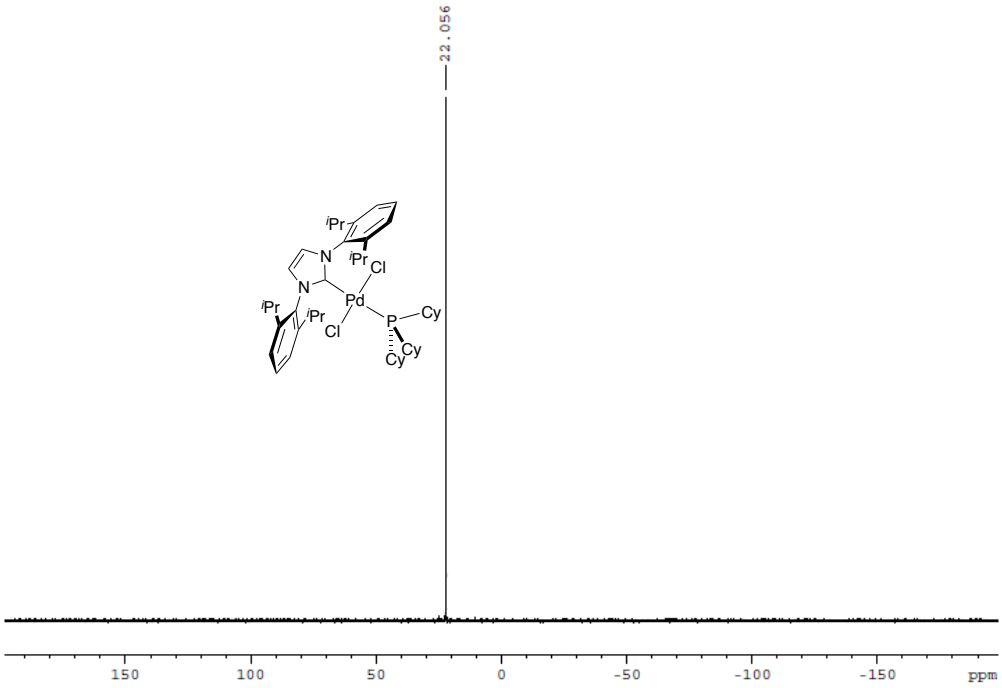
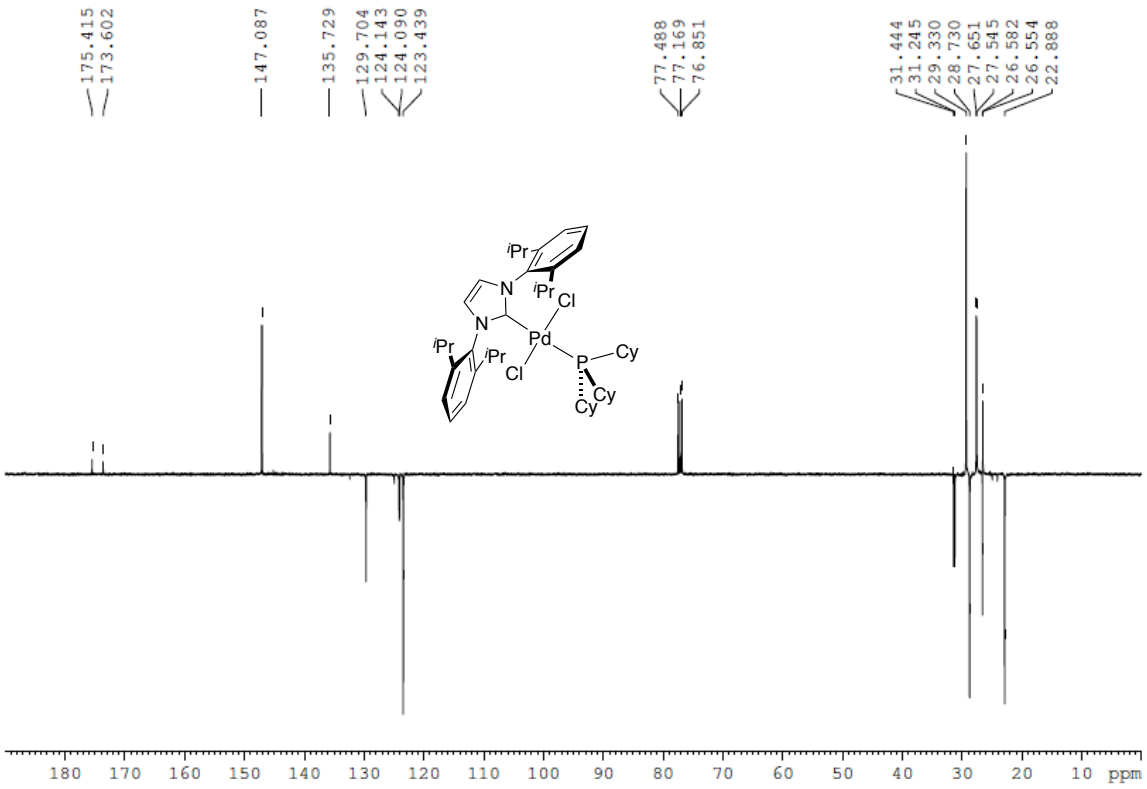
ppm

^{1}H, ^{31}P-{^{1}H} and ^{13}C-{^{1}H} NMR spectra of $[PdCl_2(IPr)\{PCy)_3\}]$ (2b)



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147.087
135.729
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124.090
123.439
77.488
77.169
76.851
31.444
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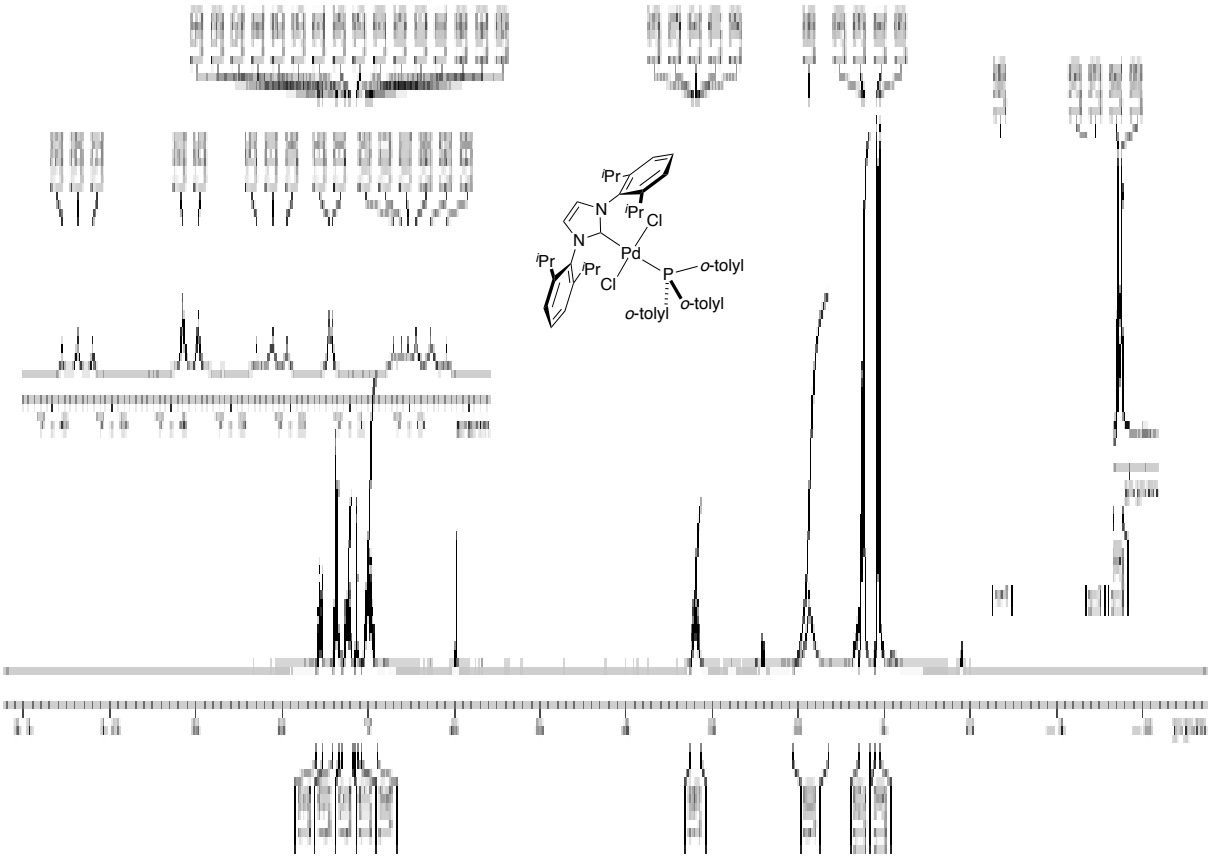
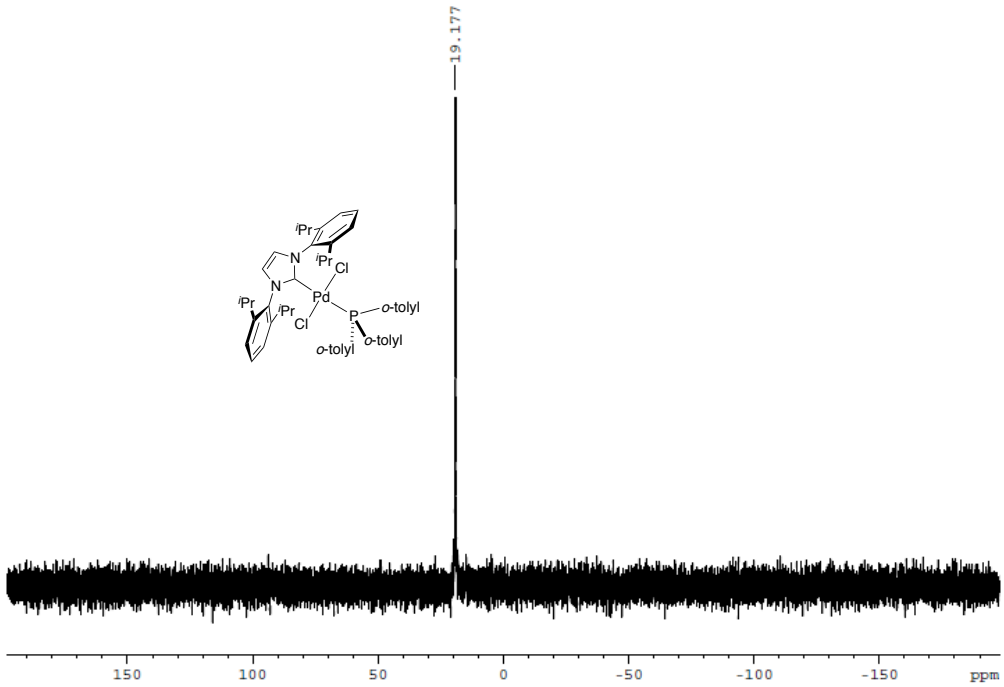
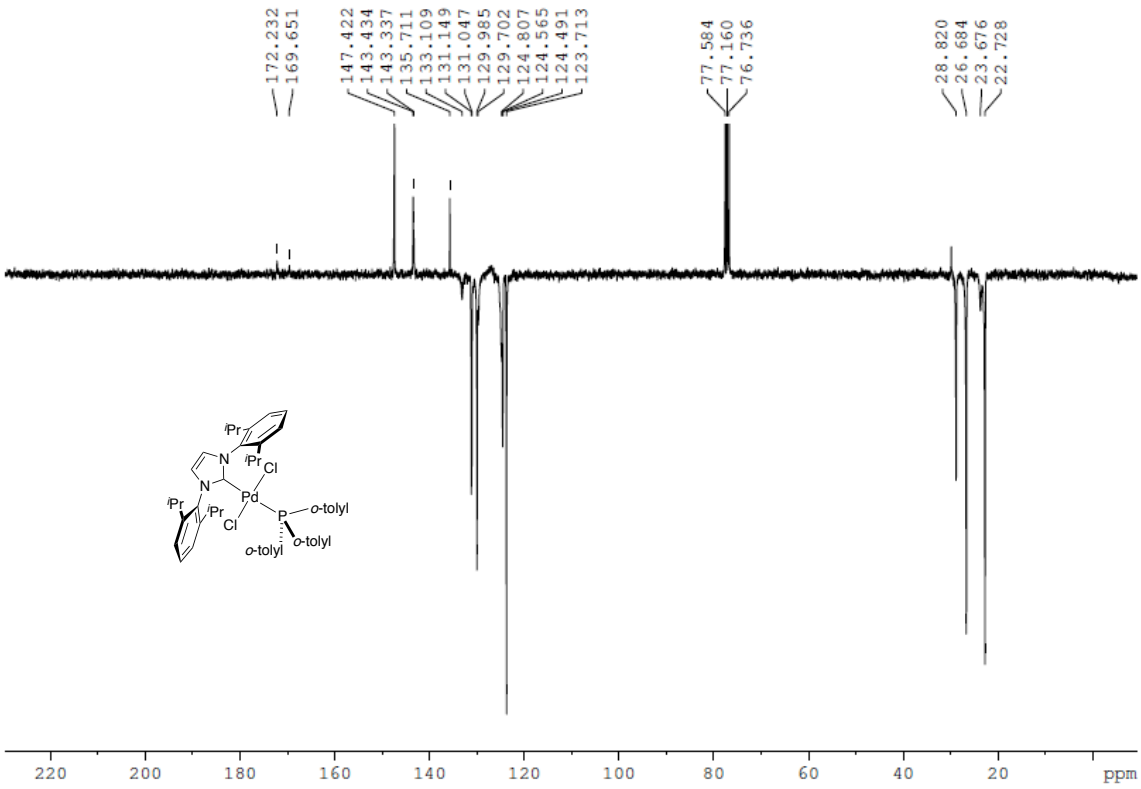
29.330
28.730
27.651
27.545
26.582
26.554
22.888
iPr
iPr
N
N
Cl
Pd
iPr
iPr
Cl
P
Cy
Cy
Cy
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

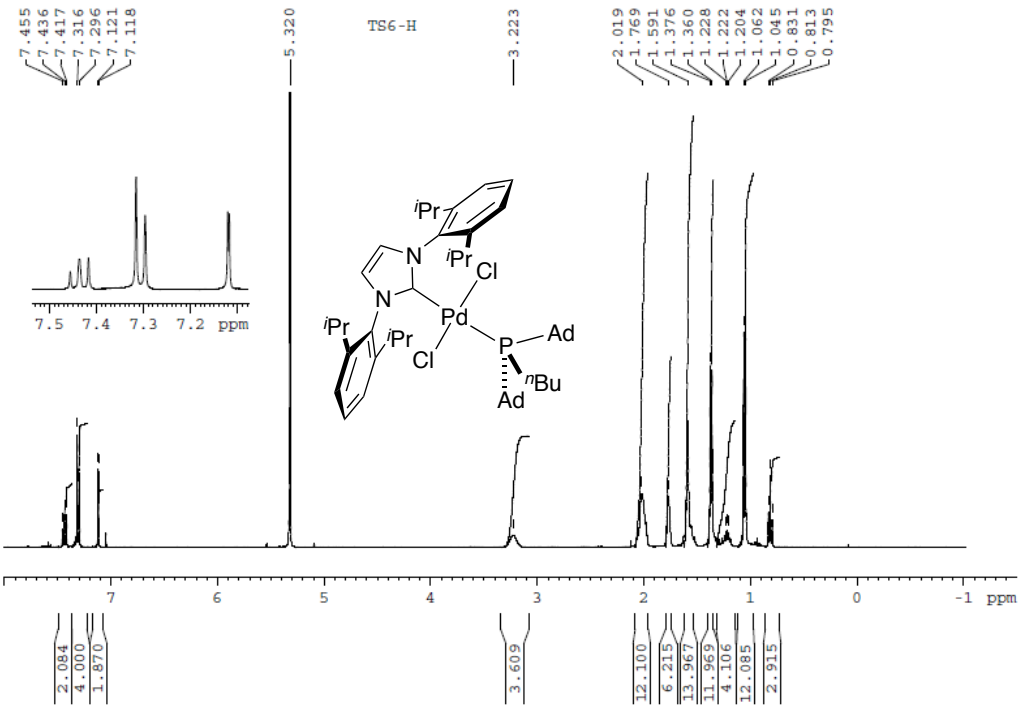
^{1}H, ^{31}P-{^{1}H} and ^{13}C-{^{1}H} NMR spectra of [$PdCl_2$(IPr){P(*o*-tolyl)$_3$}] (2c)

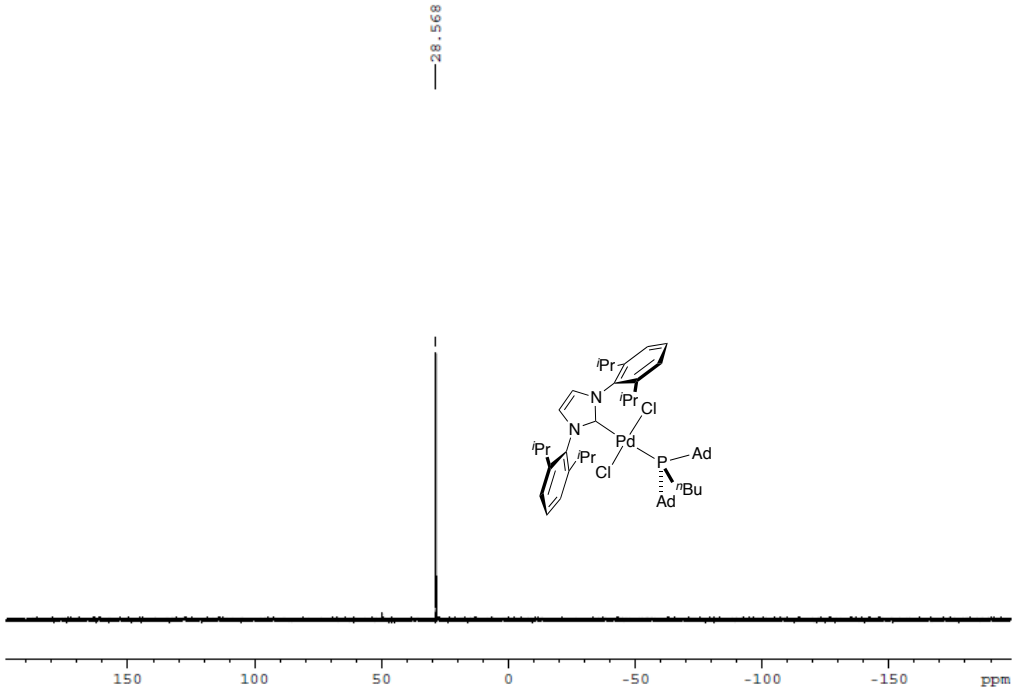






^{1}H, ^{31}P-{^{1}H} and ^{13}C-{^{1}H} NMR spectra of $[PdCl_2(IPr)\{P(1\text{-}Ad)_2(^{n}Bu)\}]$ (2d)

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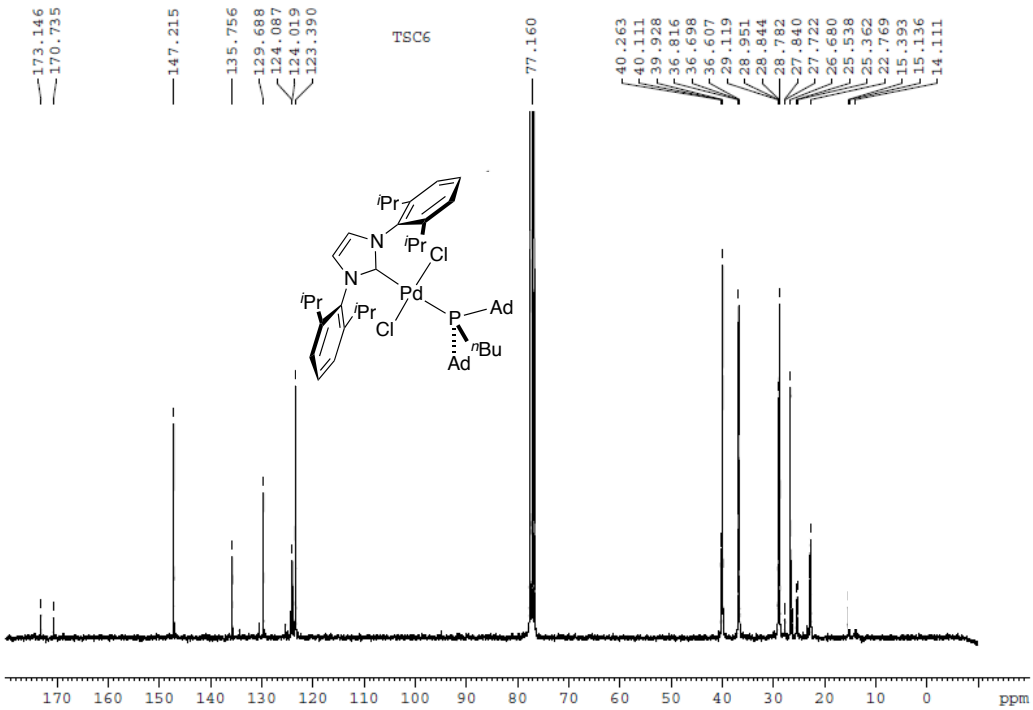
173.146
170.735
147.215
135.756
129.688
124.087
124.019
123.390
TSC6
77.160
40.263
40.111
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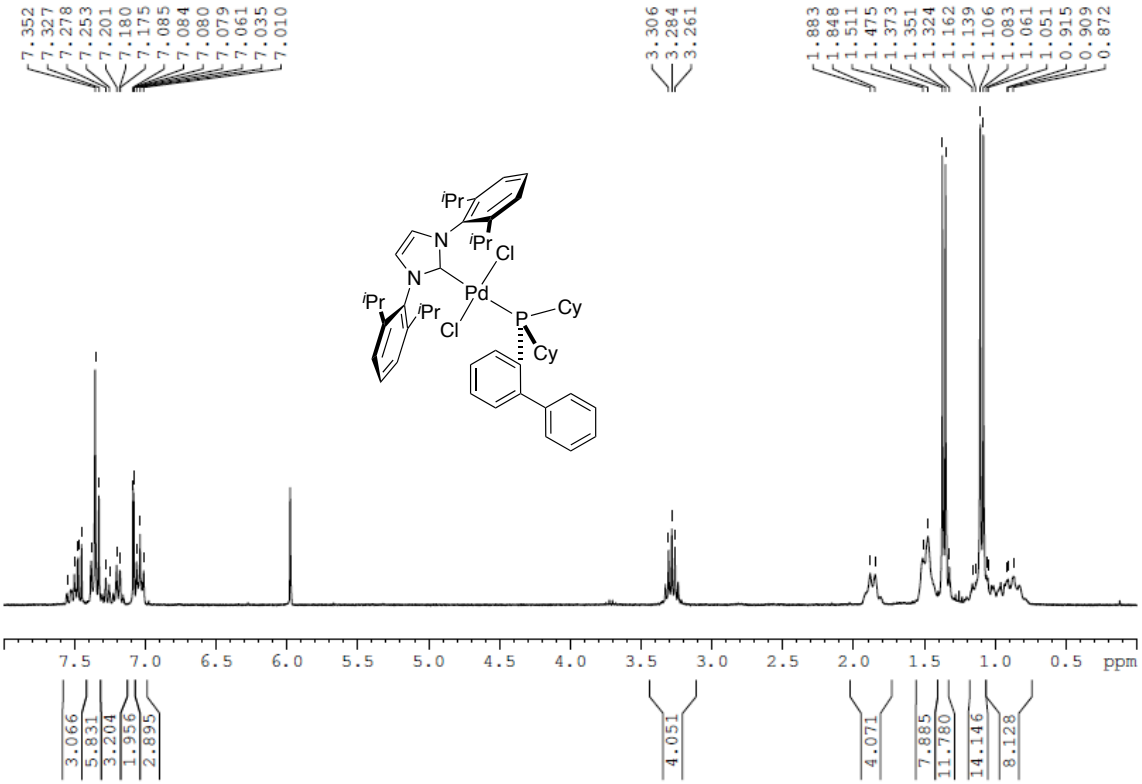
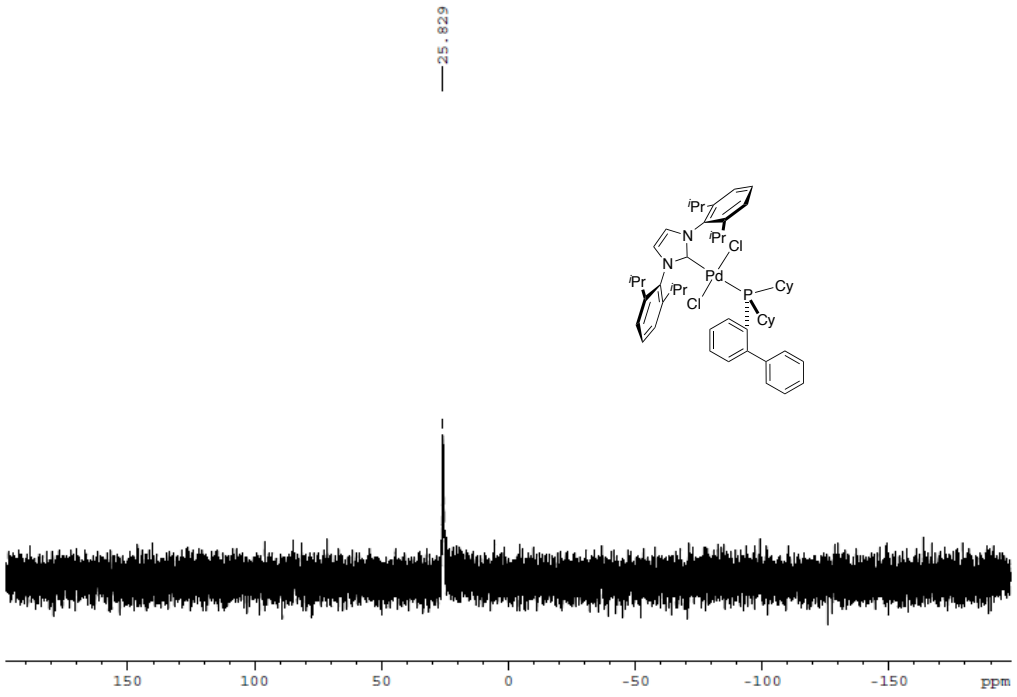
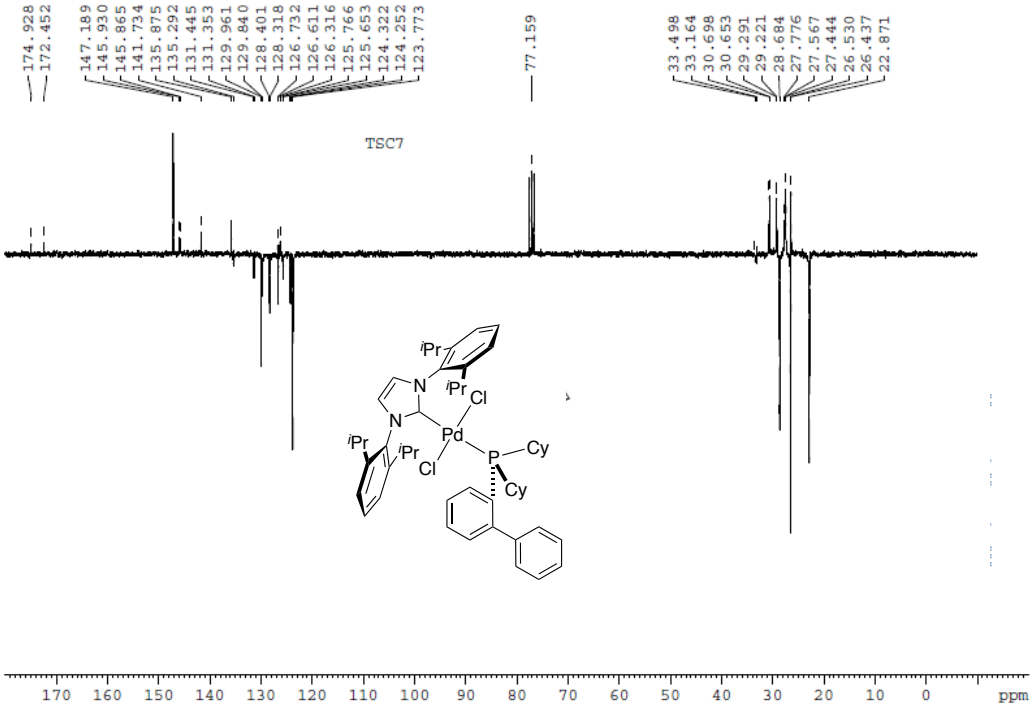
36.816
36.698
36.607
29.119
28.951
28.844
28.782
27.840
27.722
26.680
25.538
25.362
22.769
15.393
15.136
14.111
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

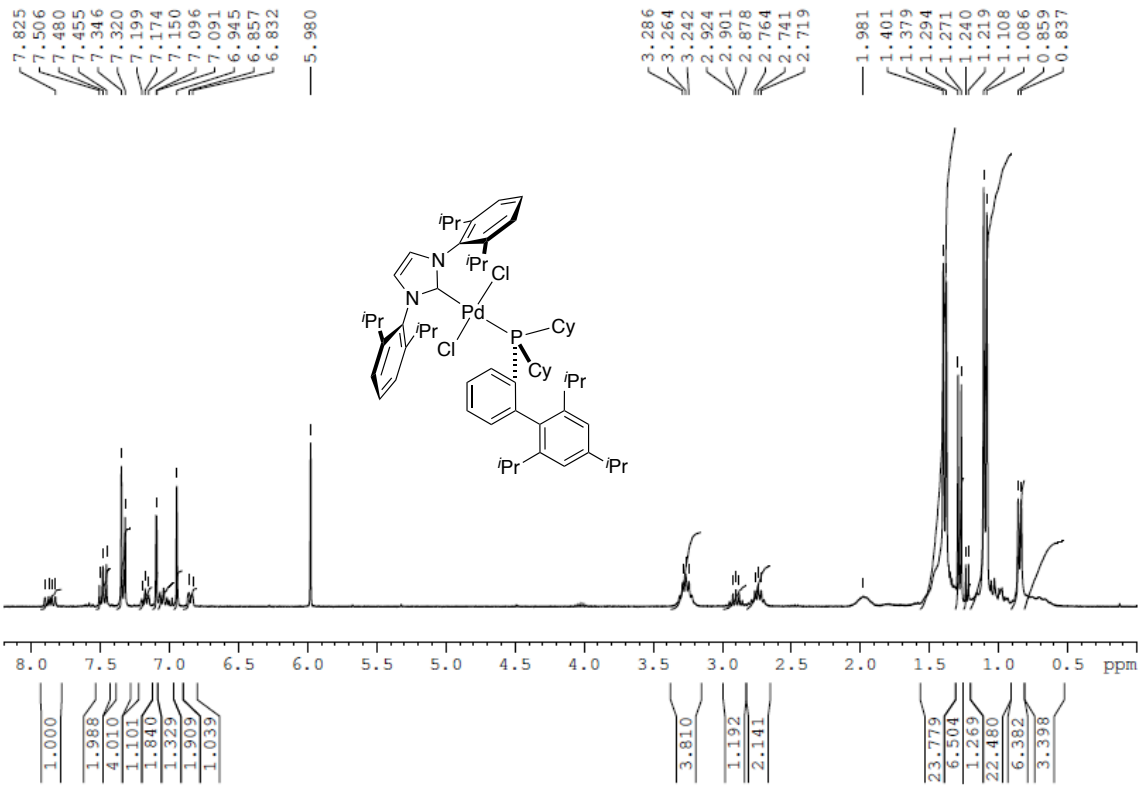
^{1}H, ^{31}P-{^{1}H} and ^{13}C-{^{1}H} NMR spectra of [$PdCl_2$(IPr){PCy_2(*o*-biphenyl)}] (2e)

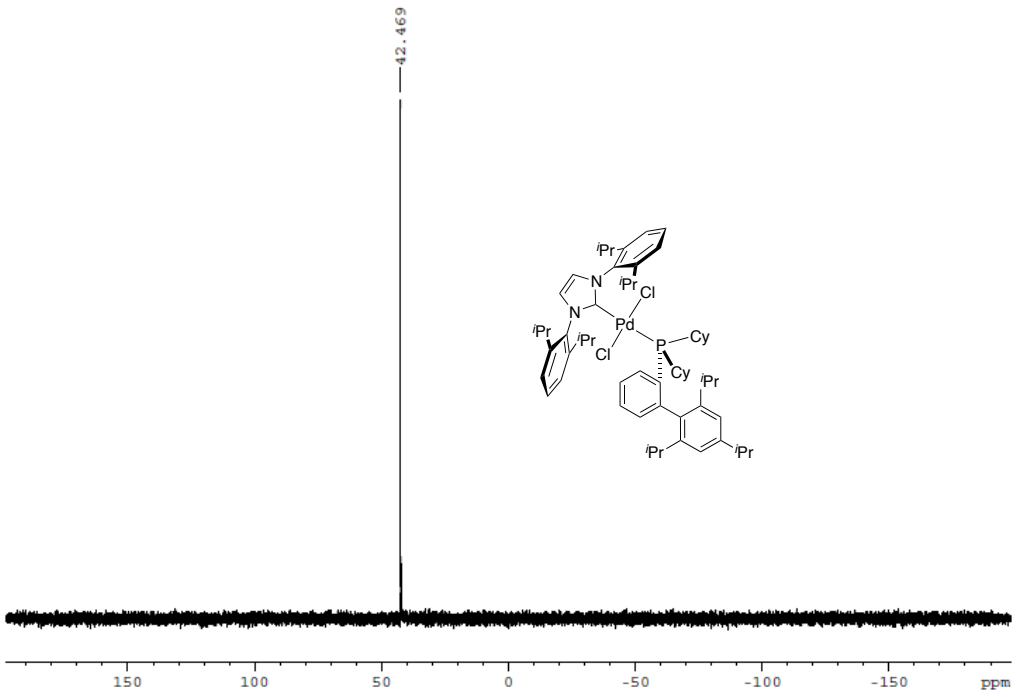






^{1}H, ^{31}P-{^{1}H} and ^{13}C-{^{1}H} NMR spectra of [$PdCl_2$(IPr)(XPhos)] (2f)

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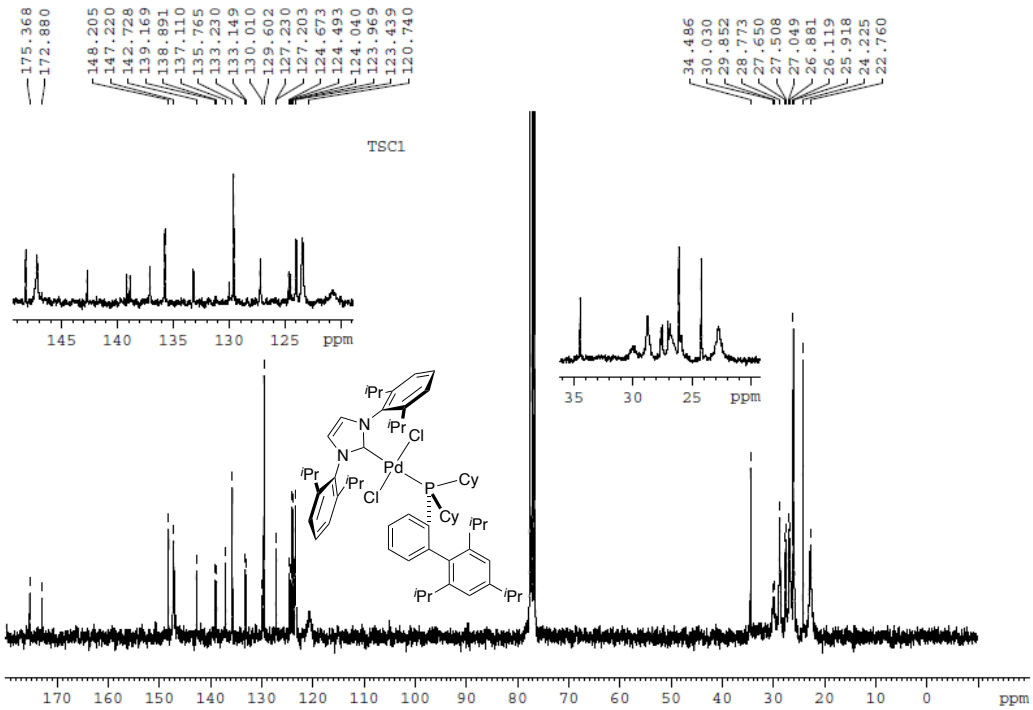
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27.049
26.881
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25.918
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TSC1
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ppm
35
30
25
ppm
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150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

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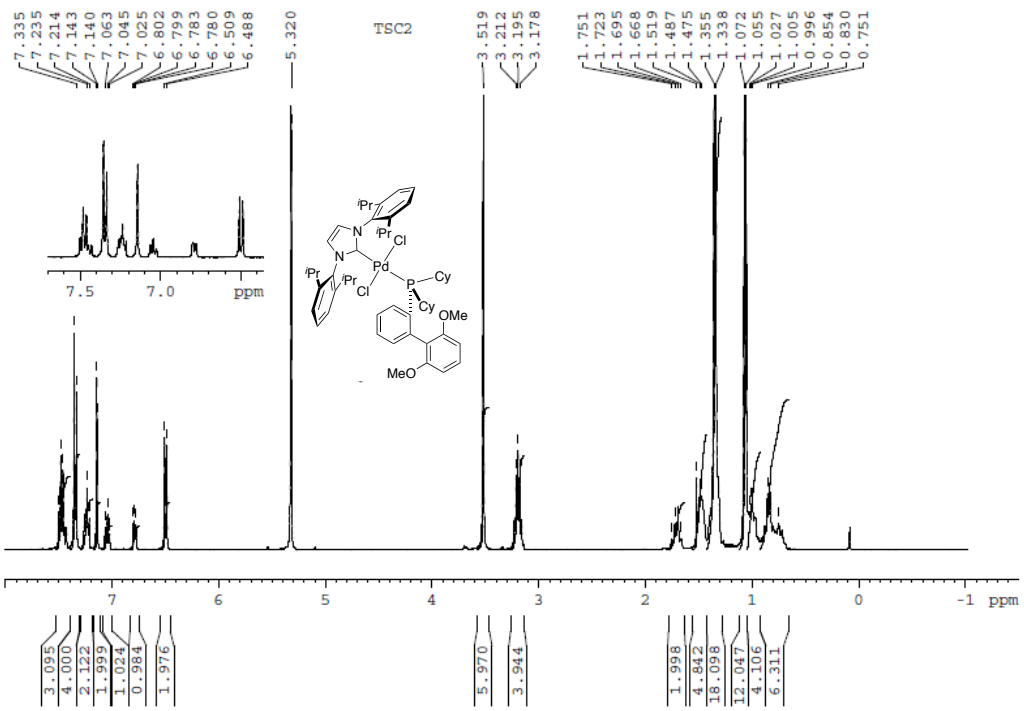
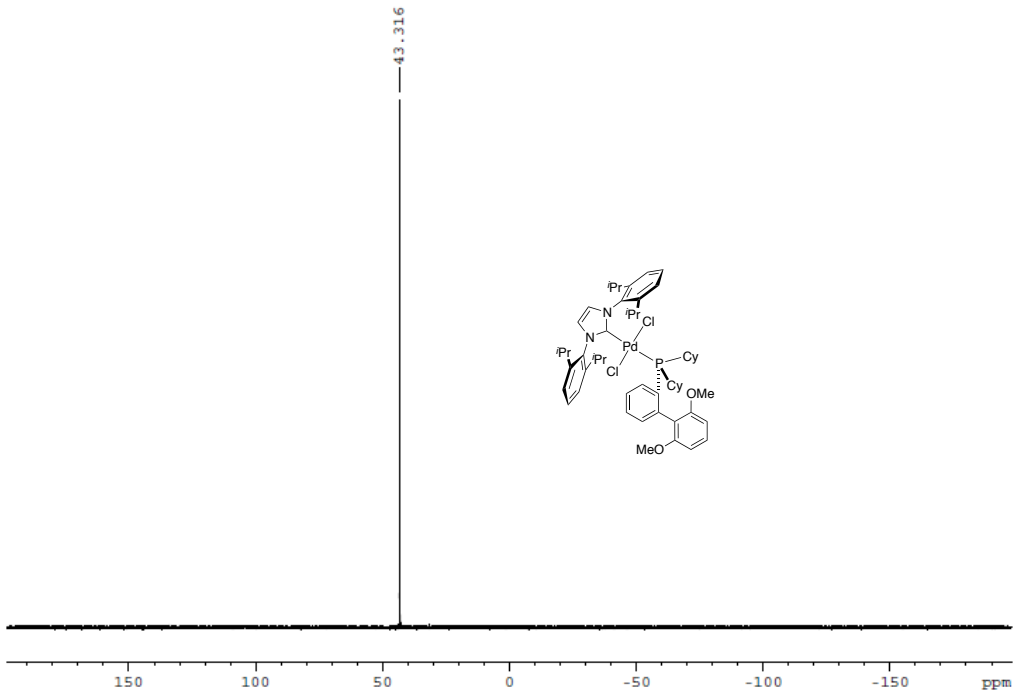
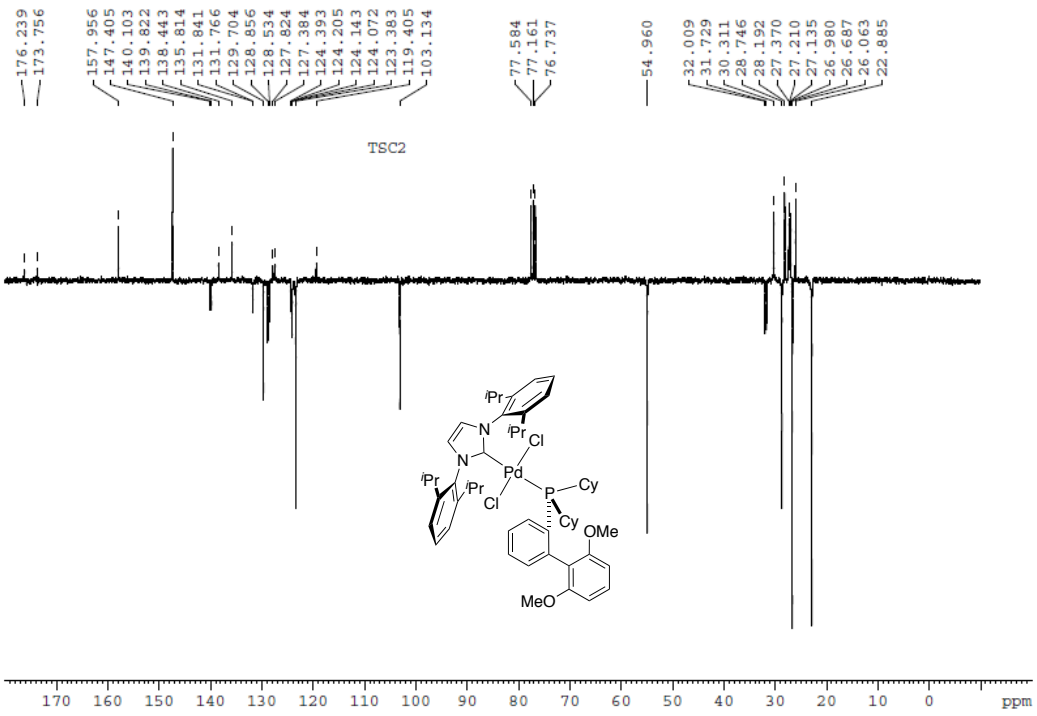
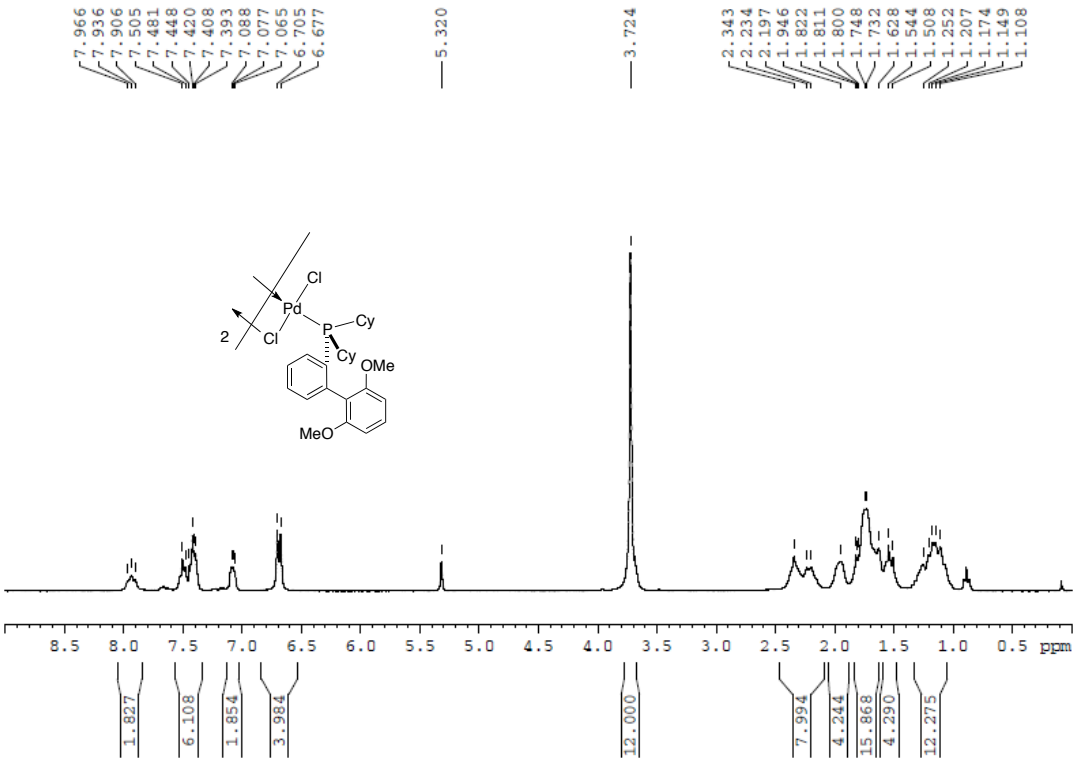
^{1}H, ^{31}P-{^{1}H} and ^{13}C-{^{1}H} NMR spectra of [$PdCl_2$(IPr)(SPhos)] (2g)

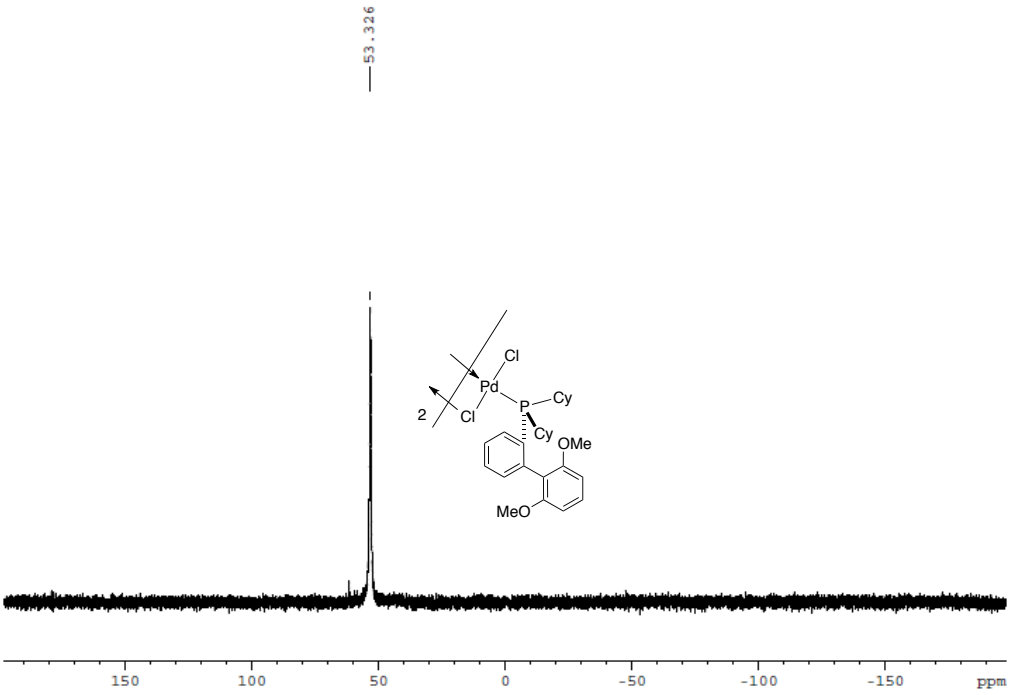






^{1}H, ^{31}P-{^{1}H} and ^{13}C-{^{1}H} NMR spectra of $[Pd(\mu\text{-}Cl)(Cl)(SPhos)]_2$ (5)

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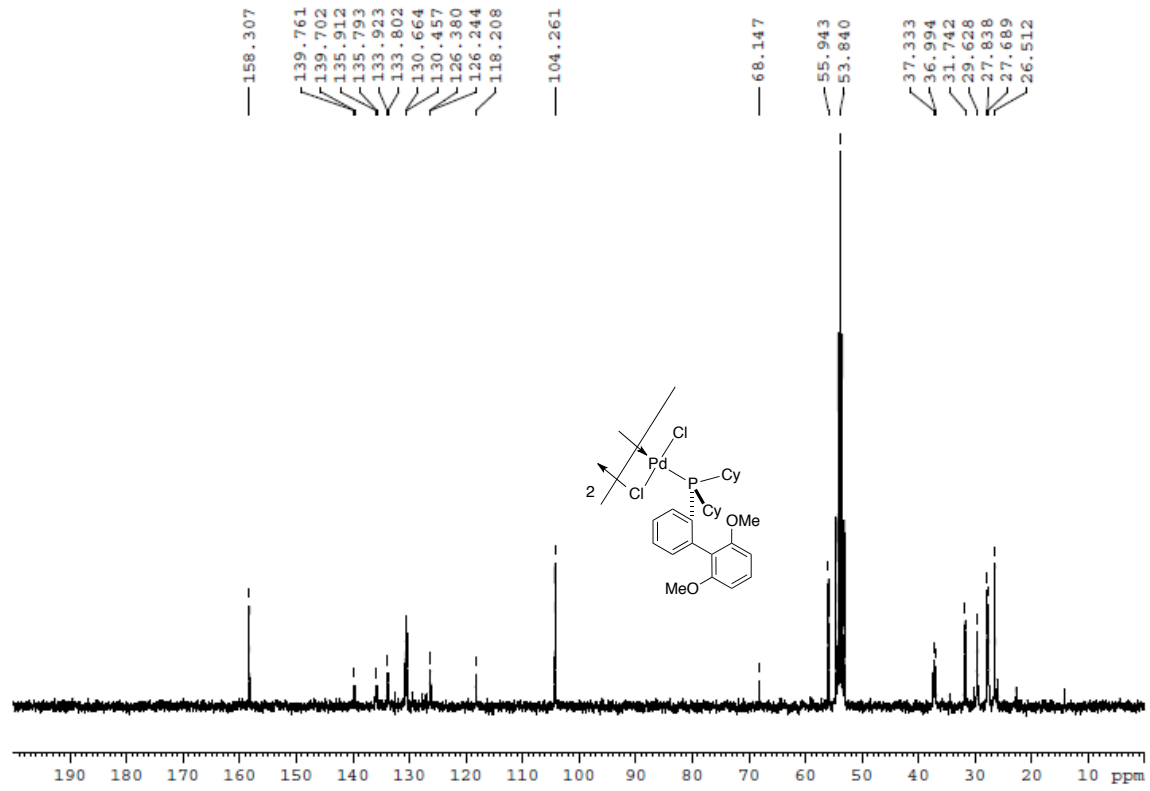
ppm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27.689
26.512
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MeO
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70
60
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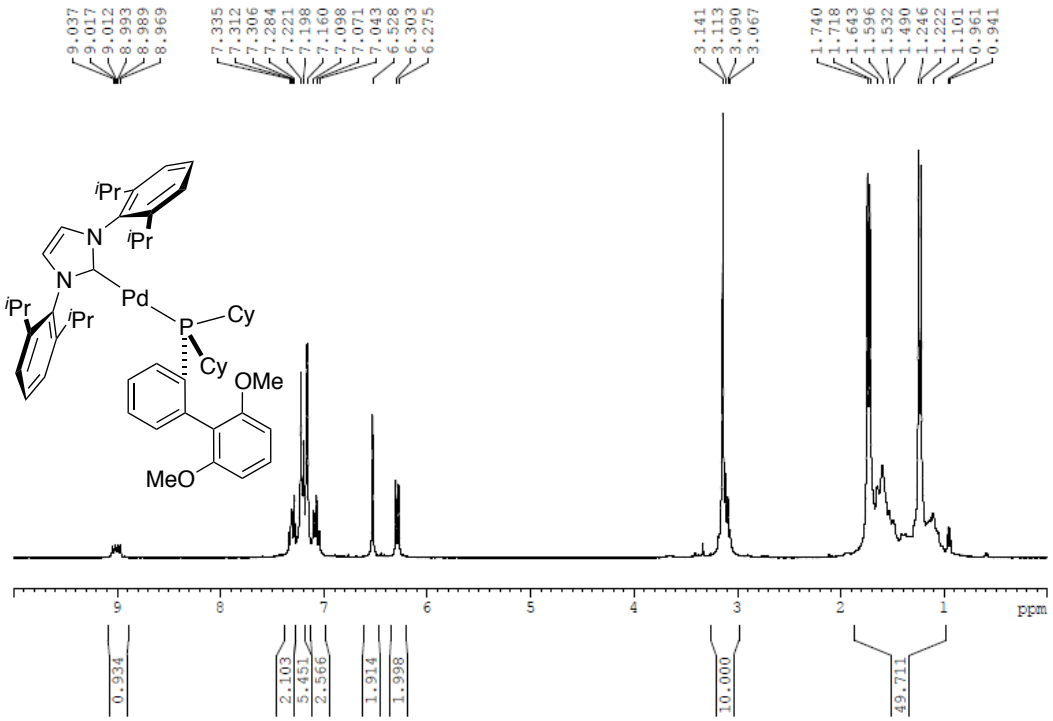
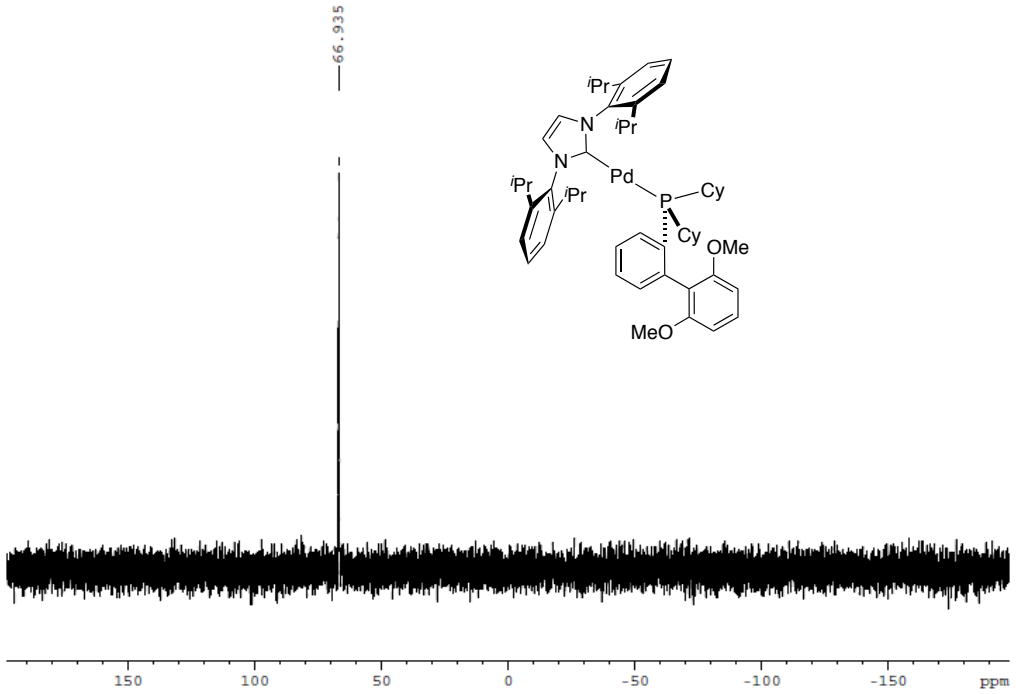
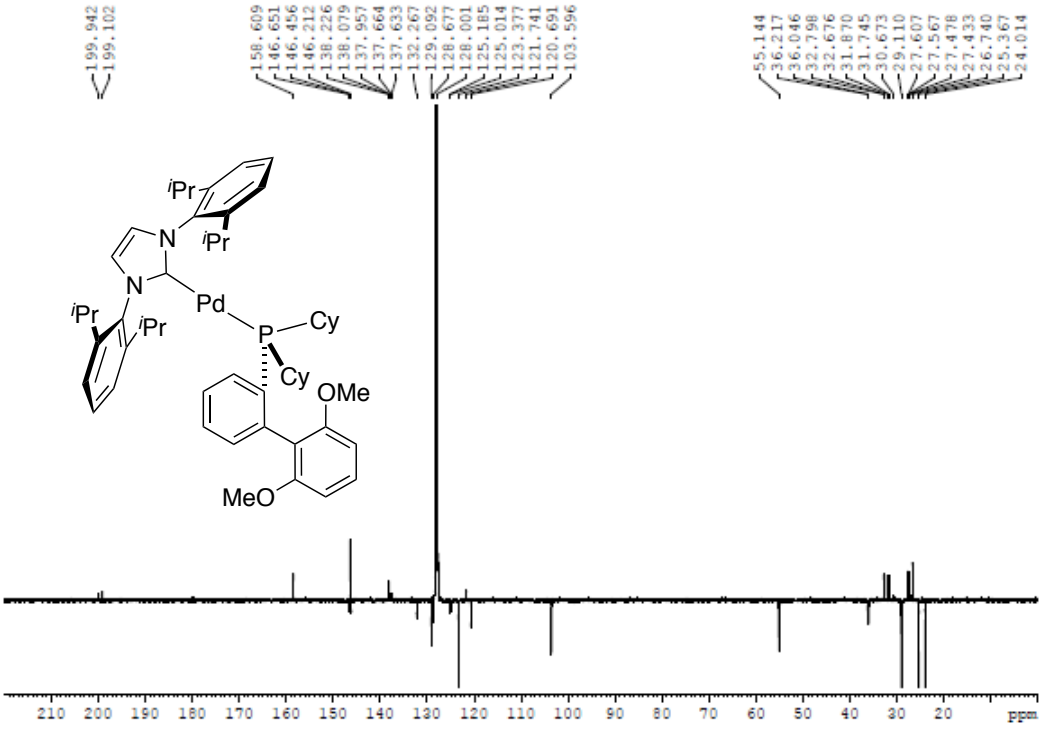
10
ppm

^{1}H, ^{31}P-{^{1}H} and ^{13}C-{^{1}H} NMR spectra of [Pd(IPr)(SPhos] (6)



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31.870
31.745
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29.110
27.607
27.567
27.478
27.433
26.740
25.367
24.014
iPr
iPr
N
N
iPr
iPr
Pd
P
Cy
Cy
OMe
MeO
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

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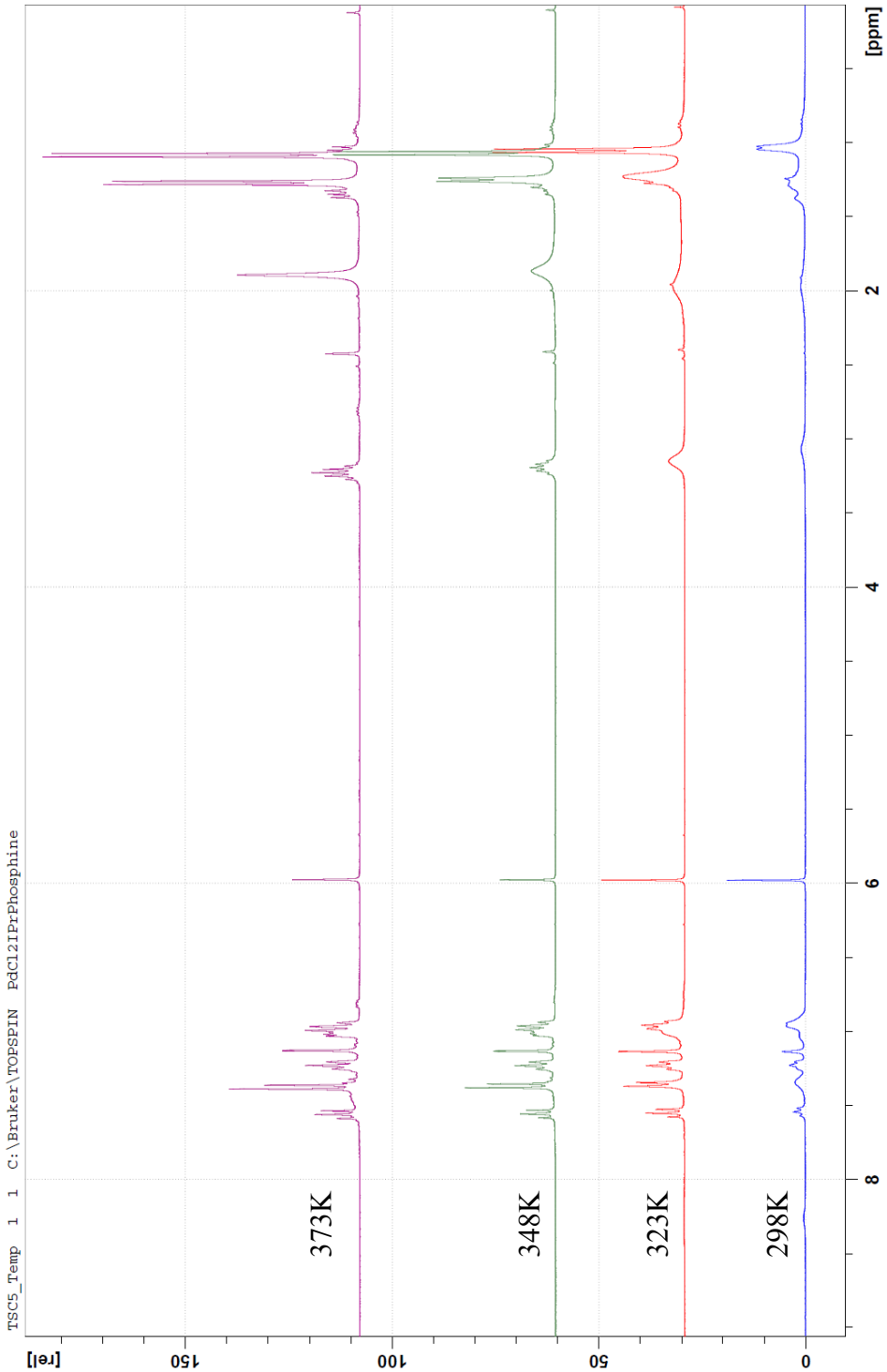
^{1}H NMR spectra of [$PdCl_2$(IPr){P(*o*-tolyl)$_3$}] (2c) at various temperatures (in $C_2D_2Cl_4$)



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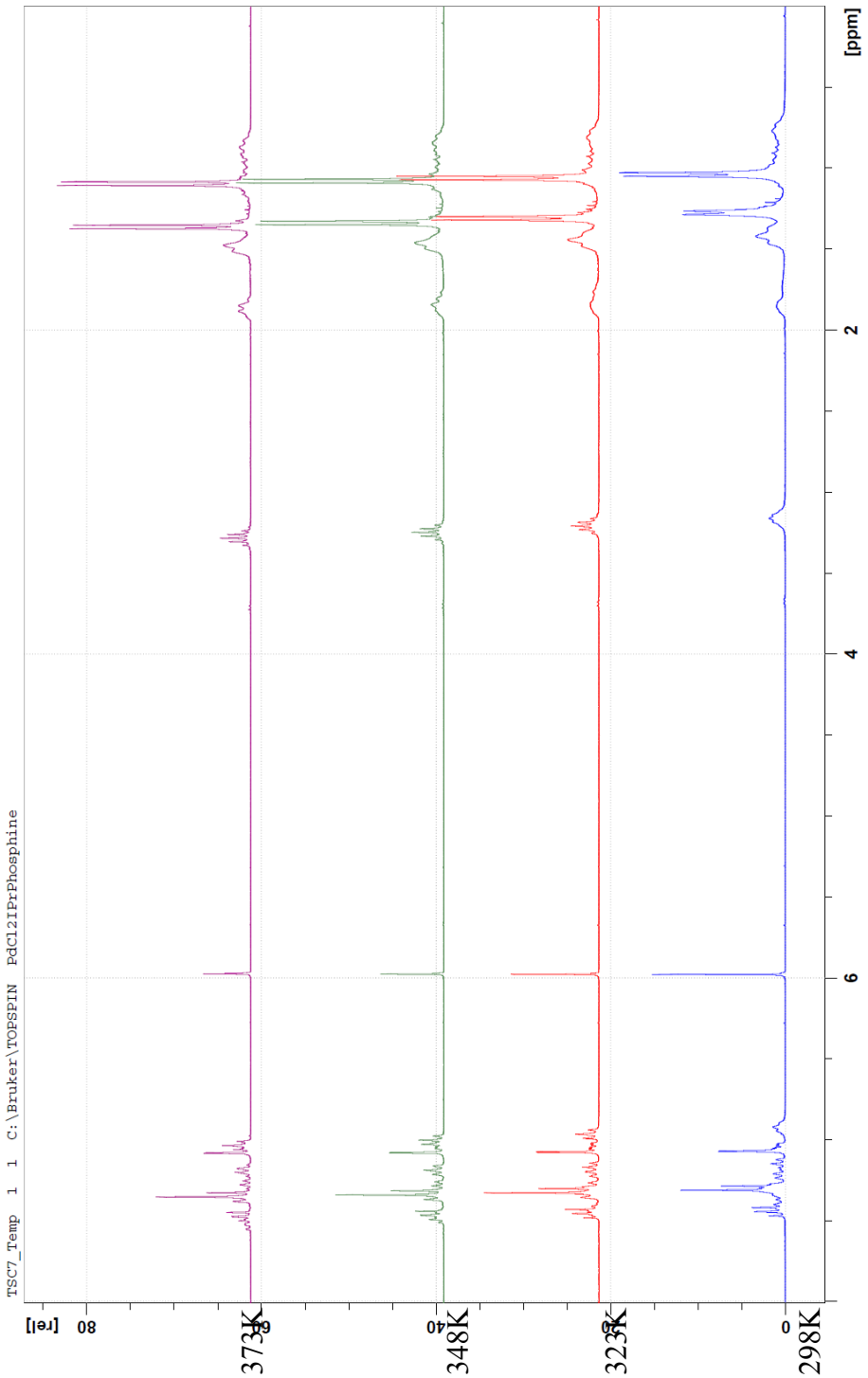
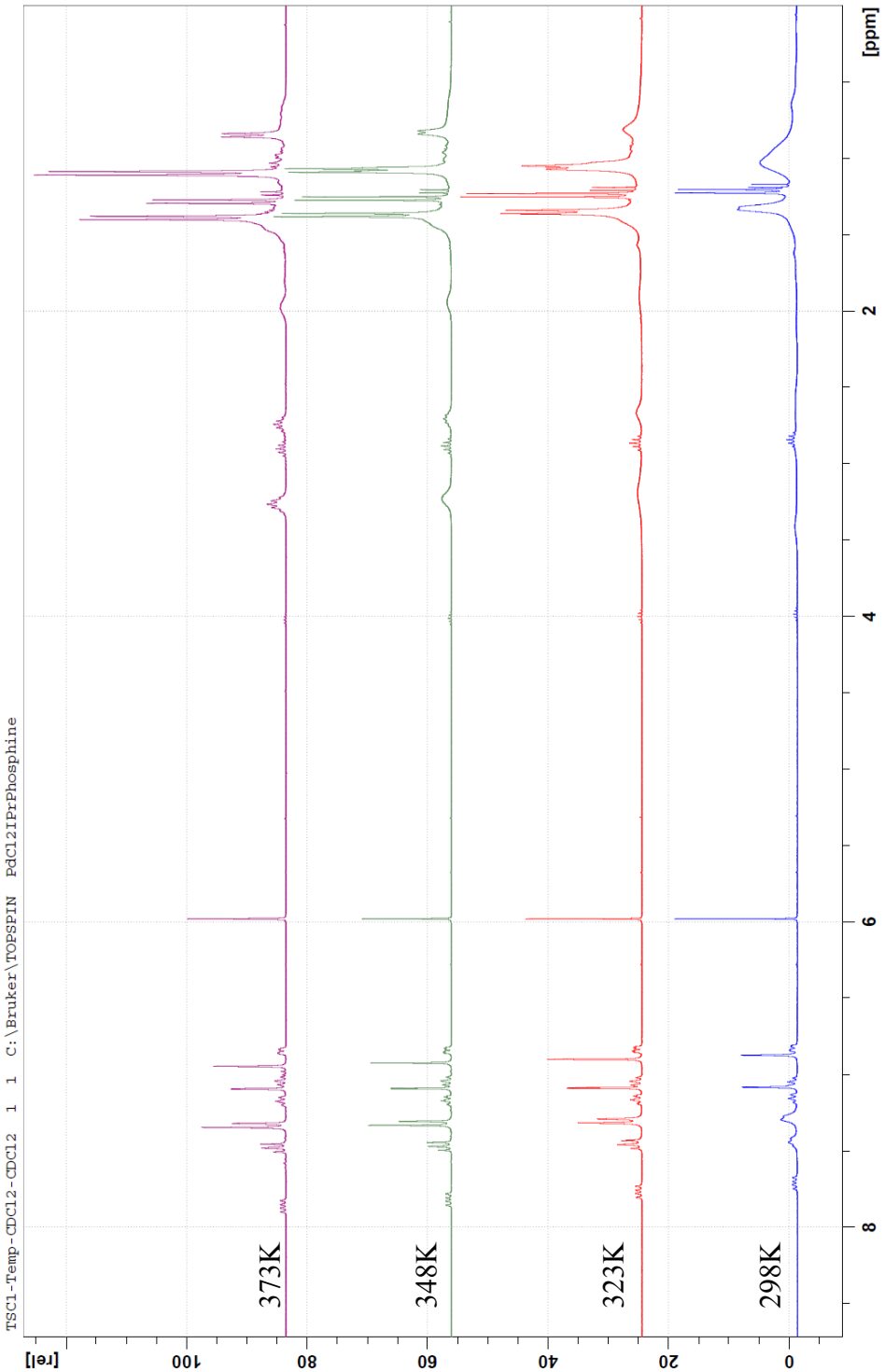
^{1}H NMR spectra of [$PdCl_2$(IPr){PCy_2(*o*-biphenyl)}] (2e) at various temperatures (in $C_2D_2Cl_4$)



^{1}H NMR spectra stacking of [$PdCl_2$(IPr)(XPhos] (2f) at increasing temperatures ($C_2D_2Cl_4$)



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Kinetic profiling for the Suzuki-Miyaura reaction mediated by 2g and 6

In a glovebox, a Radley tube was charged with phenylboronic acid (640 mg, 5.25 mmol), sodium hydroxide (300 mg, 7.25 mmol), Pd catalyst (Pd(II) complex: 4.9 mg, $5 \cdot 10^{-3}$ mmol; Pd(0) complex: 4.5 mg, $5 \cdot 10^{-3}$ mmol), and isopropanol (5 ml). Outside the glovebox, the tube was placed on a Radley carousel under argon atmosphere and 4-chlorotoluene (591.5µL, 5 mmol) was added. A sample was taken every 5 minutes during 1 hour, then every 10 minutes during 30 minutes, finally every 30 minutes during 2 hours and 30 minutes. Evolution of the reaction was followed by gas chromatography and conversion was determined ratio of integrals.

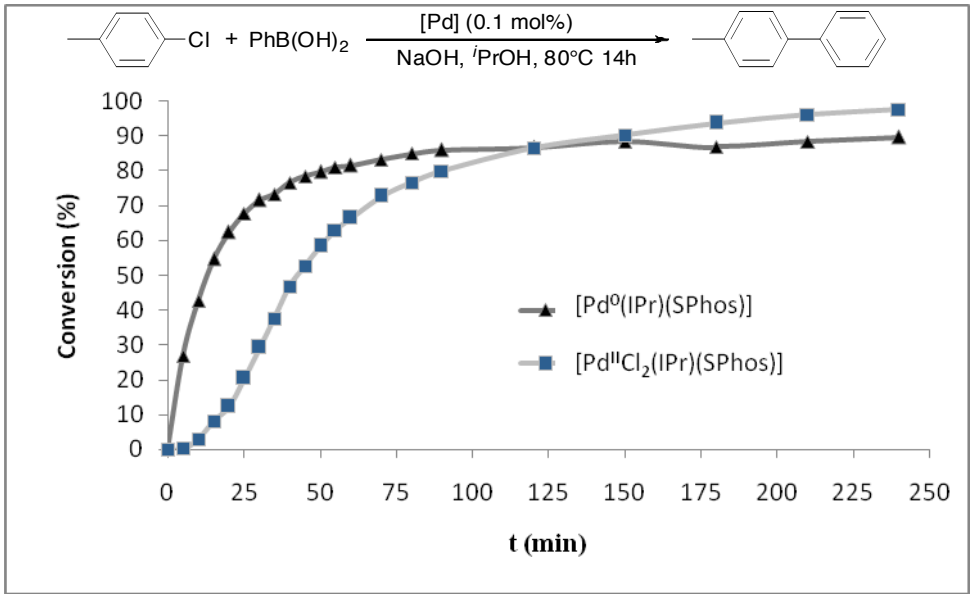

Figure S1. Comparison of [$PdCl_2$(IPr)(SPhos)](**2g**) with [Pd(IPr)(SPhos)] (**6**). Reaction conditions: 4-Me-C_6H_4 (5 mmol), $PhB(OH)_2$ (5.25 mmol), NaOH (7.5 mmol), **2g** or **6** 0.1 mol% Pd, ^{i}PrOH (5 mL), 80°C.

General procedure for the Suzuki-Miyaura reaction

In a glovebox, a 5 mL screwcap-vial fitted with a septum equipped with a magnetic stirring bar was charged with the boronic acid (1.05 mmol), the aryl chloride (if solid, 1.0 mmol) and sodium hydroxide (1.5 mmol). A 0.01 M stock solution of the pre-catalyst was prepared (0.01 mmol in 1 mL THF) and the required volume was injected in the reaction vial. Unless

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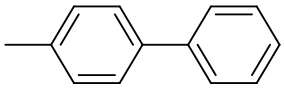
indicated otherwise, the volume injected was of 30 µL, which corresponds to a catalyst loading of 0.03 mol%. Outside the glovebox, the aryl chloride (if liquid, 1 mmol) was introduced in the vial, followed by a degassed solution of H_2O:^{i}PrOH (9:1) (0.5 mL). The mixture was heated up to 100°C and stirred during 14 hours. CH_2Cl_2 (10 mL) and water (10 mL) were then added to the reaction mixture, the phases were separated and the aqueous layer was extracted with CH_2Cl_2 (2 x 10 mL). The organic phases were then combined, dried over $MgSO_4$ and the crude product obtained after removing solvent under reduced pressure. The resulting product was purified by flash chromatography.

Cross-coupling products (Scheme 3 entries)

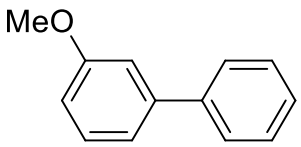
4-Methylbiphenyl[1]



The procedure afforded, after flash chromatography on silica gel (pentane), 154 mg (91%) of the product as a colourless solid.

^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.41 (s, 3H, CH_3, 3H), 7.22-7.26 (m, 1H, Ph), 7.24-7.29 (m, 2H, Ph), 7.41-7.47 (t, $^3J_{H-H}$ = 8.5 Hz, 2H, Ph), 7.48-7.53 (d, $^3J_{H-H}$ = 8.5 Hz, 2H, Ph), 7.57-7.62 (m, 2H, Ph),^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 21.2 (CH_3), 127.1 (Ar-CH), 127.1 (Ar-CH), 128.8 (Ar-CH), 129.6 (Ar-CH), 137.2 (Ar-C), 138.5 (Ar-C), 141.3 (Ar-C).

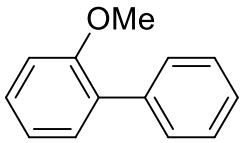
3-Phenylanisole[2]



The procedure afforded, after flash chromatography on silica gel (pentane/EtOAc (95/5)), 181 mg (98%) of the product as a colourless solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.92 (s, 3H, O-CH_3), 6.96-7.02 (m, 1H, Ph), 7.22-7.30 (m, 2H, Ph), 7.40-7.47 (m, 2H, Ph), 7.49-7.55 (m, 2H, Ph), 7.66-7.71 (m, 2H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 55.3 (OCH_3), 112.7 (Ar-CH), 113.0 (Ar-CH), 119.8 (Ar-CH), 127.3 (Ar-CH), 127.5 (Ar-CH), 128.8 (Ar-CH), 129.8 (Ar-CH), 141.2 (Ar-C), 142.8 (Ar-C), 160.0 (Ar-C).

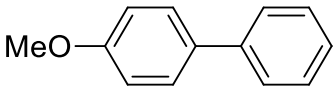
2-Phenylanisole[2]



The procedure afforded, after flash chromatography on silica gel (pentane/EtOAc (95/5)), 175.8 mg (95%) of the product as a colourless oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.88 (s, 3H, O-CH_3), 7.04-7.08 (d, $^{3}J_{H\text{-}H}$ = 7.9 Hz, 1H, Ph), 7.09-7.15 (td, $^{3}J_{H\text{-}H}$ = 7.9 Hz ,$^{4}J_{H\text{-}H}$ = 1.3 Hz, 1H, Ph), 7.38-7.44 (m, 3H, Ph), 7.47-7.53 (m, 2H, Ph), 7.61-7.65 (m, 2H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 55.6 (OCH_3), 111.3 (Ar-CH), 120.9 (Ar-CH), 127.0 (Ar-CH), 128.1 (Ar-CH), 128.7 (Ar-CH), 129.6 (Ar-CH), 130.8 (Ar-C), 131.0 (Ar-CH), 138.6 (Ar-C), 156.5 (Ar-C).

4-Phenylanisole[3]



The procedure afforded, after a flash chromatography on silica gel (pentane/EtOAc: 95/5) 138 mg (76%) of the title compound as a white powder.

^{1}H NMR ($CDCl_3$, 300 MHz) δ 3.89 (s, 3H, O-CH_3), 7.02-7.05 (m, 2H, Ph), 7.33-7.39 (m, 1H, Ph), 7.45-7.50 (m, 2H, Ph), 7.58-7.63 (m, 4H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 75.5 MHz) δ 55.4 (OCH_3), 114.3 (Ar-CH), 126.8 (Ar-CH), 126.8 (Ar-CH), 128.3 (Ar-CH), 128.8 (Ar-CH), 133.9 (Ar-C), 140.9 (Ar-C), 159.3 (Ar-C).

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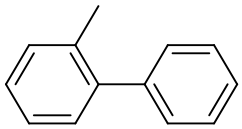
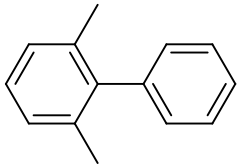
2-Methylbiphenyl[2]



The procedure afforded, after flash chromatography on silica gel (pentane), 155.5mg (92%) of the product as a colourless oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.36 (s, 3H, CH_3), 7.30-7.37 (m, 4H, Ph), 7.38-7.44 (m, 3H, Ph), 7.45-7.52 (m, 2H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 20.6 (CH_3), 125.9 (Ar-CH), 126.9 (Ar-CH), 127.4 (Ar-CH), 128.2 (Ar-CH), 129.3 (Ar-CH), 129.9 (Ar-CH), 130.4 (Ar-CH), 135.4 (Ar-C), 142.1 (Ar-C), 142.2 (Ar-C).

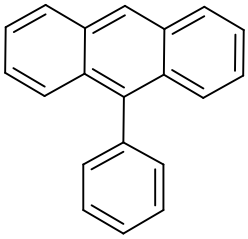
2,6-Dimethylbiphenyl[4]



The procedure afforded, after flash chromatography on silica gel (pentane), 159 mg (87%) of the product as a colourless oil.

^{1}H NMR ($CDCl_3$, 300 MHz) δ 2.11 (s, 6H, CH_3), 7.13-7.28 (m, 5H Ph), 7.36-7.43 (m, 1H, Ph), 7.45-7.52 (m, 2H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 75.5 MHz) δ 21.0 (CH_3), 126.7 (Ar-CH), 127.2 (Ar-CH), 127.4 (Ar-CH), 128.5 (Ar-CH), 129.1 (Ar-CH), 136.2 (Ar-C), 141.2 (Ar-C), 142.0 (Ar-C).

9-Phenylanthracene[5]



The procedure afforded, after a flash chromatography on silicagel (pentane/EtOAc : 95/5) 238 mg (94%) of the title compound as a yellow solid.

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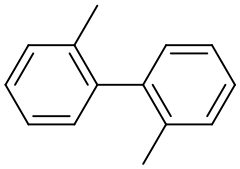
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.36-7.38 (m, 2H, Ar-H), 7.44-7.49 (m, 4H, Ar-H), 7.54-7.62 (m, 3H, Ar-H), 7.69 (d, $^{3}J_{H-H}$ = 8.7 Hz, 2H, Ar-H), 8.06 (d, $^{3}J_{H-H}$ = 8.7 Hz, 2H, Ar-H), 8.51 (s, 1H, C^{10}-H), ^{13}C-{^{1}H} NMR ($CDCl_3$, 100.6 MHz): δ = 125.4 (Ar-CH), 125.6 (Ar-CH), 126.8 (Ar-CH), 127.1 (Ar-CH), 127.8 (Ar-CH), 128.6 (Ar-CH), 130.5 (Ar-C), 131.5 (Ar-CH), 131.7 (Ar-C), 137.3 (Ar-C), 139.1 (Ar-C).

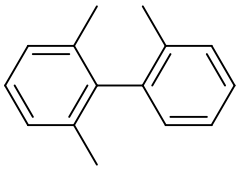
2,2'-Dimethylbiphenyl[6]



The procedure afforded, after flash chromatography on silica gel (pentane), 160.4 mg (88%) of the product as a colourless oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.11 (s, 6H, CH_3), 7.14-7.18 (m, 2H, Ph), 7.24-7.33 (m, 6H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 20.0 (CH_3), 125.7 (Ar-CH), 127.3 (Ar-CH), 129.4 (Ar-CH), 129.9 (Ar-CH), 135.9 (Ar-C), 141.7 (Ar-C).

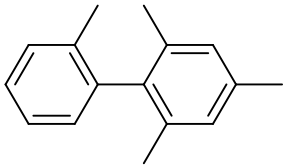
2,2',6-Trimethylbiphenyl[2]



The procedure afforded, after flash chromatography on silica gel (pentane), 152 mg (76%) of the product as a colourless oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.07 (s, 6H, CH_3), 2.09 (s, 3H, CH_3), 7.00-7.15 (m, 1H, Ph), 7.20-7.24 (d, $^{3}J_{H-H}$ = 8 Hz, 2H, Ph), 7.25-7.30 (m, 1H, Ph), 7.31-7.41 (m, 3H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 19.5 (CH_3), 20.5 (CH_3), 126.2 (Ar-CH), 127.1 (Ar-CH), 127.1 (Ar-CH), 127.4 (Ar-CH), 128.9 (Ar-CH), 130.1 (Ar-CH), 135.7 (Ar-C), 135.9 (Ar-C), 140.7 (Ar-C), 141.2. (Ar-C)

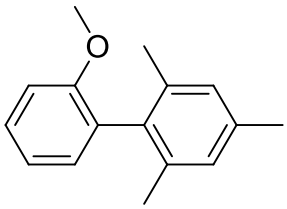
2,2',4,6-Tetramethylbiphenyl[7]



The procedure afforded, after flash chromatography on silica gel (pentane), 157 mg (74%) of the product as a colourless oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.98 (s, 6H, CH_3), 2.04 (s, 3H, CH_3), 2.39 (s, 3H, CH_3), 7.00 (s, 2H, Ph), 7.04-7.13 (d, $^{3}J_{H\text{-}H}$= 0.8 Hz, 1H, Ph), 7.24-7.38 (m, 3H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 19.6 (CH_3), 20.3 (CH_3), 21.2 (CH_3), 126.1 (Ar-CH), 127.0 (Ar-CH), 128.1 (Ar-CH), 129.3 (Ar-CH), 130.0 (Ar-CH), 135.8 (Ar-C), 135.9 (Ar-C), 136.4 (Ar-C), 138.3 (Ar-C), 140.7 (Ar-C).

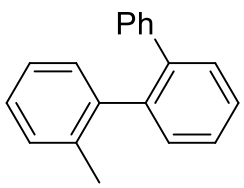
2,4,6-Trimethyl-2'-methoxybiphenyl[8]



The procedure afforded, after flash chromatography on silica gel (pentane/EtOAc (95/5)), 202 mg (89%) of the product as a colourless oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.13 (s, 6H, CH_3), 2.46 (s, 3H, CH_3), 3.85 (s, 3H, O-CH_3), 7.05-7.18 (m, 5H, Ph), 7.41-7.49 (m, 1H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 20.5 (CH_3), 21.3 (CH_3), 55.4 (OCH_3), 110.9 (Ar-CH), 120.7 (Ar-CH), 128.1 (Ar-CH), 128.4 (Ar-CH), 129.6 (Ar-CH), 131.1 (Ar-C), 135.4 (Ar-CH), 136.6 (Ar-C), 136.6 (Ar-C), 156.8 (Ar-C).

2-*o*-Tolylbiphenyl[9]



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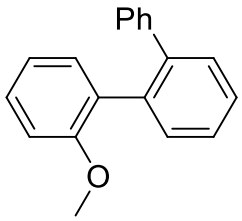
The procedure afforded, after flash chromatography on silica gel (pentane), 230 mg (94%) of the product as a colourless solid.

^{1}H NMR (CDCl3, 400 MHz) δ 2.01 (s, 3H, CH_3), 7.12-7.28 (m, 9H, Ph), 7.37-7.41 (d, $^{3}J_{H-H}$ = 7.1 Hz, 1H, Ph), 7.44-7.58 (m, 3H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 20.2 (CH_3), 125.4 (Ar-CH), 126.5 (Ar-CH), 127.1 (Ar-CH), 127.2 (Ar-CH), 127.6 (Ar-CH), 127.8 (Ar-CH), 129.5 (Ar-CH), 129.8 (Ar-CH), 130.1 (Ar-CH), 130.7 (Ar-CH), 130.8 (Ar-CH), 135.9 (Ar-CH), 140.4 (Ar-C), 141.1 (Ar-C), 141.4 (Ar-C), 141.5 (Ar-C).

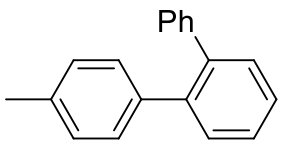
2-Phenyl, 2'-methoxybiphenyl[10]



The procedure afforded, after flash chromatography on silica gel (pentane/EtOAc (95/5)), 247 mg (95%) of the product as a colourless solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.39 (s, 3H, O-CH_3), 6.71-6.77 (d, $^{3}J_{H-H}$=8.5 Hz, 1H, Ph), 6.93-6.99 (t, $^{3}J_{H-H}$=7.5 Hz, 1H, Ph), 7.15-7.30 (m, 7H, Ph), 7.41-7.52 (m, 4H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 55.0 (OCH_3), 110.8 (Ar-CH), 120.5 (Ar-CH), 126.3 (Ar-CH), 127.3 (Ar-CH), 127.5 (Ar-CH), 127.7 (Ar-CH), 128.6 (Ar-CH), 129.1 (Ar-CH), 129.8 (Ar-CH), 130.8 (Ar-C), 131.0 (Ar-CH), 131.7 (Ar-CH), 137.4 (Ar-C), 141.8 (Ar-C), 142.3 (Ar-C), 156.4 (Ar-C).

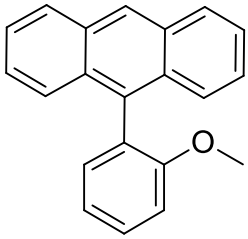
2-Phenyl, 4'-methylbiphenyl[11]



The procedure afforded, after flash chromatography on silica gel (pentane), 218 mg (89%) of the product as a colourless solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 2.35 (s, 3H, CH_3), 7.04-7.11 (m, 4H, Ph), 7.18-7.29 (m, 5H, Ph), 7.41-7.50 (m, 4H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 21.2 (CH_3), 126.3 (Ar-CH), 127.4 (Ar-CH), 127.6 (Ar-CH), 128.0 (Ar-CH), 128.7 (Ar-CH), 129.9 (Ar-CH), 130.0 (Ar-CH), 130.7 (Ar-CH), 136.2 (Ar-C), 138.7 (Ar-C), 140.6 (Ar-C), 141.8 (Ar-C).

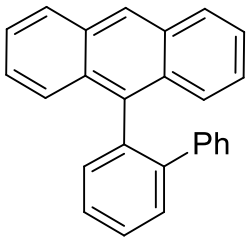
9-(2-Methoxyphenyl)-anthracene[8]



The procedure afforded, after flash chromatography on silica gel (pentane/EtOAc (95/5)), 196 mg (69%) of the product as a yellow solid.

1H NMR ($CDCl_3$, 400 MHz) δ 3.62 (s, 3H, O-CH_3), 7.14-7.21 (m, 2H, Ar), 7.24-7.30 (m, 1H, Ar), 7.30-7.38 (m, 2H, Ar), 7.41-7.49 (t, $^{3}J_{H\text{-}H}$ = 8 Hz, 2H, Ar), 7.55 (t, $^{3}J_{H\text{-}H}$ = 8 Hz, 1H, Ar), 7.64 (d, $^{3}J_{H\text{-}H}$ = 8 Hz, 2H, Ar), 8.05 (d, $^{3}J_{H\text{-}H}$ = 8 Hz, 2H, Ar), 8.50 (s, 1H, Ar), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 55.7 (OCH_3), 111.4 (Ar-CH), 120.8 (Ar-CH), 125.1 (Ar-CH), 125.3 (Ar-CH), 126.7 (Ar-CH), 126.9 (Ar-CH), 127.4 (Ar-C), 128.5 (Ar-CH), 129.4 (Ar-CH), 130.5 (Ar-C), 131.6 (Ar-C), 133.0 (Ar-CH), 133.9 (Ar-C), 158.1 (Ar-C).

9-(*o*-Biphenyl)anthracene[12]



The procedure, using 0.06 mol% of catalyst, after flash chromatography on silica gel (pentane/EtOAc (95/5)), afforded 193 mg (58%) of the product as a yellow solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 6.80-6.88 (m, 3H, Ar), 6.95-7.00 (m, 2H, Ar), 7.29-7.35 (m, 2H, Ar), 7.36-7.44 (m, 3H, Ar), 7.51-7.58 (m, 1H, Ar), 7.60-7.69 (m, 4H, Ar), 7.95 (d, $^{3}J_{H\text{-}H}$ =

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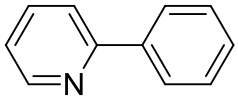
8.8 Hz, 2H, Ar), 8.38 (s, 1H, Ar), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 125.0 (Ar-CH), 125.4 (Ar-CH), 126.5 (Ar-CH), 126.6 (Ar-CH), 127.0 (Ar-CH), 127.3 (Ar-CH), 127.5 (Ar-CH), 128.3 (Ar-CH), 128.5 (Ar-CH), 128.5 (Ar-CH), 130.4 (Ar-CH), 130.5 (Ar-C), 131.2 (Ar-C), 132.5 (Ar-CH), 136.3 (Ar-C), 137.1 (Ar-C), 141.3 (Ar-C), 143.3 (Ar-C).

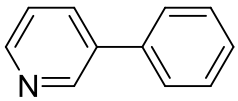
2-Phenylpyridine[13]



The procedure afforded, after flash chromatography on silica gel (CH_2Cl_2), 75 mg (48%) of the product as colourless oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.20-7.27 (m, 1H, Ar), 7.40-7.54 (m, 3H, Ar), 7.72-7.79 (m, 2H, Ar), 7.98-8.06 (m, 2H, Ar), 8.69-8.76 (dt, $^{3}J_{H\text{-}H}$ = 6 Hz, $^{4}J_{H\text{-}H}$ = 2.0 Hz, 1H, Ar), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 120.7 (Ar-CH), 122.2 (Ar-CH), 127.0 (Ar-CH), 128.9 (Ar-CH), 129.0 (Ar-CH), 136.9 (Ar-CH), 139.5 (Ar-C), 149.8 (Ar-CH), 157.6 (Ar-C).

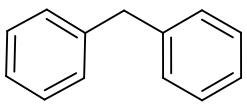
3-Phenylpyridine[14]



The procedure afforded, after flash chromatography on silica gel (pentane/EtOAc (85/15)), 152mg (98%) of the product as colourless oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.36-7.43 (m, 2H, Ar), 7.47-7.51 (m, 2H, Ar), 7.58-7.60 (m, 2H, Ar), 7.87-7.90 (m, 1H, Ar), 8.61 (d, $J_{H\text{-}H}$ = 3.7 Hz, 1H, Ar), 8.87 (d, $J_{H\text{-}H}$ = 1.5 Hz, 1H, Ar), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 123.7 (Ar-CH), 127.3 (Ar-CH), 128.3 (Ar-CH), 129.2 (Ar-CH), 134.6 (Ar-CH), 136.9 (Ar-CH), 137.9 (Ar-C), 148.3 (Ar-C), 148.4 (Ar-CH).

Diphenylmethane[15]



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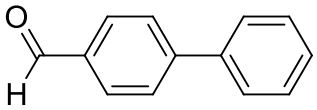
The procedure afforded, after flash chromatography on silica gel (pentane), 90 mg (53%) of the product as colourless oil.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 3.94 (s, Ph-CH_2-Ph, 2H), 7.12-7.18 (m, 6H, Ph), 7.21-7.27 (m, 4H, Ph), ^{13}C-{^{1}H} NMR ($CDCl_3$, 100.6 MHz) δ 42.0 (CH_2), 126.2 (Ar-CH), 128.6 (Ar-CH), 129.0 (Ar-CH), 141.2 (Ar-C).

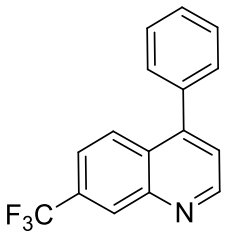
4-Formyl-1,1'-biphenyl[16]



The procedure, using 0.06 mol% of catalyst, after flash chromatography on silica gel (pentane/EtOAc (95/5)), afforded 153 mg (84%) of the product as a crystalline solid.

^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.39-7.51 (m, 3H, Ph), 7.61-7.66 (m, 2H, Ph), 7.72-7.76 (dt, $^{3}J_{H\text{-}H}$ = 8.3 Hz, $J_{H\text{-}H}$=1.3 Hz, 2H, Ph), 7.92-7.97 (dt, $^{3}J_{H\text{-}H}$ = 8.3 Hz, $^{4}J_{H\text{-}H}$ = 1.8 Hz, 2H, Ph), 10.05 (s, 1H, H-C=O), ^{13}C-{^{1}H} NMR ($CDCl_3$ 100.6 MHz) δ 127.4 (Ar-CH), 127.7 (Ar-CH), 128.5 (Ar-CH), 129.1 (Ar-CH), 130.3 (Ar-CH), 135.2 (Ar-C), 139.7 (Ar-C), 147.2 (Ar-C), 191.9 (C=O).

4-Phenyl-7-(trifluoromethyl)quinoline



The procedure, using 0.06 mol% of catalyst, after a flash chromatography on silica gel (pentane/EtOAc: 1/0 to 95/5) afforded 200 mg (73%) of the title compound as a white solid.

^{1}H NMR ($CDCl_3$, 300 MHz): δ 7.42-7.58 (m, 6H, Ar), 7.64-7.67 (m, 1H, Ar), 8.05 (d, $^{3}J_{H\text{-}H}$ = 8.8 Hz, 1H, Ar), 8.49 (s, 1H, Ar), 9.02 (d, $^{3}J_{H\text{-}H}$ = 4.3 Hz, 1H, Ar), ^{13}C NMR ($CDCl_3$, 75.5 MHz): δ 122.2 (q, $^{4}J_{C\text{-}F}$ = 3.1 Hz, Ar-CH), 123.0 (s, Ar-CH), 125.8 (s, Ar-C), 127.4 (s, Ar-

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CH), 127.8 (q, $^{3}J_{C\text{-}F}$ = 4.1 Hz, Ar-CH), 128.4 (s, Ar-C), 128.9 (s, Ar-CH), 128.9 (s, Ar-CH), 129.5 (s, Ar-CH), 131.2 (q, $^{1}J_{C\text{-}F}$ = 32.8 Hz, Ar-C-*C*F_3), 137.2 (s, Ar-C), 147.8 (s, Ar-C), 148.6 (s, Ar-C), 151.4 (s, Ar-CH). HRMS (CI) calcd. $C_{16}H_{10}F_3N$: $(M + H)^+$, 274.0844; found: $(M + H)^+$, 274.0835.

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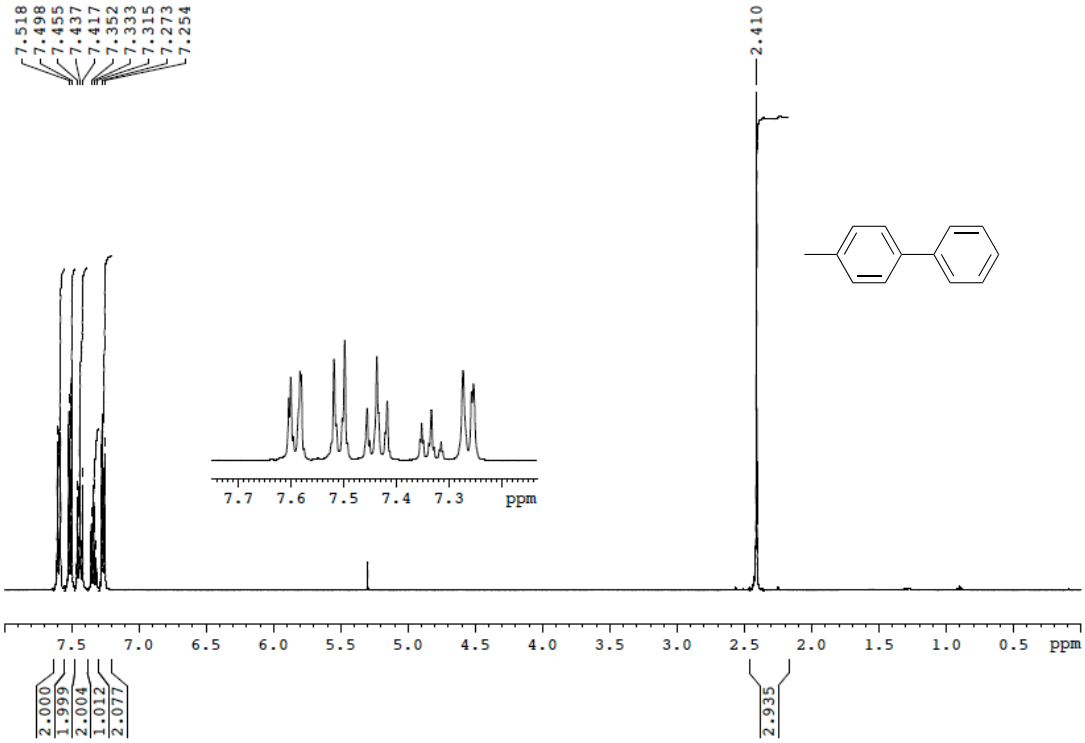
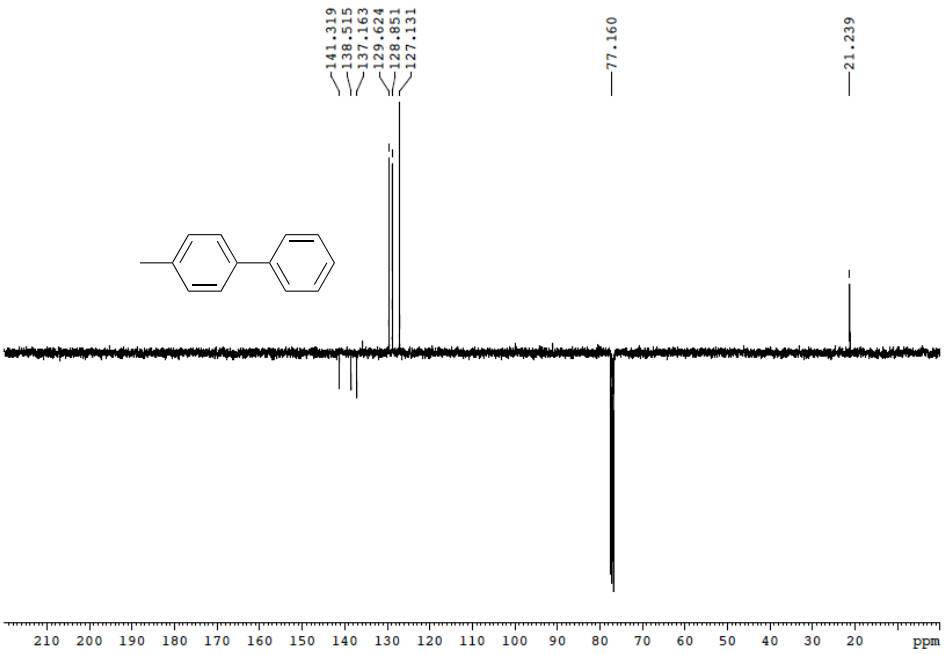
NMR spectra of products

^{1}H and ^{13}C-{^{1}H} NMR spectra of 4-methylbiphenyl





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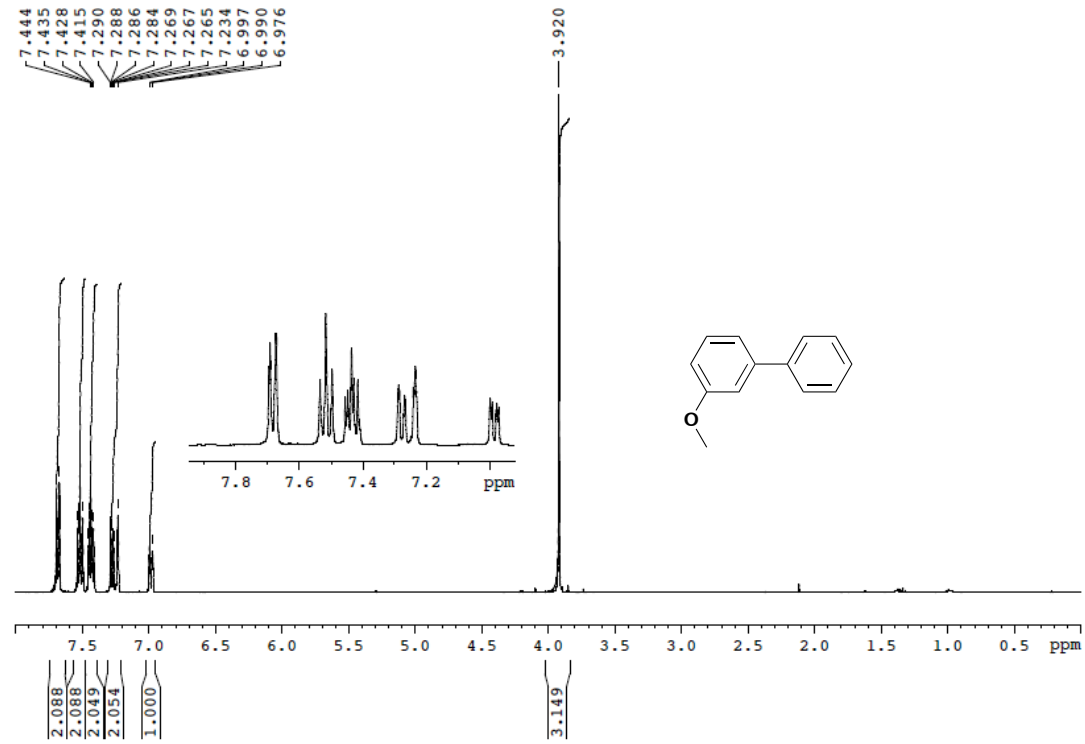
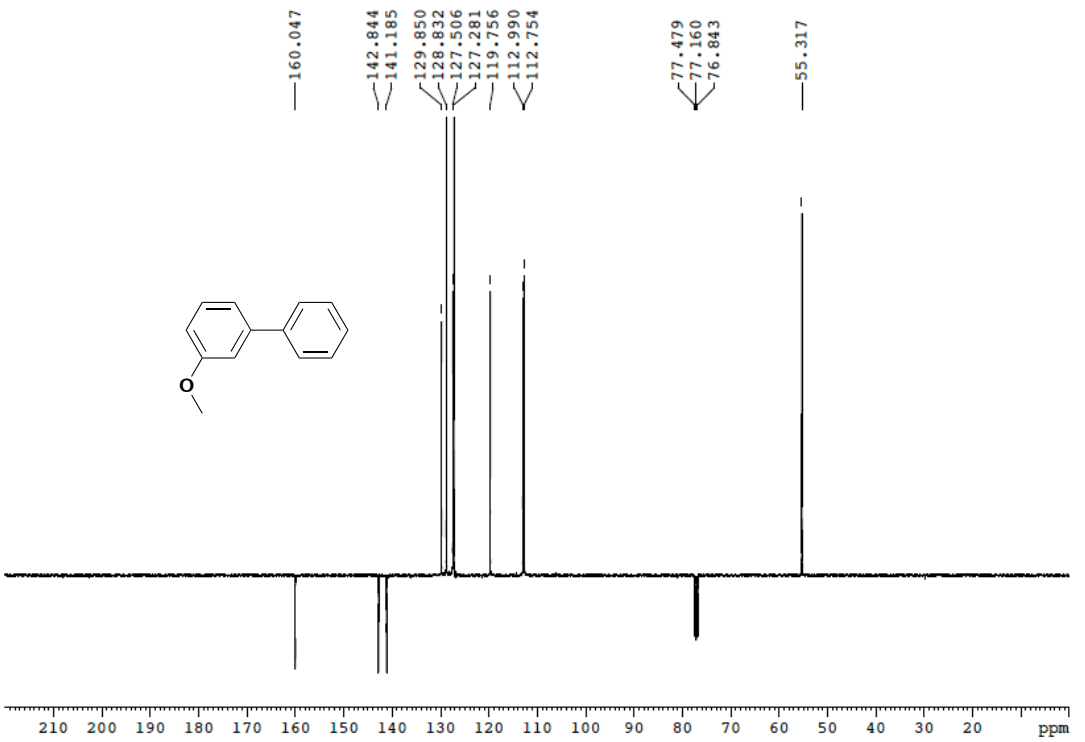
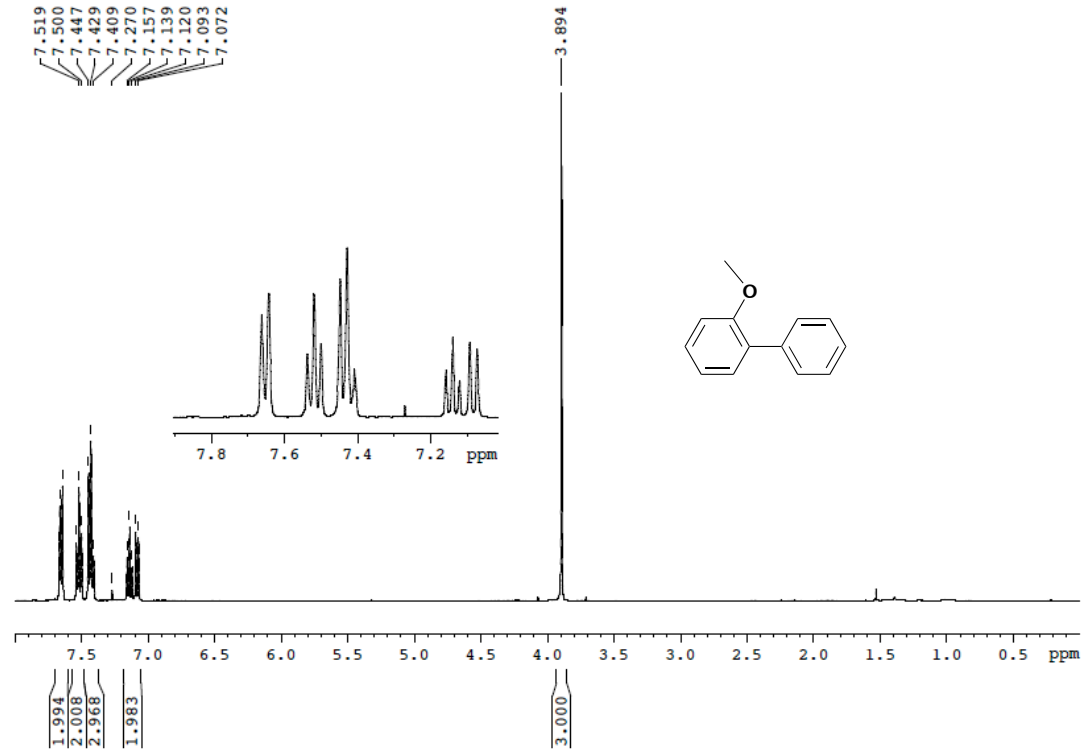
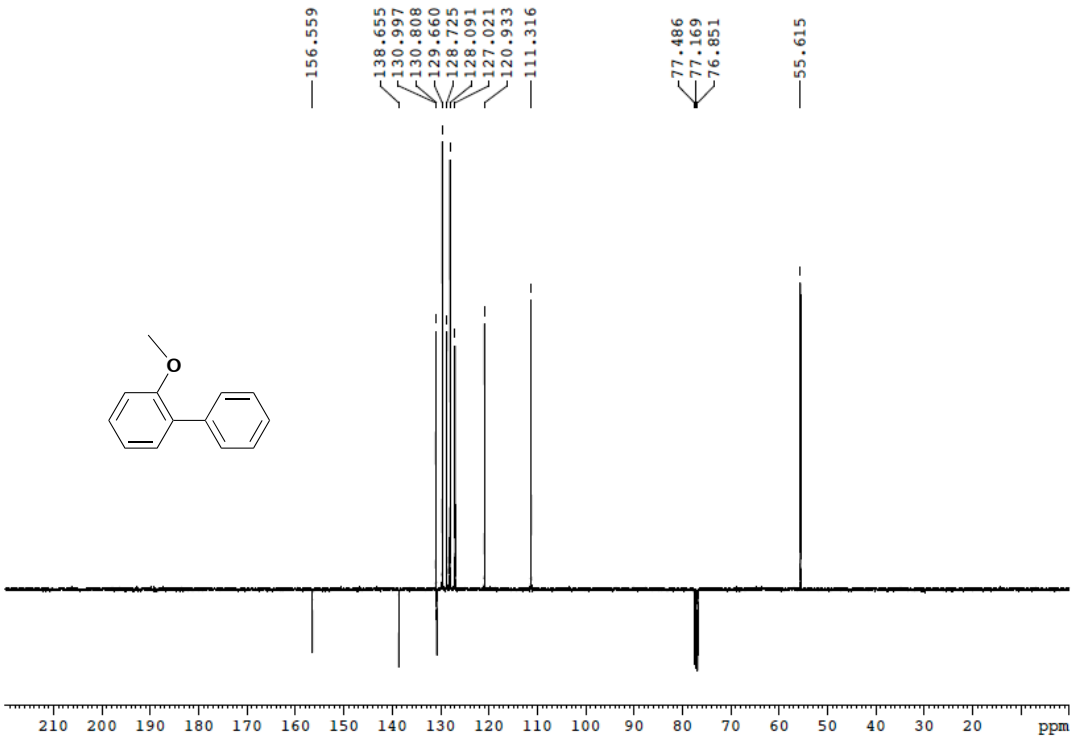
^{1}H and ^{13}C-{^{1}H} NMR spectra of 3-phenylanisole





^{1}H and ^{13}C-{^{1}H} NMR spectra of 2-phenylanisole:





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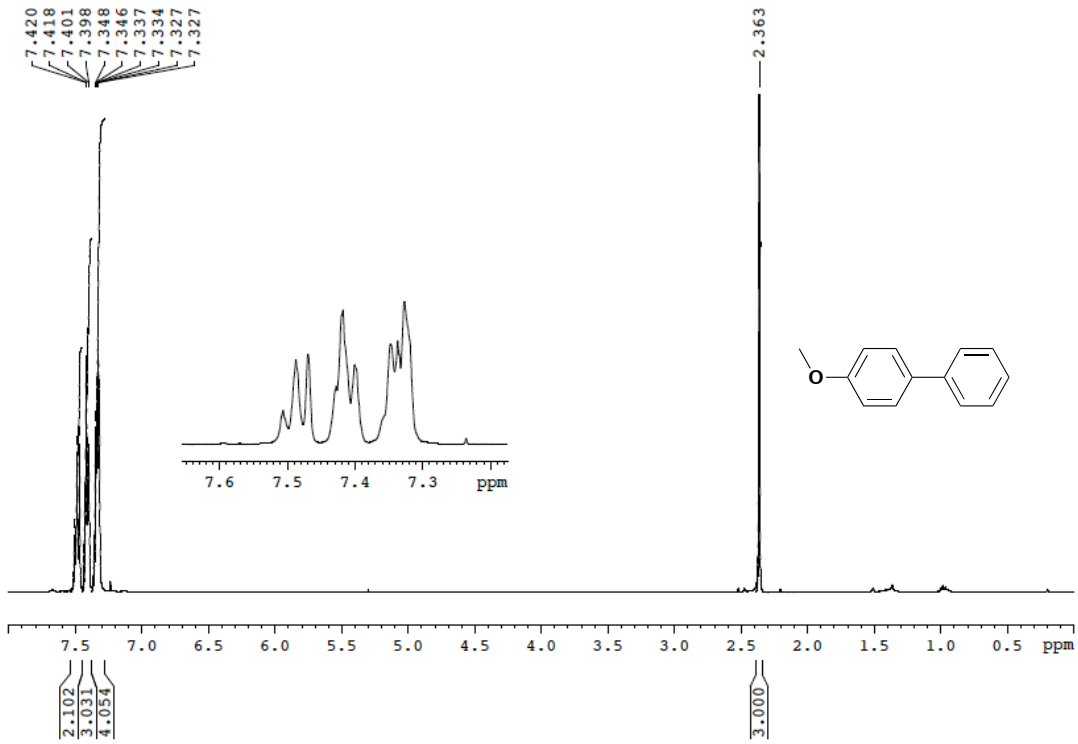
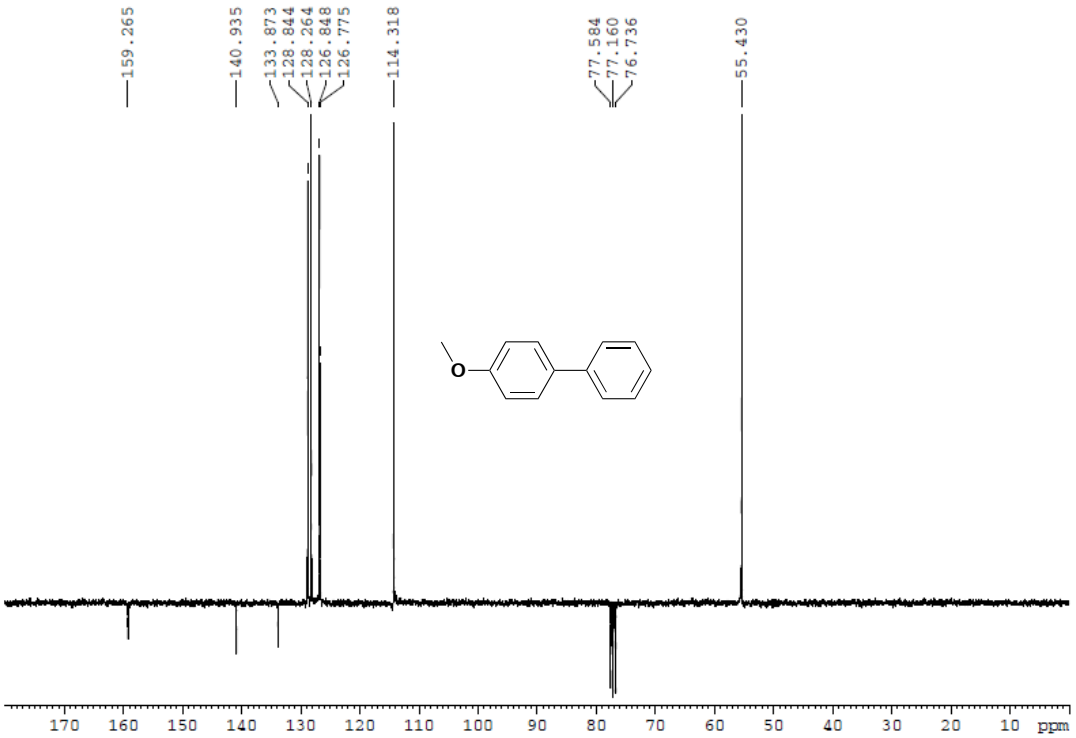
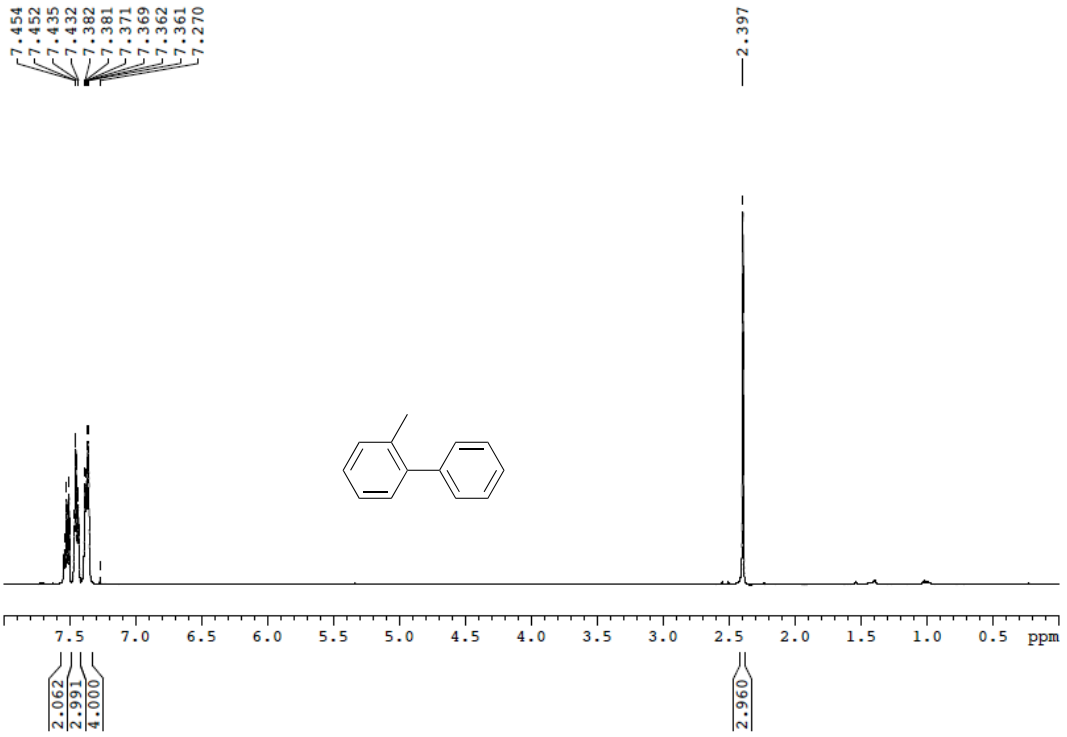
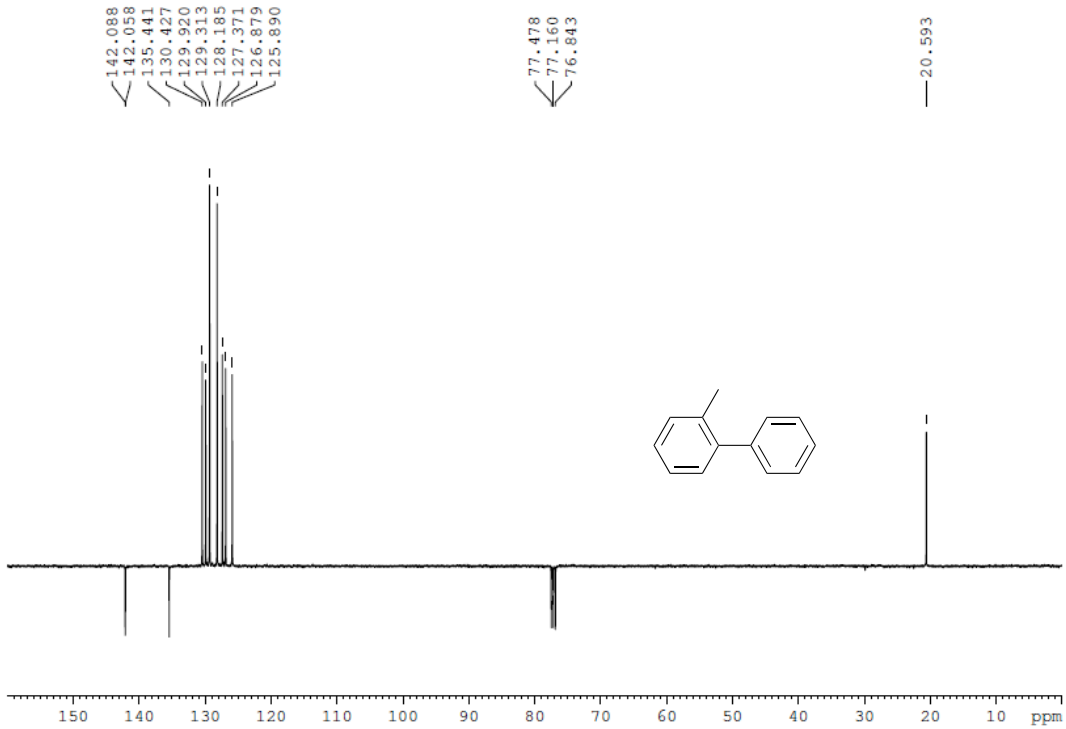
^{1}H and ^{13}C-{^{1}H} NMR spectra of 4-phenylanisole



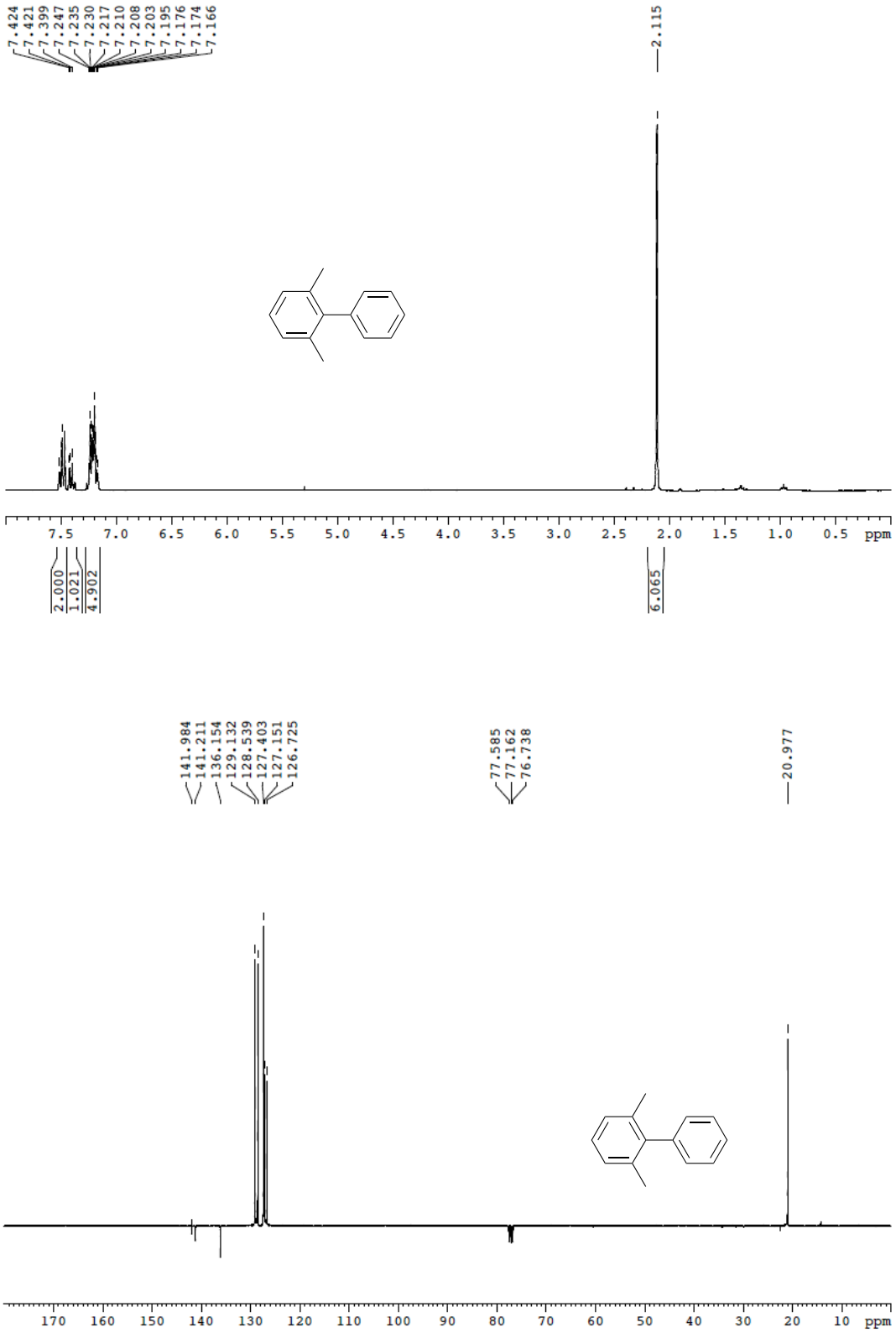


^{1}H and ^{13}C-{^{1}H} NMR spectra of 2-methylbiphenyl





^{1}H and ^{13}C-{^{1}H} NMR spectra of 2,6-dimethylbiphenyl



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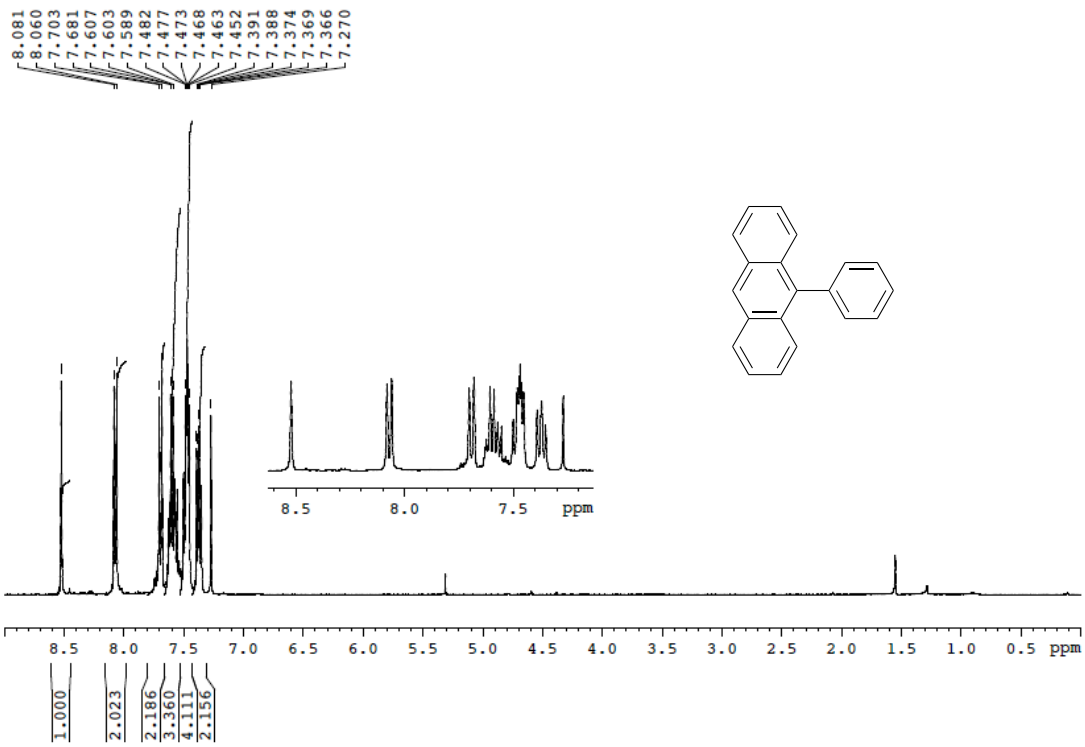
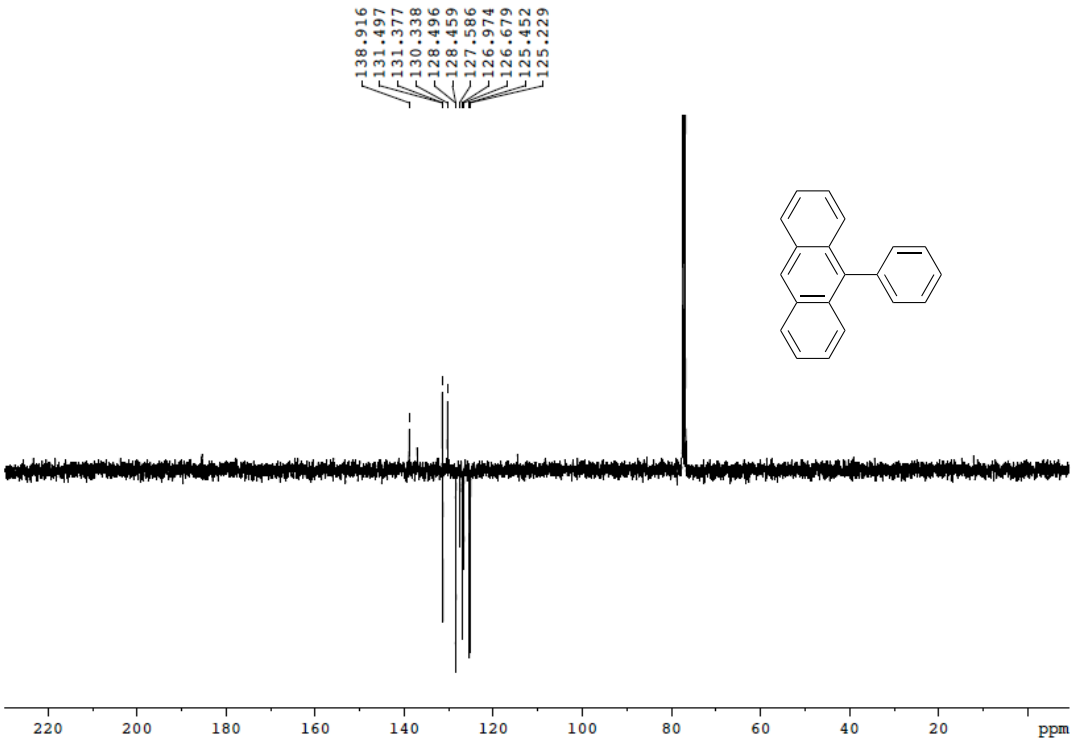
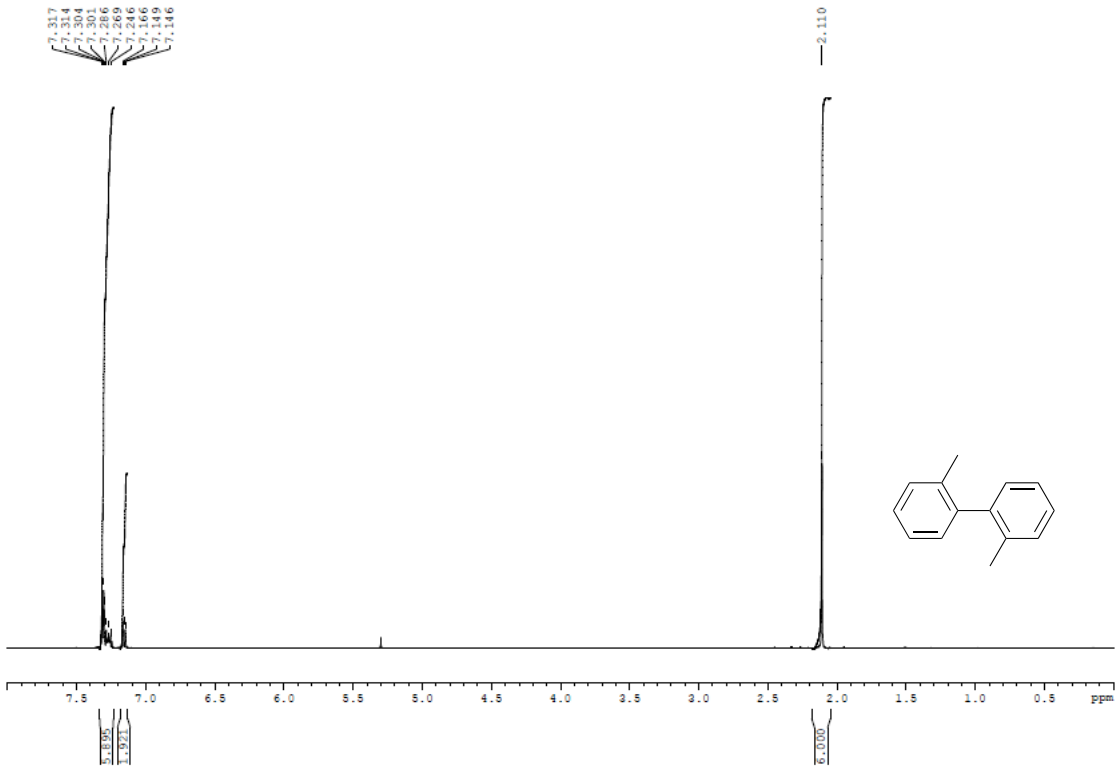
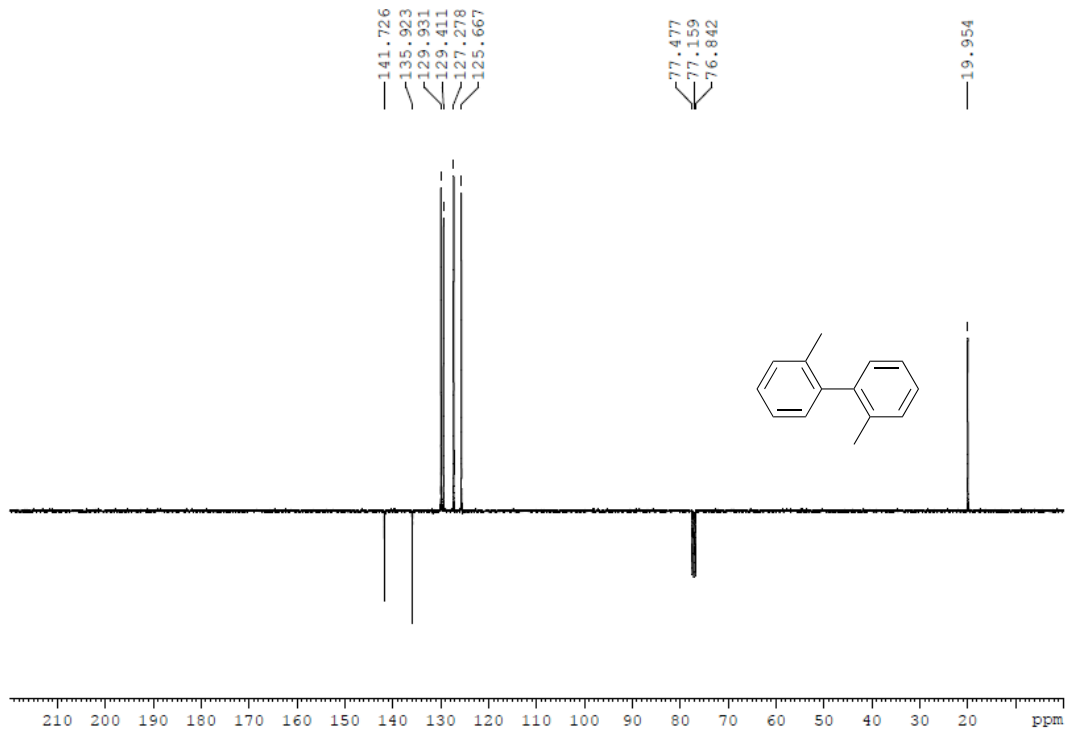
^{1}H and ^{13}C-{^{1}H} NMR spectra of 9-phenylanthracene





^{1}H and ^{13}C-{^{1}H} NMR spectra of 2,2'-dimethylbiphenyl





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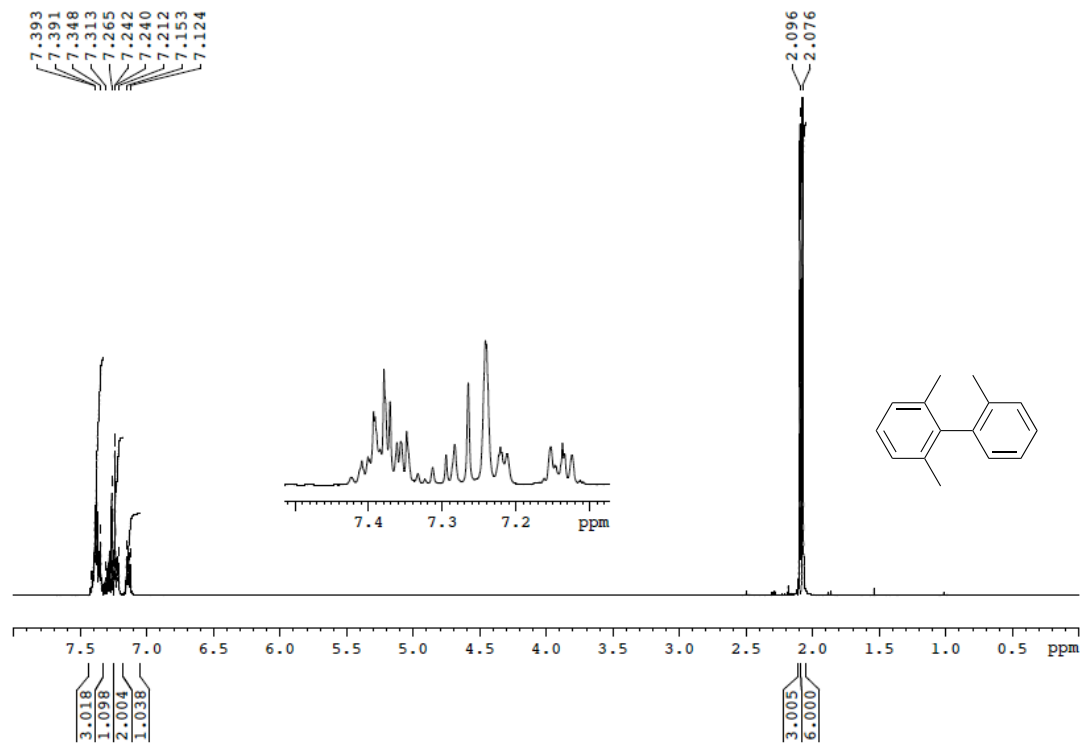
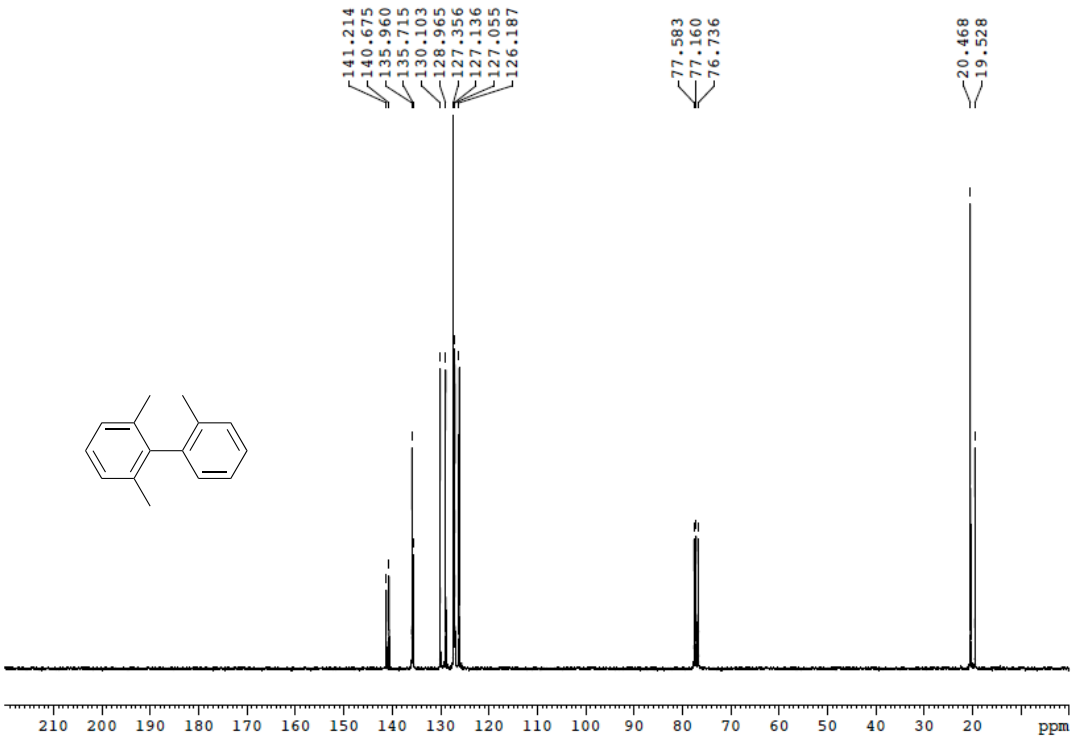
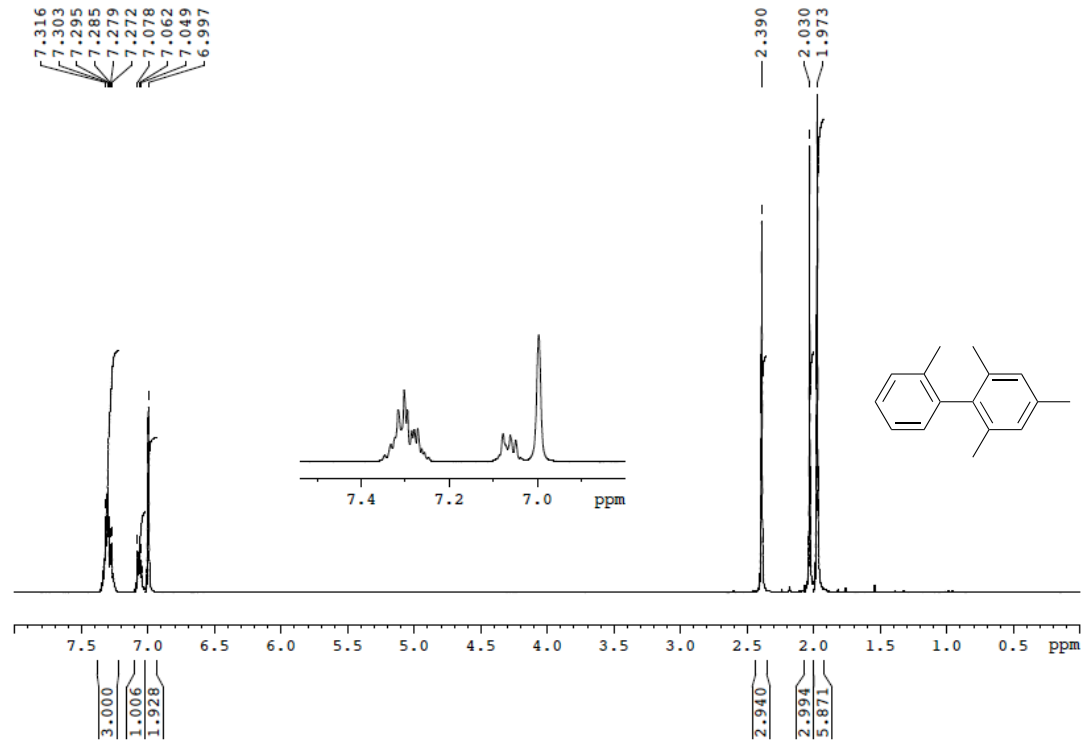
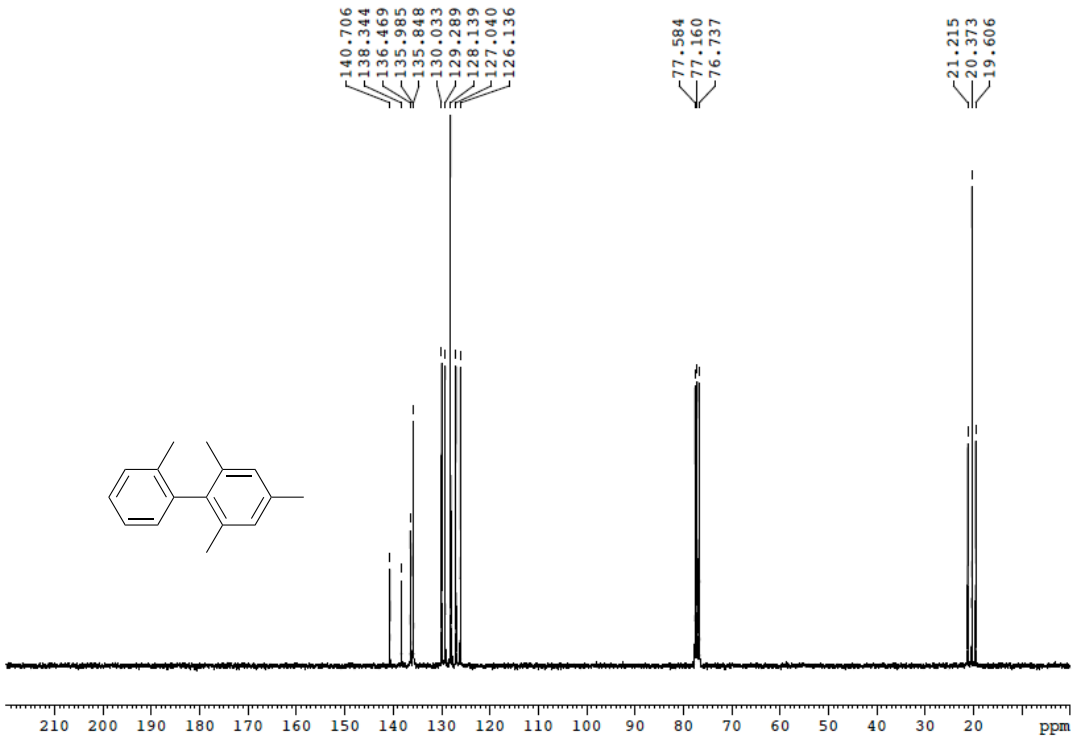
^{1}H and ^{13}C-{^{1}H} NMR Spectra of 2,2',6-trimethylbiphenyl





^{1}H and ^{13}C-{^{1}H} NMR spectra of 2,2',4,6-tetramethylbiphenyl:





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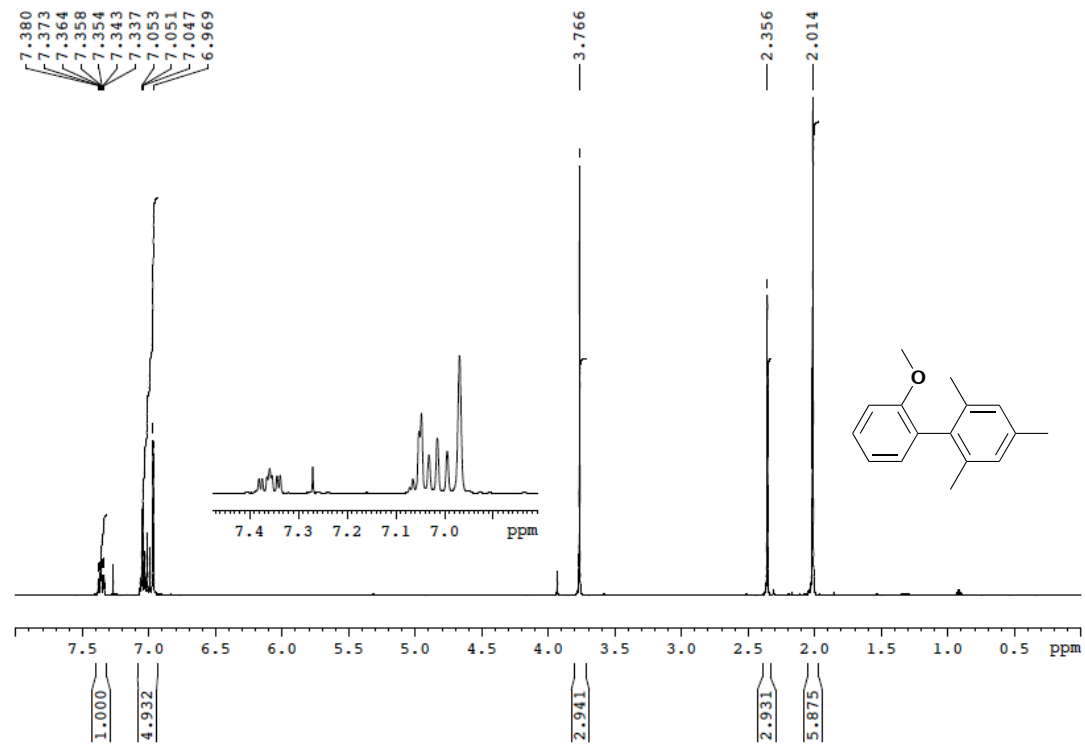
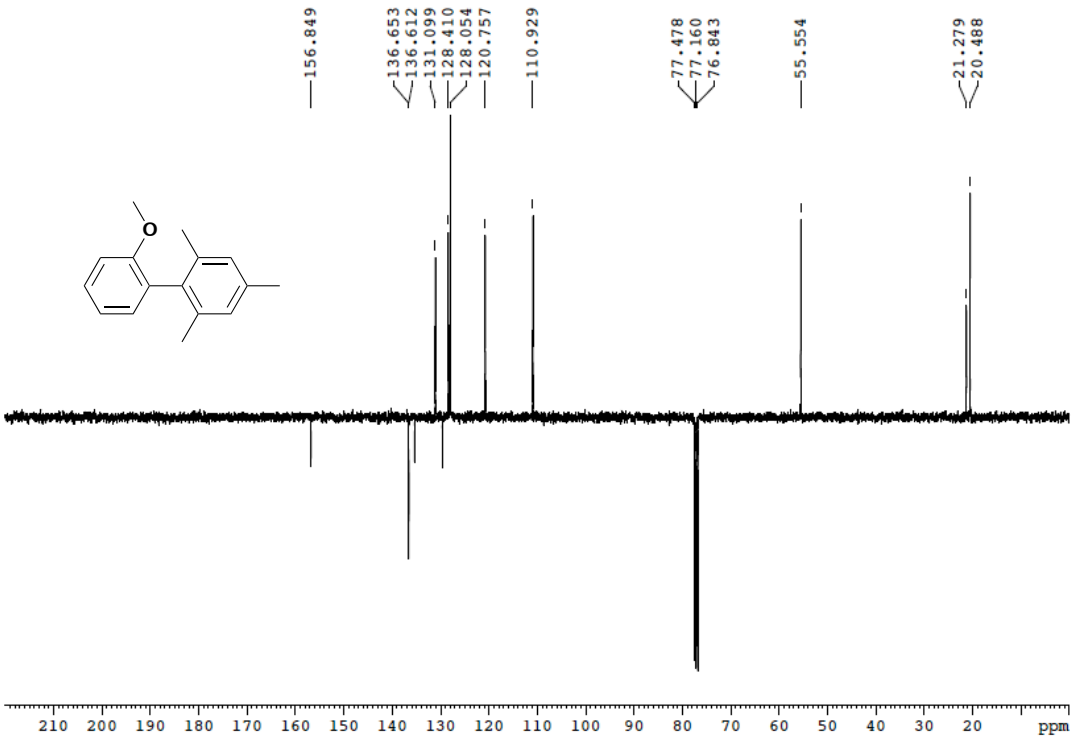
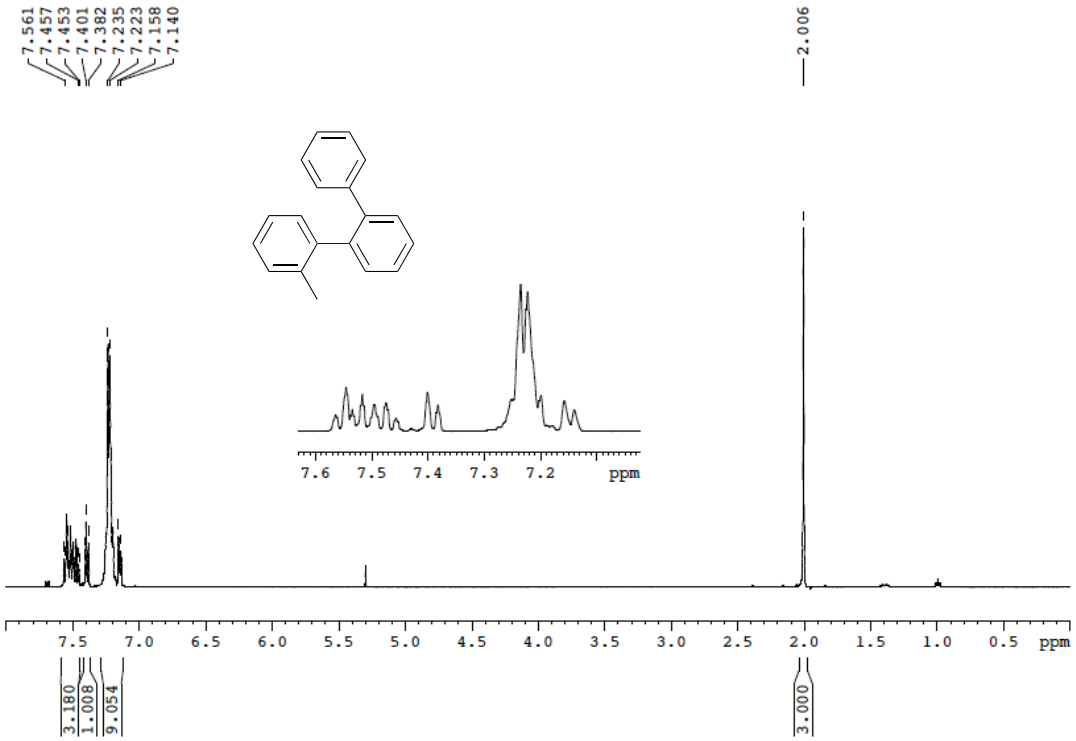
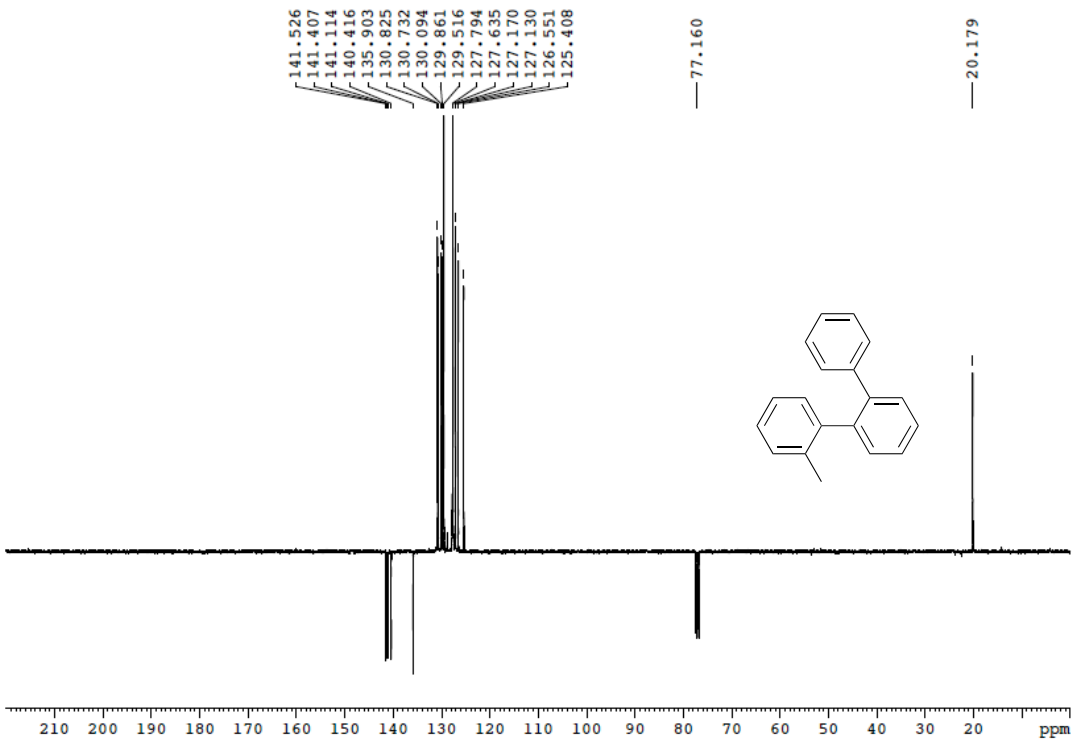
^{1}H and ^{13}C-{^{1}H} NMR spectra of 2,4,6-trimethyl-2'-methoxybiphenyl



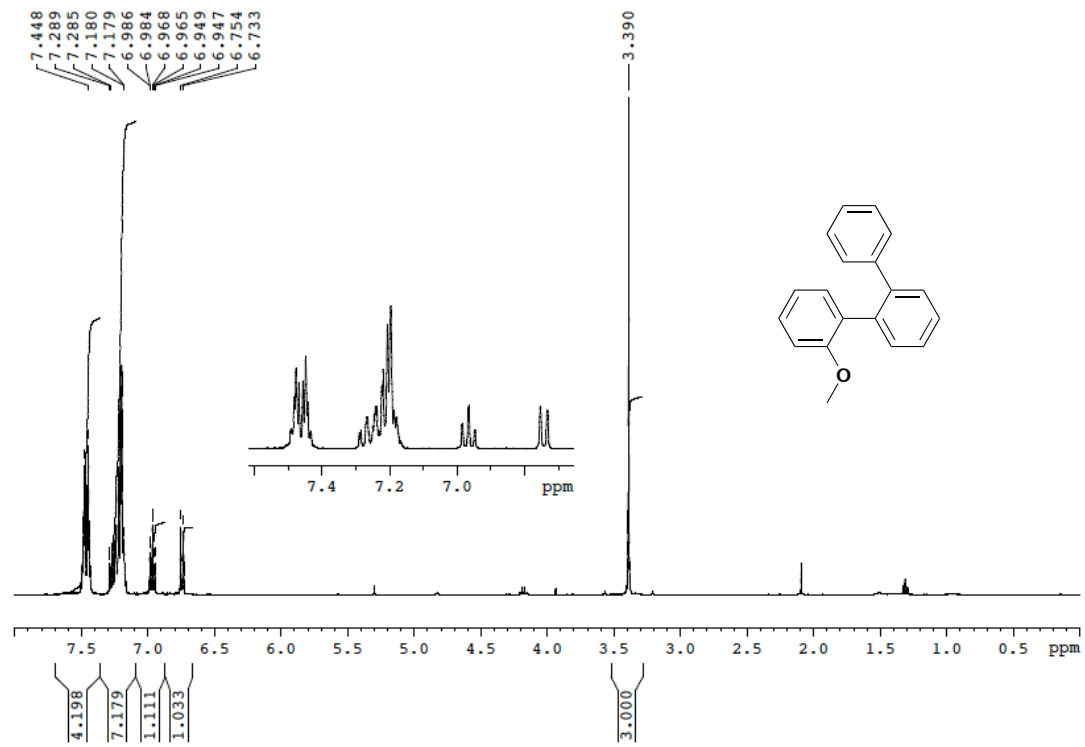


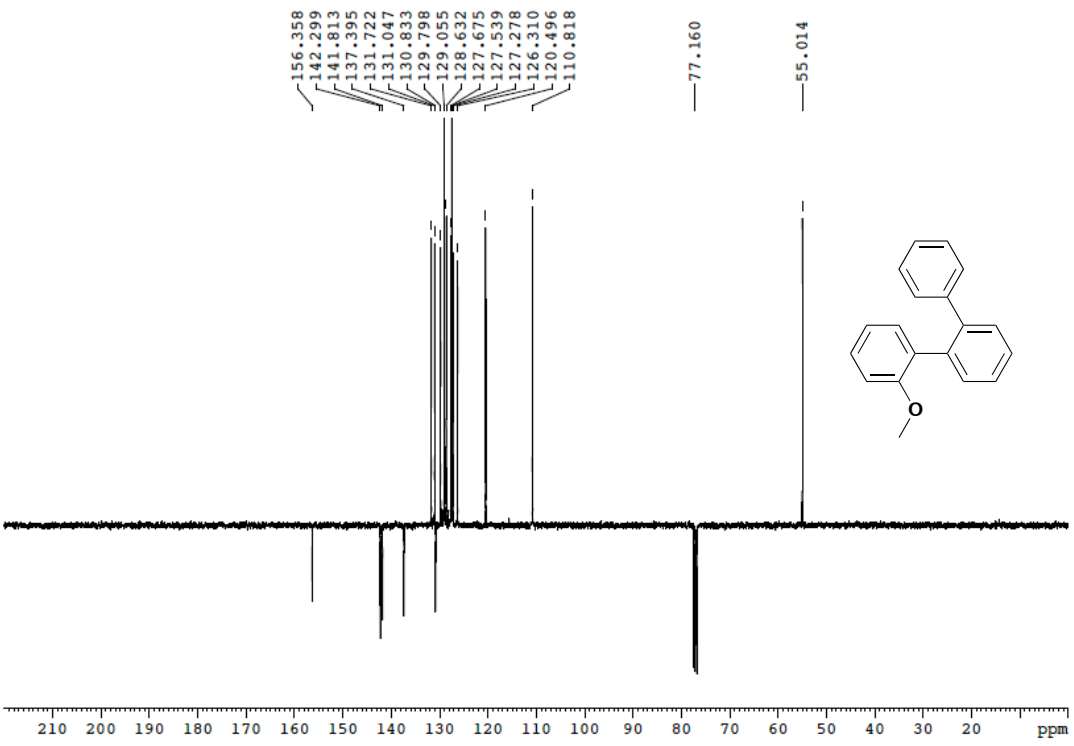
^{1}H and ^{13}C-{^{1}H} NMR Spectra of 2-*o*-tolylbiphenyl





^{1}H and ^{13}C-{^{1}H} NMR spectra of 2-phenyl-2'-methoxybiphenyl





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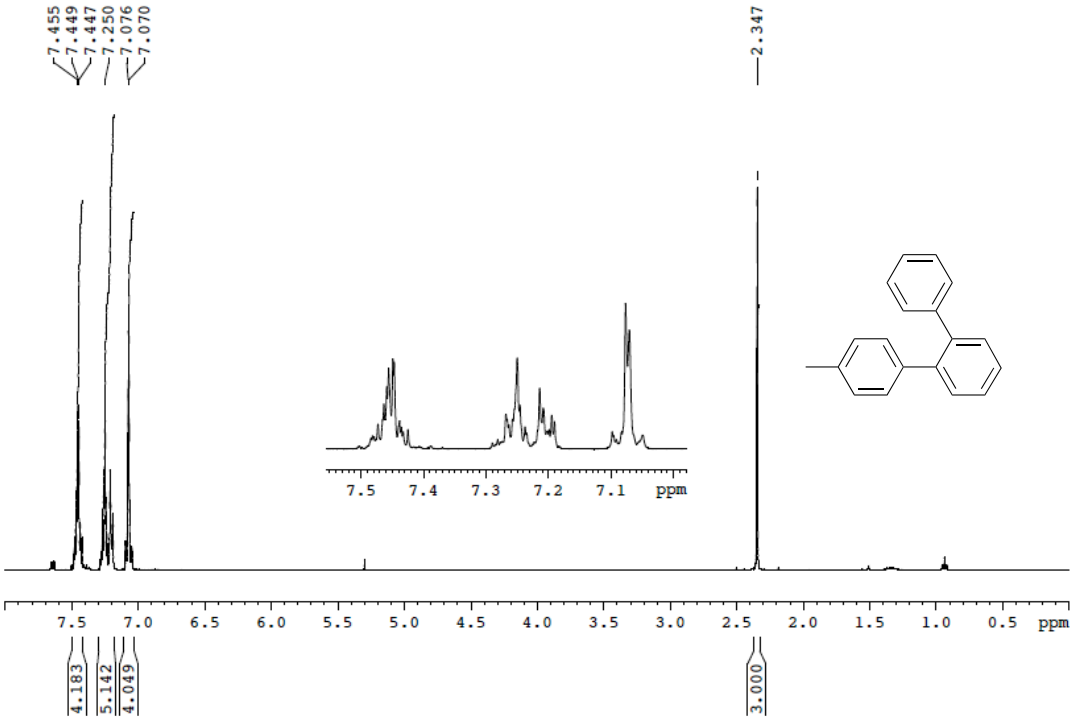
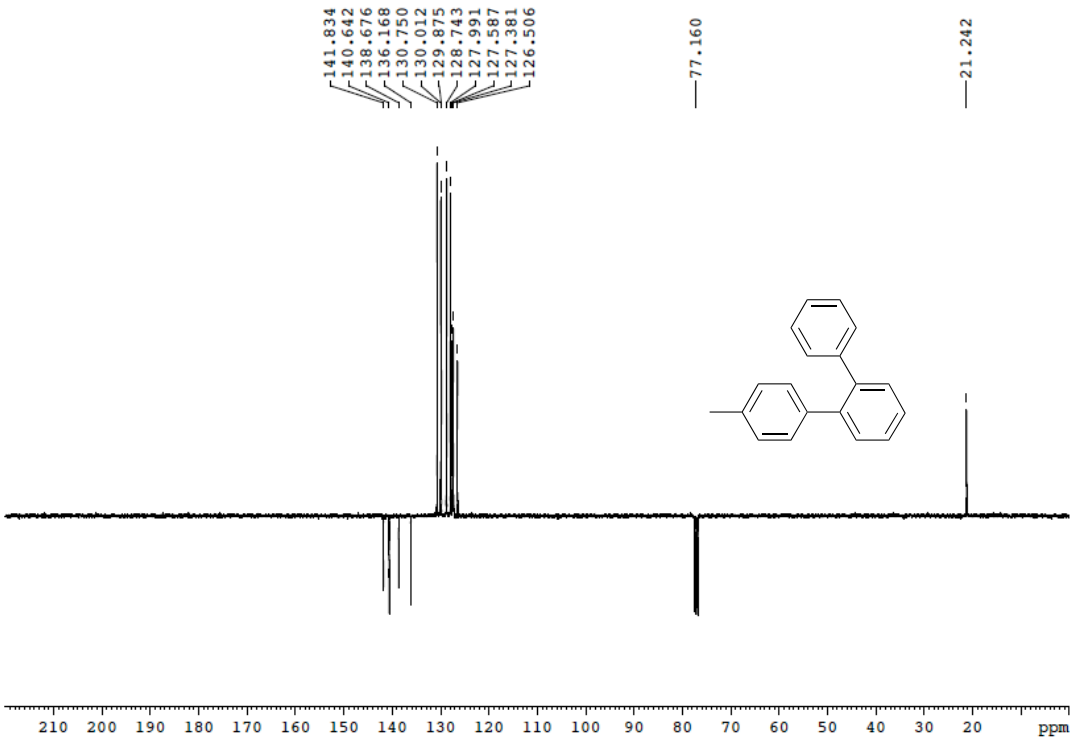
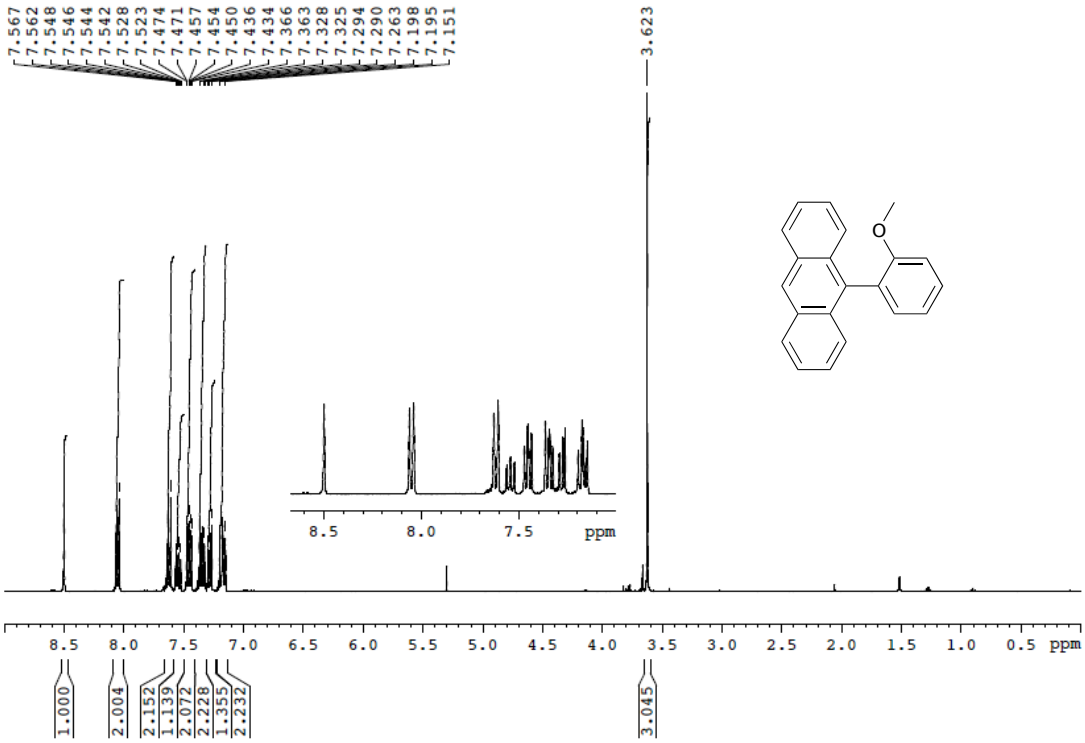
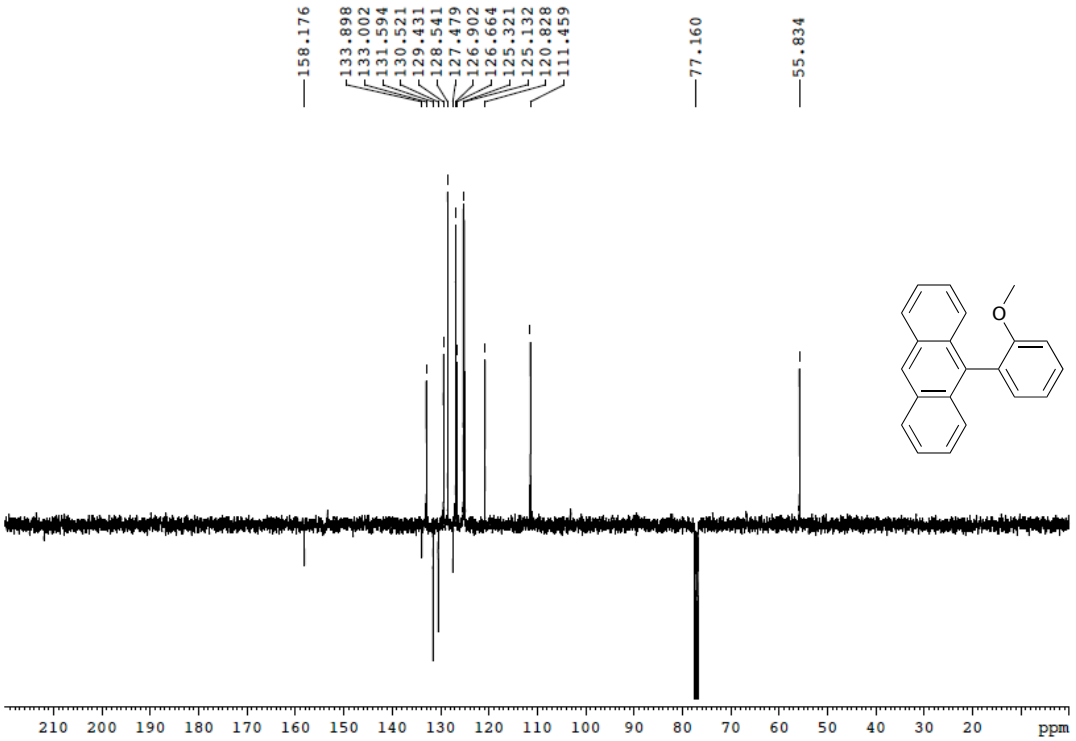
^{1}H and ^{13}C-{^{1}H} NMR spectra of 2-phenyl,4'-methylbiphenyl



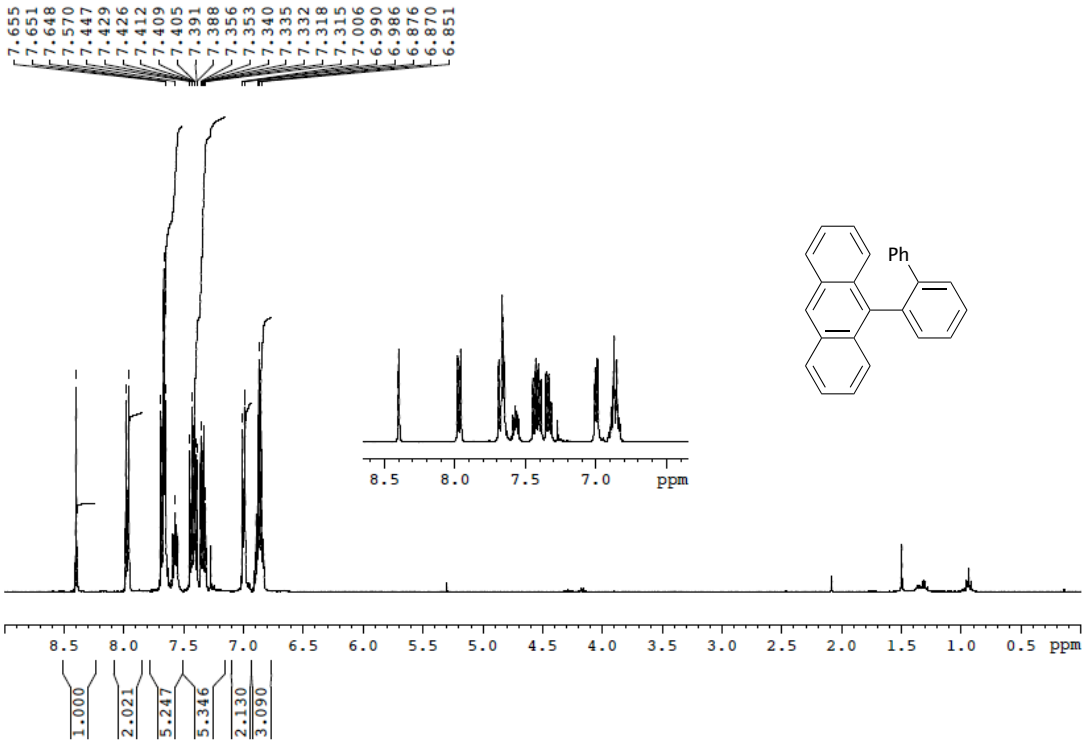


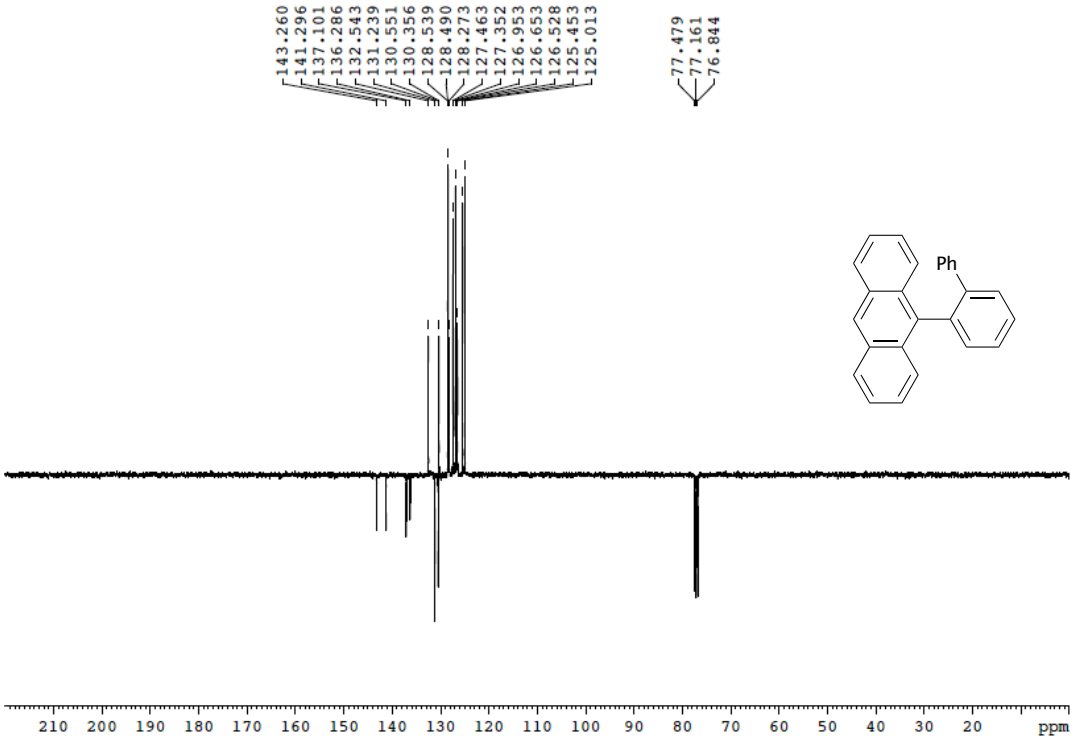
^{1}H and ^{13}C-{^{1}H} NMR spectra of 9-(2-methoxyphenyl)anthracene:



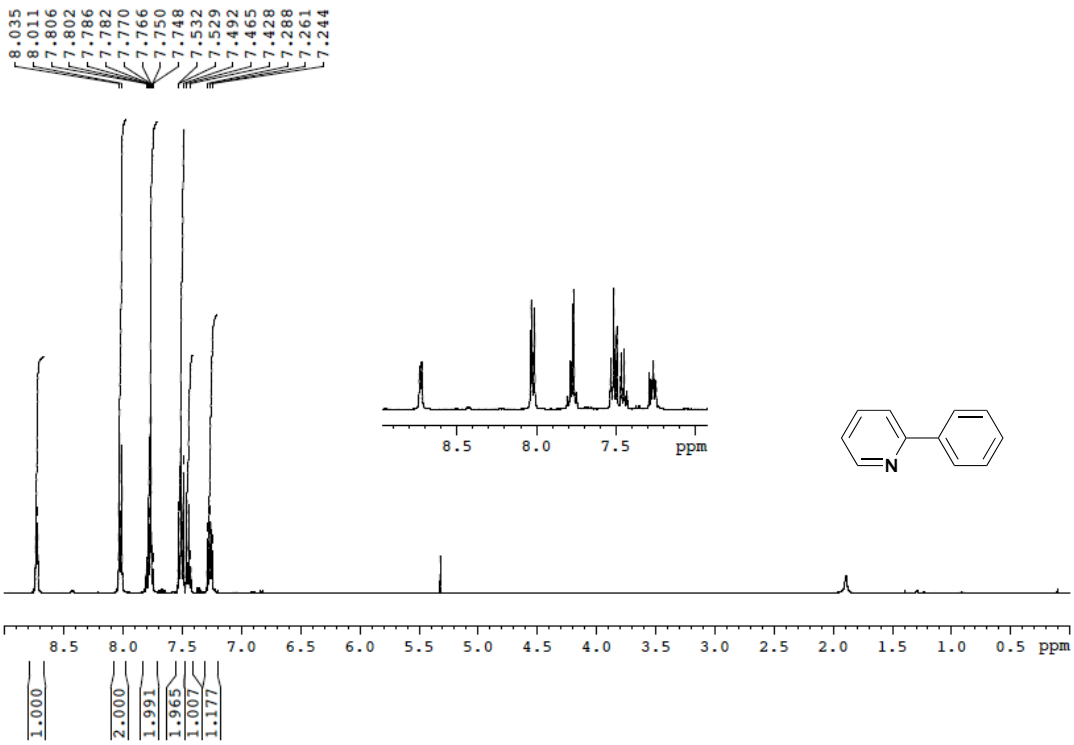


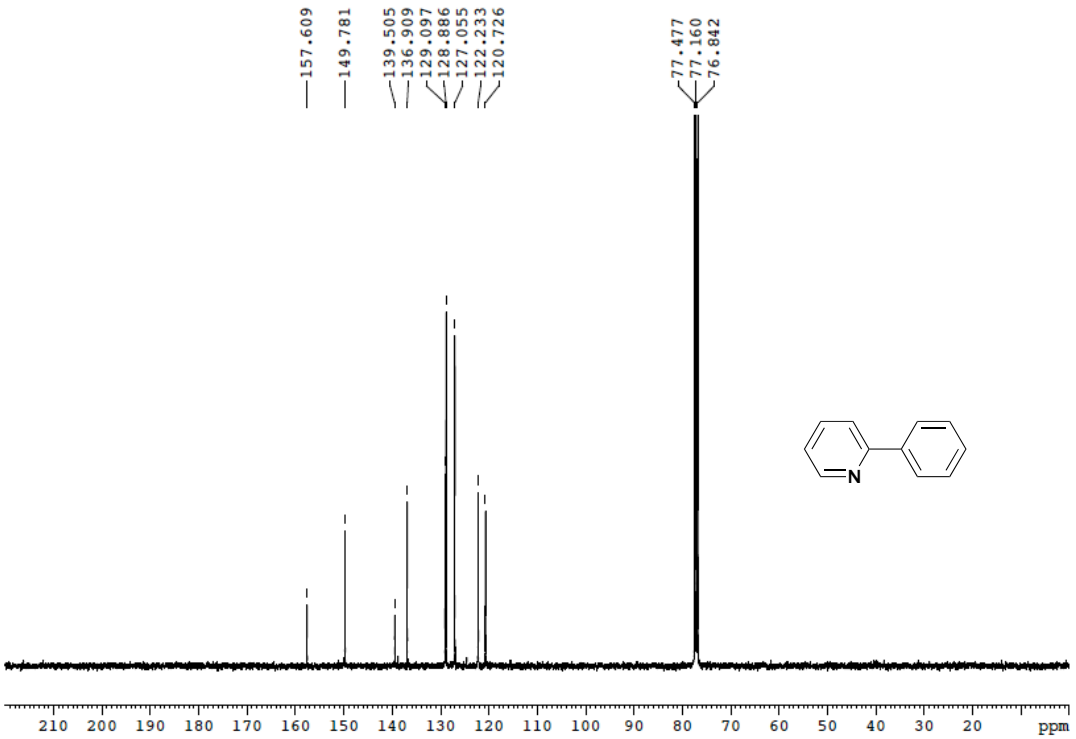
^{1}H and ^{13}C-{^{1}H} NMR spectra of 9-(*o*-biphenyl)anthracene





^{1}H and ^{13}C-{^{1}H} NMR spectra of 2-phenylpyridine





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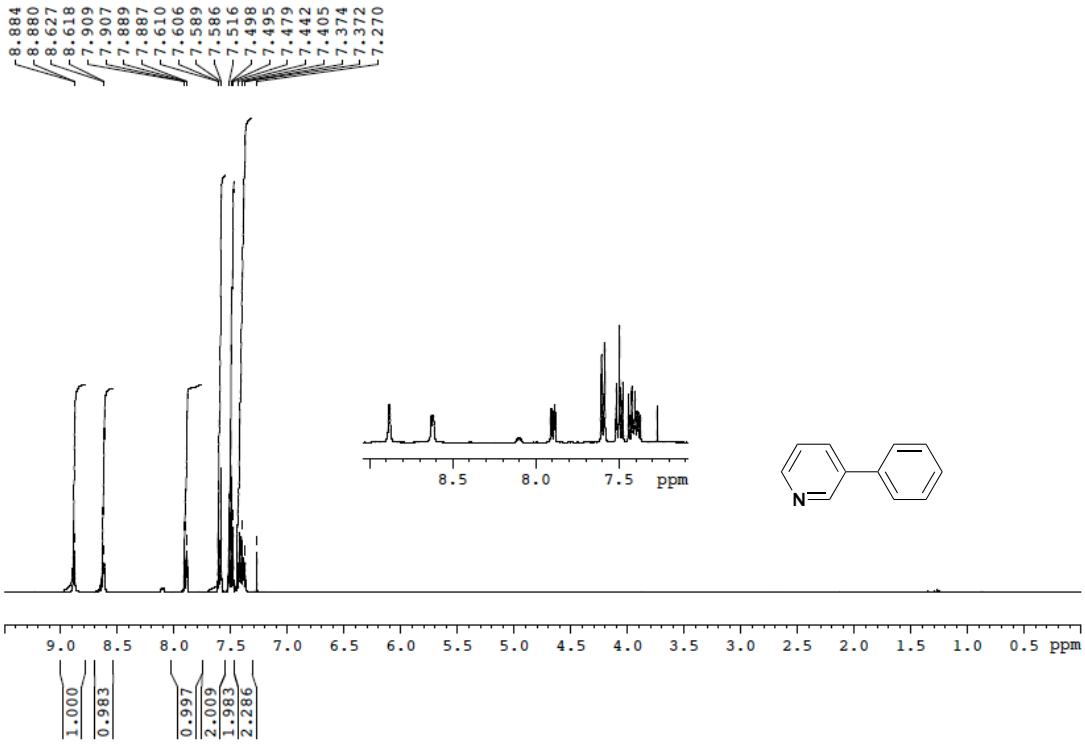
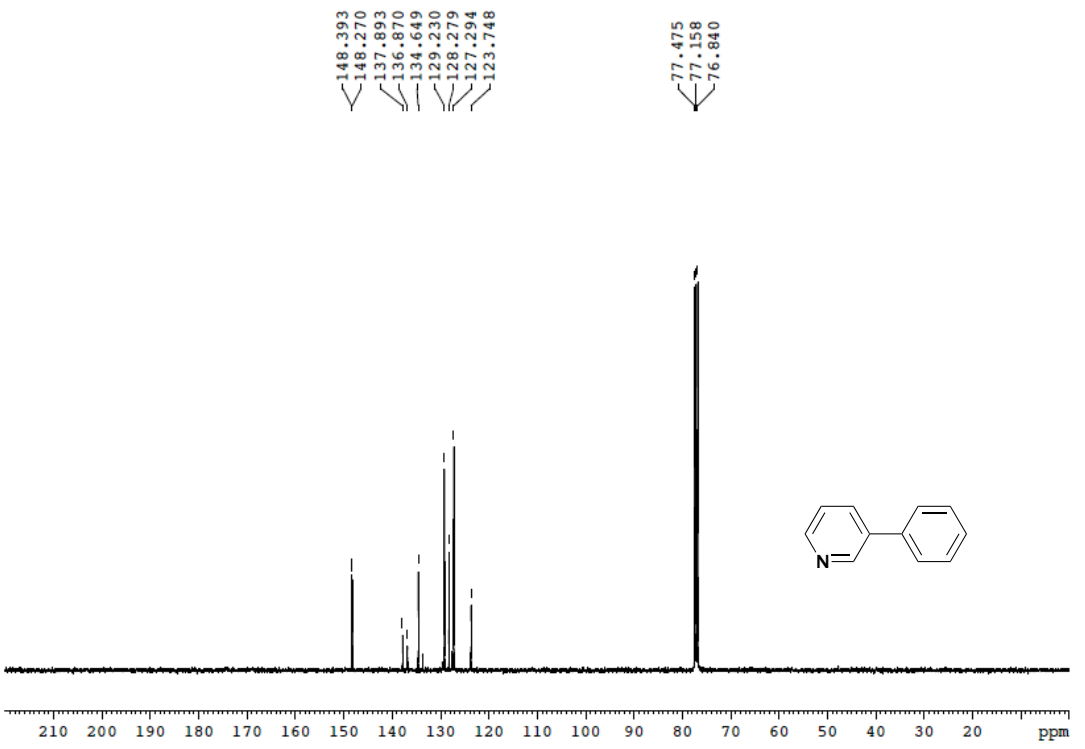
^{1}H and ^{13}C-{^{1}H} NMR spectra of 3-phenylpyridine





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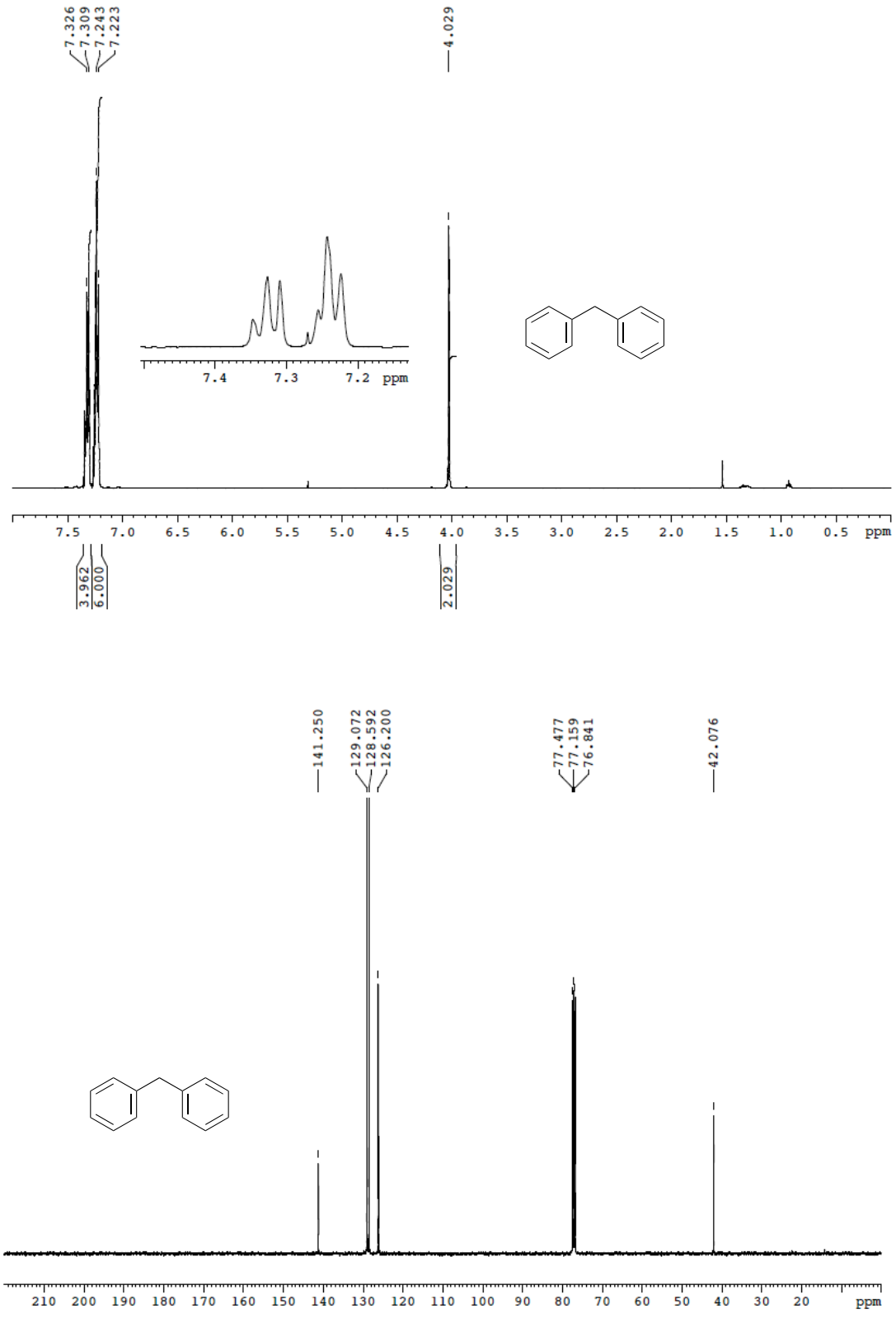
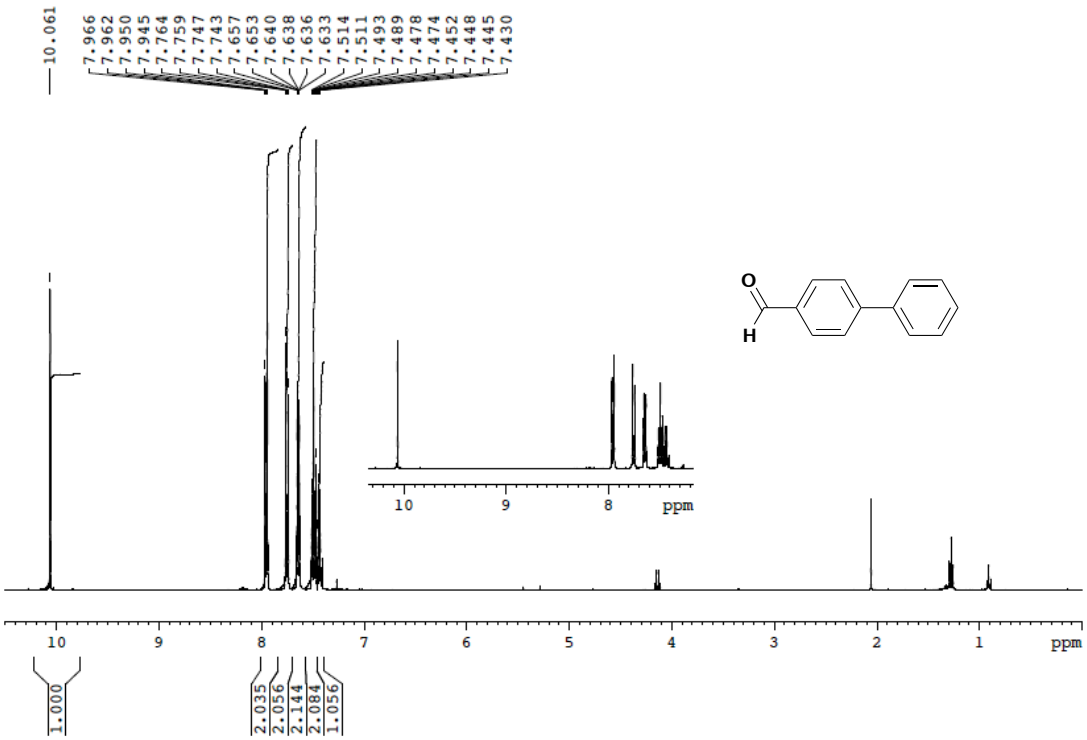
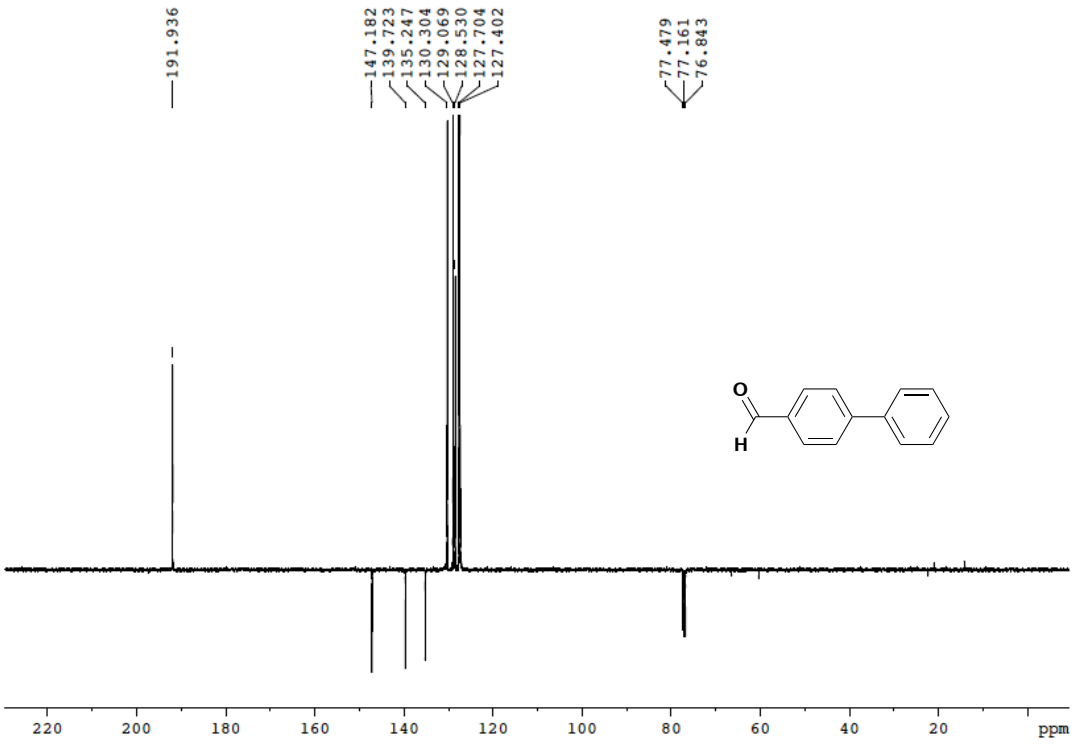
^{1}H and ^{13}C-{^{1}H} NMR spectra of diphenylmethane

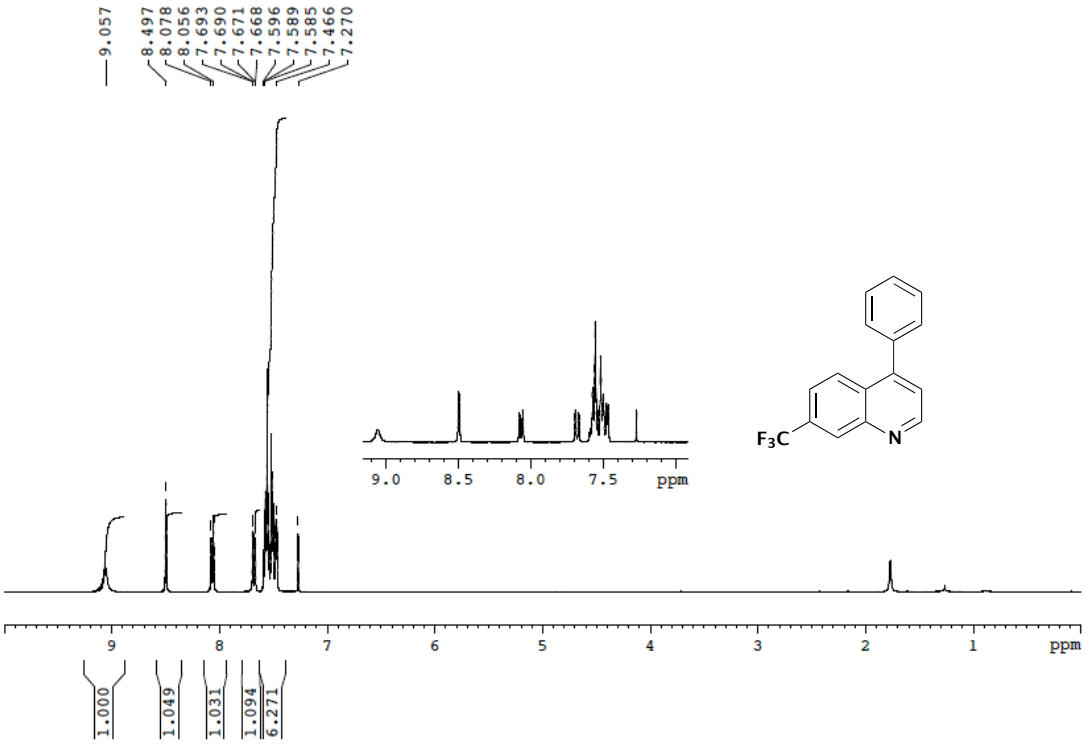


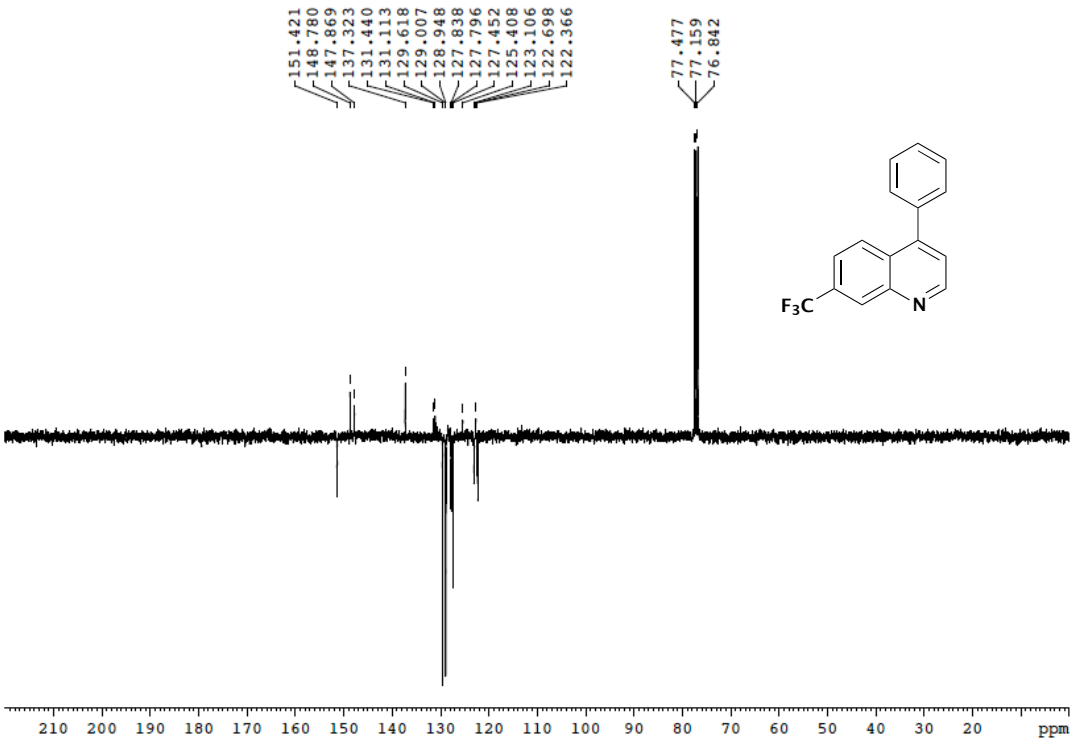
^{1}H and ^{13}C-{^{1}H} NMR spectra of 4-formyl-1,1'-biphenyl





^{1}H and ^{13}C-{^{1}H} NMR spectra of 4-phenyl-7-(trifluoromethyl)quinoline





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Crystal data and structure refinement

$[PdCl_2(IPr)\{PPh_3\}]$ (2a)

Empirical formula	$C_{45}H_{51}Cl_2N_2PPd$	
Formula weight	828.15	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 12.7651(7) Å	α= 90°
	b = 13.7447(9) Å	β= 90°
	c = 47.075(3) Å	γ = 90°
Volume	8259.4(8) $Å^3$	
Z	8	
Density (calculated)	1.332 Mg/m^3	
Absorption coefficient	0.650 mm^{-1}	
F(000)	3440	
Crystal size	0.100 x 0.100 x 0.100 mm^3	
Theta range for data collection	2.62 to 27.75°.	
Index ranges	$-16 \le h \le 16$, $-17 \le k \le 17$, $-52 \le l \le 60$	
Reflections collected	81368	
Independent reflections	17555 [R(int) = 0.0772]	
Completeness to theta = 25.00°	99.4 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.8295	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17555 / 0 / 919	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0546, wR2 = 0.1194	
R indices (all data)	R1 = 0.0587, wR2 = 0.1221	
Absolute structure parameter	0.04(2)	
Largest diff. peak and hole	0.431 and -0.771 $e.Å^{-3}$	

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$[PdCl_2(IPr)\{PCy_3\}]$ (2b)

Empirical formula	$C_{45}H_{69}Cl_2N_2PPd$	
Formula weight	846.29	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 10.687(2) Å	α= 90°
	b = 14.147(3) Å	β= 95.572(6)°
	c = 15.029(3) Å	γ = 90°
Volume	2261.5(7) $Å^3$	
Z	2	
Density (calculated)	1.243 Mg/m^3	
Absorption coefficient	0.595 mm^{-1}	
F(000)	896	
Crystal size	0.1200 x 0.1200 x 0.1000 mm^3	
Theta range for data collection	2.24 to 25.33°.	
Index ranges	$-8 \le h \le 12$, $-16 \le k \le 17$, $-18 \le l \le 17$	
Reflections collected	14317	
Independent reflections	7509 [R(int) = 0.0399]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.7527	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7509 / 1 / 460	
Goodness-of-fit on F^2	0.826	
Final R indices [I>2sigma(I)]	R1 = 0.0419, wR2 = 0.0953	
R indices (all data)	R1 = 0.0498, wR2 = 0.1116	
Absolute structure parameter	-0.02(3)	
Largest diff. peak and hole	1.130 and -0.732 $e.Å^{-3}$	

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$[PdCl_2(IPr)\{P(o\text{-tolyl})_3\}]$ (2c)

Empirical formula	$C_{48}H_{57}Cl_2N_2PPd$	
Formula weight	870.23	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	I-4	
Unit cell dimensions	a = 24.122(4) Å	α= 90°
	b = 24.122(4) Å	β= 90°
	c = 18.253(3) Å	γ = 90°
Volume	10620(3) $Å^3$	
Z	8	
Density (calculated)	1.089 Mg/m^3	
Absorption coefficient	0.509 mm^{-1}	
F(000)	3632	
Crystal size	0.2000 x 0.2000 x 0.2000 mm^3	
Theta range for data collection	1.19 to 25.32°.	
Index ranges	$-23 \le h \le 29$, $-26 \le k \le 29$, $-17 \le l \le 21$	
Reflections collected	33423	
Independent reflections	9699 [R(int) = 0.0659]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.7469	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9699 / 0 / 487	
Goodness-of-fit on F^2	1.085	
Final R indices [I>2sigma(I)]	R1 = 0.0541, wR2 = 0.1571	
R indices (all data)	R1 = 0.0652, wR2 = 0.1662	
Absolute structure parameter	-0.01(3)	
Largest diff. peak and hole	0.990 and -0.458 $e.Å^{-3}$	

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$[PdCl_2(IPr)\{P(^nBu)(1\text{-}Ad)_2\}]\cdot 0.5CH_2Cl_2$ (2d)

Empirical formula	$C_{51.50}H_{76}Cl_3N_2PPd$	
Formula weight	966.86	
Temperature	125(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.854(3) Å	α= 93.602(5)°
	b = 16.741(4) Å	β= 91.002(6)°
	c = 21.852(4) Å	γ = 92.724(7)°
Volume	5051.5(18) $Å^3$	
Z	4	
Density (calculated)	1.271 Mg/m^3	
Absorption coefficient	0.593 mm^{-1}	
F(000)	2044	
Crystal size	0.21 x 0.18 x 0.03 mm^3	
Theta range for data collection	0.93 to 25.35°.	
Index ranges	$-16 \le h \le 15$, $-20 \le k \le 20$, $-26 \le l \le 25$	
Reflections collected	39296	
Independent reflections	18263 [R(int) = 0.1179]	
Completeness to theta = 25.00°	98.8 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.000 and 0.540	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18263 / 4 / 1059	
Goodness-of-fit on F^2	1.340	
Final R indices [I>2sigma(I)]	R1 = 0.0966, wR2 = 0.2788	
R indices (all data)	R1 = 0.1360, wR2 = 0.3680	
Largest diff. peak and hole	2.829 and -2.955 $e.Å^{-3}$	

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$[PdCl_2(IPr)\{PCy_2(o\text{-biphenyl})\}]$ (2e)

Empirical formula	$C_{51}H_{67}Cl_2N_2PPd$	
Formula weight	916.38	
Temperature	93(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 11.928(2) Å	α= 90°
	b = 13.362(3) Å	β= 92.804(5)°
	c = 30.789(5) Å	γ = 90°
Volume	4901(2) $Å^3$	
Z	4	
Density (calculated)	1.242 Mg/m^3	
Absorption coefficient	0.5545 mm^{-1}	
F(000)	1928.00	
Crystal size	0.10 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.0 to 50.7°.	
Index ranges	$-14 \le h \le 14$, $-15 \le k \le 16$, $-36 \le l \le 36$	
Reflections collected	29822	
Independent reflections	8941 [R(int) = 0.0546]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Multiscan	
Max. and min. transmission	0.946 and 0.8386	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8941 / 0 / 514	
Goodness-of-fit on F^2	0.964	
Final R indices [I>2sigma(I)]	R1 = 0.0425, wR2 = 0.0904	
R indices (all data)	R1 = 0.0681, wR2 = 0.0904	
Largest diff. peak and hole	0.44 and -0.51 $e.Å^{-3}$	

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$[PdCl_2(IPr)(XPhos)]\cdot 1.5CH_2Cl_2$ (2f)

Empirical formula	$C_{61.50}H_{88}Cl_5N_2PPd$	
Formula weight	1169.96	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.320(3) Å	α= 103.505(8)°
	b = 12.759(2) Å	β= 104.578(7)°
	c = 21.547(5) Å	γ = 93.875(9)°
Volume	3158.4(11) $Å^3$	
Z	2	
Density (calculated)	1.230 Mg/m^3	
Absorption coefficient	0.567 mm^{-1}	
F(000)	1234	
Crystal size	0.12 x 0.12 x 0.03 mm^3	
Theta range for data collection	2.02 to 25.39°.	
Index ranges	$-14 \le h \le 14$, $-12 \le k \le 15$, $-25 \le l \le 25$	
Reflections collected	32216	
Independent reflections	11488 [R(int) = 0.0479]	
Completeness to theta = 25.00°	99.4 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.000 and 0.849	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11488 / 2 / 639	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0808, wR2 = 0.2344	
R indices (all data)	R1 = 0.0913, wR2 = 0.2451	
Largest diff. peak and hole	3.902 and -1.177 $e.Å^{-3}$	

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$[PdCl_2(IPr)(SPhos)]$ (2g)

Empirical formula	$C_{53}H_{71}Cl_2N_2O_2PPd$	
Formula weight	976.39	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 18.580(3) Å	α= 90°
	b = 14.0874(19) Å	β= 90.472(3)°
	c = 19.401(3) Å	γ = 90°
Volume	5077.7(12) $Å^3$	
Z	4	
Density (calculated)	1.277 Mg/m^3	
Absorption coefficient	0.542 mm^{-1}	
F(000)	2056	
Crystal size	0.10 x 0.10 x 0.03 mm^3	
Theta range for data collection	2.10 to 25.36°.	
Index ranges	$-21 \le h \le 22$, $-16 \le k \le 16$, $-23 \le l \le 23$	
Reflections collected	50611	
Independent reflections	9288 [R(int) = 0.0564]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.000 and 0.893	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9288 / 0 / 550	
Goodness-of-fit on F^2	1.109	
Final R indices [I>2sigma(I)]	R1 = 0.0504, wR2 = 0.1297	
R indices (all data)	R1 = 0.0596, wR2 = 0.1409	
Largest diff. peak and hole	1.044 and -0.800 $e.Å^{-3}$	

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$[Pd(\mu\text{-}Cl)(Cl)(SPhos)]_2$ (5)

Empirical Formula	$C_{52}H_{70}Cl_4O_4P_2Pd_2$	
Formula Weight	1175.68	
Crystal Color, Habit	orange, prism	
Crystal Dimensions	0.120 X 0.120 X 0.050 mm	
Crystal System	triclinic	
Lattice Type	Primitive	
Lattice Parameters	a = 9.390(10) Å	α = 103.70(2)º
	b = 10.444(11) Å	β = 103.29(2)º
	c = 13.80(2) Å	γ = 96.525(10)º
	V = 1259(3) Å3	
Space Group	P-1 (#2)	
Z value	1	
Dcalc	1.551 g/cm3	
F000	604.00	
μ(MoKα)	10.347 cm-1	
Diffractometer	Saturn70	
Radiation	MoKα (λ = 0.71075 Å)	
Voltage, Current	50kV, 16mA	
Temperature	-180.0ºC	
Detector Aperture	70 x 70 mm	
Pixel Size	0.034 mm	
2θmax	50.6º	
No. of Reflections Measured	Total: 11553	Unique: 4471 (Rint = 0.1775)
Corrections	Lorentz-polarization	
	Absorption	
	(trans. factors: 0.387 - 0.950)	
Structure Solution	Direct Methods	
Refinement	Full-matrix least-squares on F2	
Function Minimized	Σ w (Fo2 - Fc2)2	
Least Squares Weights	w = 1/ [σ2(Fo2) + (0.2000 . P)2 + 0.0000 . P] where P = (Max(Fo2,0) + 2Fc2)/3	
2θmax cutoff	50.6º	
Anomalous Dispersion	All non-hydrogen atoms	
No. Observations (All reflections)	4471	
No. Variables	289	
Reflection/Parameter Ratio	15.47	
Residuals: R1 (I>2.00σ(I))	0.1309	
Residuals: R (All reflections)	0.1367	
Residuals: wR2 (All reflections)	0.3519	
Goodness of Fit Indicator	1.404	
Max Shift/Error in Final Cycle	0.003	
Maximum peak in Final Diff. Map	3.78 e-/Å^3	
Minimum peak in Final Diff. Map	-4.06 e-/Å^3	

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[Pd(IPr)(SPhos)] (6)

Empirical formula	$C_{53}H_{71}N_2O_2PPd$	
Formula weight	905.49	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 17.831(2) Å	α= 90°
	b = 14.5302(19) Å	β= 99.784(5)°
	c = 18.802(3) Å	γ = 90°
Volume	4800.7(11) $Å^3$	
Z	4	
Density (calculated)	1.253 Mg/m^3	
Absorption coefficient	0.461 mm^{-1}	
F(000)	1920	
Crystal size	0.150 x 0.150 x 0.150 mm^3	
Theta range for data collection	2.02 to 25.35°.	
Index ranges	$-21 \le h \le 18$, $-17 \le k \le 12$, $-21 \le l \le 22$	
Reflections collected	25152	
Independent reflections	8670 [R(int) = 0.2327]	
Completeness to theta = 25.00°	99.2 %	
Absorption correction	Multiscan	
Max. and min. transmission	1.0000 and 0.5095	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8670 / 0 / 532	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0875, wR2 = 0.2141	
R indices (all data)	R1 = 0.1272, wR2 = 0.2548	
Largest diff. peak and hole	2.118 and -4.074 $e.Å^{-3}$	

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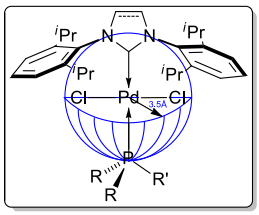
%V_{Bur} and topographical steric maps calculated using SambVca



General considerations

The buried volumes and the steric maps have been calculated on the NHC ligand as in the X-ray structure of the Pd complexes. The points in space defining the steric map were located with the Samb*V*ca package developed by Cavallo.[17]

To build the steric maps, the optimised geometry of the complexes under analysis has been placed with the Pd center at the origin, with the Pd-NHC or phosphine bonds aligned along the z-axis at positive z values, at a Pd-NHC/P distance of 2.1 Å. The radius *R* of the sphere around the metal centre was set to 3.5 Å, while for the atoms we adopted the Bondi radii[18] scaled by 1.17, and a mesh of 0.1 Å was used to scan the sphere for buried voxels.

https://www.molnac.unisa.it/OMtools/sambvca.php

%V_{Bur} of IPr in the complex [$PdCl_2$(IPr){PPh_3}] (2a)

Number of atoms : 29
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 28 29

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C -135.12400 -46.33000 -7.96600	C -132.29200 -47.95600 -10.96400	C -136.64200 -48.76000 -6.45200
C -132.90800 -46.68800 -7.76900	C -134.24100 -47.55700 -12.48700	C -135.04200 -46.05700 -4.21600
C -133.51900 -47.35200 -6.78500	C -133.62300 -43.23700 -7.98700	C -133.87500 -46.60400 -3.37200
C -133.64900 -45.21600 -9.61500	C -132.22700 -42.87900 -7.46000	C -135.82600 -45.04400 -3.40200
C -133.49900 -43.83700 -9.35800	C -134.53400 -42.02400 -7.96100	C -136.54400 -49.27800 -7.87200
C -133.16800 -43.03500 -10.43600	C -135.84000 -47.69900 -6.00900	C -135.27000 -50.09400 -8.08500
C -132.97700 -43.56000 -11.69300	C -135.91800 -47.19200 -4.70900	C -137.77100 -50.07000 -8.29600
C -133.12000 -44.91100 -11.89100	C -136.81200 -47.80200 -3.83900	N -133.91500 -46.06800 -8.48900
C -133.48700 -45.78300 -10.86800	C -137.59300 -48.86100 -4.24800	N -134.87600 -47.13500 -6.91500
C -133.63600 -47.26200 -11.11600	C -137.52700 -49.32000 -5.54100	

Atoms and radius in the parameter file

H 1.29	C 1.99	N 1.81
C2 1.99	N2 1.81	O 1.78
C3 1.99	N3 1.81	F 1.72

Si 2.45	S 2.10	Br 2.16
P 2.11	Cl 2.05	

Coordinates scaled to put the metal at the origin

C 1.86329 -0.69442 0.67523	C 4.69529 -2.32042 -2.32277	C 0.34529 -3.12442 2.18923
C 4.07929 -1.05242 0.87223	C 2.74629 -1.92142 -3.84577	C 1.94529 -0.42142 4.42523
C 3.46829 -1.71642 1.85623	C 3.36429 2.39858 0.65423	C 3.11229 -0.96842 5.26923
C 3.33829 0.41958 -0.97377	C 4.76029 2.75658 1.18123	C 1.16129 0.59158 5.23923
C 3.48829 1.79858 -0.71677	C 2.45329 3.61158 0.68023	C 0.44329 -3.64242 0.76923
C 3.81929 2.60058 -1.79477	C 1.14729 -2.06342 2.63223	C 1.71729 -4.45842 0.55623
C 4.01029 2.07558 -3.05177	C 1.06929 -1.55642 3.93223	C -0.78371 -4.43442 0.34523
C 3.86729 0.72458 -3.24977	C 0.17529 -2.16642 4.80223	N 3.07229 -0.43242 0.15223
C 3.50029 -0.14742 -2.22677	C -0.60571 -3.22542 4.39323	N 2.11129 -1.49942 1.72623
C 3.35129 -1.62642 -2.47477	C -0.53971 -3.68442 3.10023	XX 0.00000 0.00000 0.00000

Results : Volumes in Angs^3

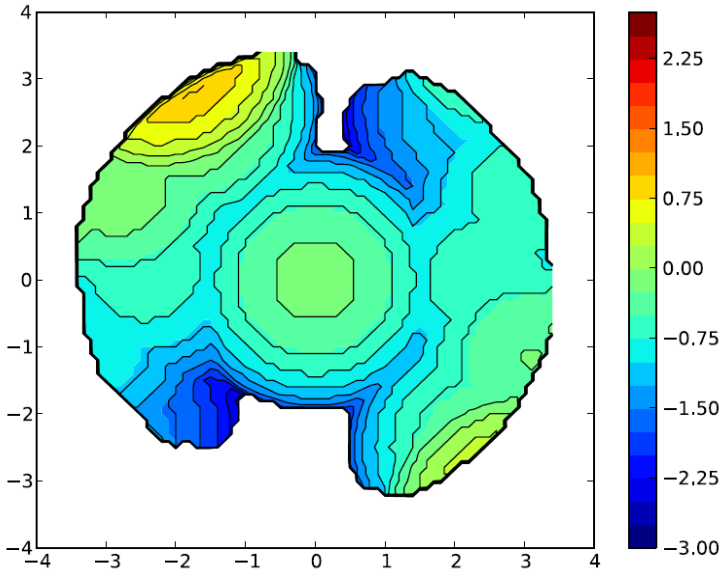
N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
117.976	61.559	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
65.712	34.288	99.967

The $\%V_{Bur}$ of *IPr* is: **34.3**

Steric map of IPr in the complex [$PdCl_2$(IPr){PPh_3}] (2a)



$\%V_{Bur}$ of PPh_3 in the complex [$PdCl_2$(IPr){PPh_3}] (2a)

Number of atoms : 19
Atom that is coordinated : 19
Atoms that define the axis : 3
ID of these atoms : 1 7 13

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050

H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C -133.20000 -40.70700 42.97400	C -135.00600 -41.65700 40.58900	C -133.95300 -44.58700 46.04700
C -133.58400 -40.15600 44.16900	C -135.99800 -41.88200 39.63600	C -135.30400 -44.39000 46.25900
C -133.41300 -38.79700 44.41700	C -136.49300 -43.14300 39.44500	C -136.03200 -43.62000 45.39000
C -132.84100 -38.00900 43.46700	C -136.01800 -44.19900 40.18100	C -135.42900 -43.04300 44.30900
C -132.45000 -38.52700 42.27000	C -135.01100 -43.97400 41.13300	P -133.26000 -42.48000 42.63000
C -132.62500 -39.88300 42.00500	C -134.06400 -43.22100 44.06800	
C -134.53100 -42.69600 41.33700	C -133.34900 -44.00700 44.95200	

Atoms and radius in the parameter file

H 1.29	N3 1.81	P 2.11
C2 1.99	N 1.81	S 2.10
C3 1.99	O 1.78	Cl 2.05
C 1.99	F 1.72	Br 2.16
N2 1.81	Si 2.45	

Coordinates scaled to put the metal at the origin

C -1.83900 2.54203 0.80485	C -3.64500 1.59203 -1.58015	C -2.59200 -1.33797 3.87785
C -2.22300 3.09303 1.99985	C -4.63700 1.36703 -2.53315	C -3.94300 -1.14097 4.08985
C -2.05200 4.45203 2.24785	C -5.13200 0.10603 -2.72415	C -4.67100 -0.37097 3.22085
C -1.48000 5.24003 1.29785	C -4.65700 -0.94997 -1.98815	C -4.06800 0.20603 2.13985
C -1.08900 4.72203 0.10085	C -3.65000 -0.72497 -1.03615	P -1.89900 0.76903 0.46085
C -1.26400 3.36603 -0.16415	C -2.70300 0.02803 1.89885	XX 0.00000 0.00000 0.00000
C -3.17000 0.55303 -0.83215	C -1.98800 -0.75797 2.78285	

Results : Volumes in Angs^3

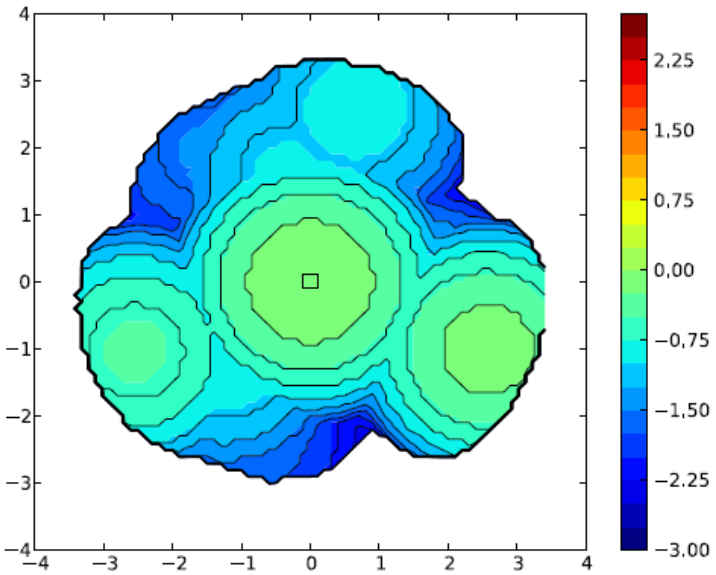
N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
122.485	57.050	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
68.223	31.777	99.967

The $\%V_{Bur}$ of *PPh₃* is: **31.8**

Steric map of PPh_3 in the complex $[PdCl_2(IPr)\{PPh_3\}]$ (2a)



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%V_{Bur} of IPr in the complex [$PdCl_2$(IPr){PCy_3}] (2b)

Number of atoms : 29
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 28 29

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C	28.96000	-17.49800	46.43000	C	31.00100	-15.87400	43.05600	C	26.20500	-17.00300	48.22900
C	29.85100	-15.42500	46.45400	C	30.95100	-18.29800	42.40700	C	26.06900	-16.39700	44.41400
C	28.53700	-15.28000	46.65300	C	31.99900	-17.08600	48.52200	C	25.91100	-14.91700	44.10000
C	31.41100	-17.31300	46.04000	C	32.55400	-15.71500	48.86600	C	25.25700	-17.23800	43.40900
C	31.75900	-17.58900	44.71300	C	32.54900	-18.11900	49.51900	C	27.20400	-17.00400	49.37800
C	33.05400	-18.05400	44.45800	C	26.57600	-16.79200	46.89400	C	27.08400	-15.67100	50.12900
C	33.96100	-18.22500	45.47800	C	25.67400	-16.70000	45.85000	C	26.92000	-18.16200	50.34200
C	33.60700	-17.93400	46.76500	C	24.31700	-16.82600	46.17100	N	30.11000	-16.77800	46.30500
C	32.34400	-17.46300	47.08700	C	23.91300	-17.04400	47.47500	N	27.99400	-16.55700	46.63100
C	30.79100	-17.29600	43.56100	C	24.85400	-17.12000	48.49100				

Atoms and radius in the parameter file

H	1.29	N3	1.81	P	2.11
C2	1.99	N	1.81	S	2.10
C3	1.99	O	1.78	Cl	2.05
C	1.99	F	1.72	Br	2.16
N2	1.81	Si	2.45		

Coordinates scaled to put the metal at the origin

C	0.23098	2.08508	0.09540	C	2.27198	3.70908	-3.27860	C	-2.52402	2.58008	1.89440
C	1.12198	4.15808	0.11940	C	2.22198	1.28508	-3.92760	C	-2.66002	3.18608	-1.92060
C	-0.19202	4.30308	0.31840	C	3.26998	2.49708	2.18740	C	-2.81802	4.66608	-2.23460
C	2.68198	2.27008	-0.29460	C	3.82498	3.86808	2.53140	C	-3.47202	2.34508	-2.92560
C	3.02998	1.99408	-1.62160	C	3.81998	1.46408	3.18440	C	-1.52502	2.57908	3.04340
C	4.32498	1.52908	-1.87660	C	-2.15302	2.79108	0.55940	C	-1.64502	3.91208	3.79440
C	5.23198	1.35808	-0.85660	C	-3.05502	2.88308	-0.48460	C	-1.80902	1.42108	4.00740
C	4.87798	1.64908	0.43040	C	-4.41202	2.75708	-0.16360	N	1.38098	2.80508	-0.02960
C	3.61498	2.12008	0.75240	C	-4.81602	2.53908	1.14040	N	-0.73502	3.02608	0.29640
C	2.06198	2.28708	-2.77360	C	-3.87502	2.46308	2.15640	XX	0.00000	0.00000	0.00000

Results : Volumes in Angs^3

N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
121.820	57.715	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
67.853	32.147	99.967

The %V_{Bur} of *IPr* is: **32.1**

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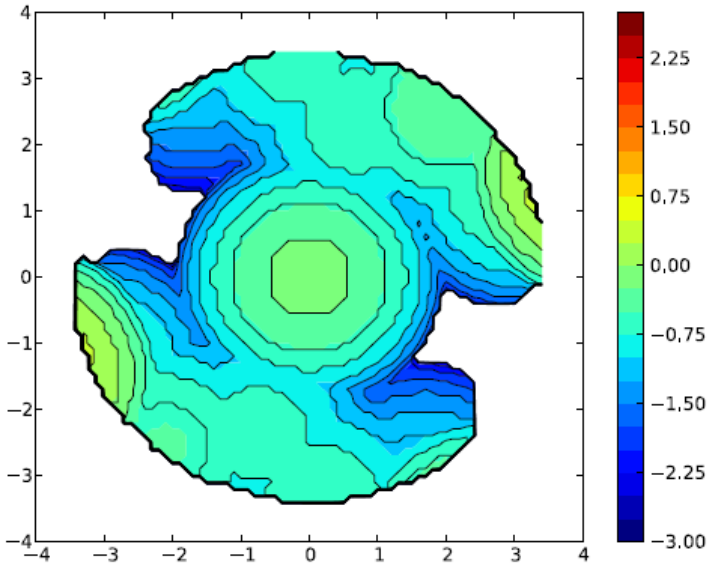
Steric map of IPr in the complex [$PdCl_2$(IPr){PCy_3}] (2b)



%V_{Bur} of PCy_3 in the complex [$PdCl_2$(IPr){PCy_3}] (2b)

Number of atoms : 19
Atom that is coordinated : 19
Atoms that define the axis : 3
ID of these atoms : 1 7 13

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C 28.99900 -22.82600 47.52400	C 28.10200 -23.96200 44.33900	C 24.00000 -21.59700 45.81000
C 28.44700 -24.23500 47.77100	C 28.11500 -24.29000 42.84000	C 23.66900 -20.88400 47.12600
C 29.14800 -24.89500 48.97300	C 29.46500 -23.93700 42.19900	C 24.53400 -21.40300 48.23600
C 30.64400 -24.92300 48.78800	C 29.86200 -22.50000 42.48500	C 26.01100 -21.28200 47.89500
C 31.21100 -23.52200 48.53800	C 29.84600 -22.19100 43.97600	P 28.17700 -21.78800 46.23800
C 30.52300 -22.87900 47.33100	C 26.35800 -21.98600 46.57600	
C 28.43600 -22.47400 44.55400	C 25.46800 -21.45700 45.44800	

Atoms and radius in the parameter file

H 1.29	N3 1.81	P 2.11
C2 1.99	N 1.81	S 2.10
C3 1.99	O 1.78	Cl 2.05
C 1.99	F 1.72	Br 2.16
N2 1.81	Si 2.45	

Coordinates scaled to put the metal at the origin

C 0.06956 -2.99761 1.22483	C -0.82744 -4.13361 -1.96017	C -4.92944 -1.76861 -0.48917
C -0.48244 -4.40661 1.47183	C -0.81444 -4.46161 -3.45917	C -5.26044 -1.05561 0.82683
C 0.21856 -5.06661 2.67383	C 0.53556 -4.10861 -4.10017	C -4.39544 -1.57461 1.93683
C 1.71456 -5.09461 2.48883	C 0.93256 -2.67161 -3.81417	C -2.91844 -1.45361 1.59583
C 2.28156 -3.69361 2.23883	C 0.91656 -2.36261 -2.32317	P -0.75244 -1.95961 -0.06117
C 1.59356 -3.05061 1.03183	C -2.57144 -2.15761 0.27683	XX 0.00000 0.00000 0.00000
C -0.49344 -2.64561 -1.74517	C -3.46144 -1.62861 -0.85117	

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Results : Volumes in Angs^3

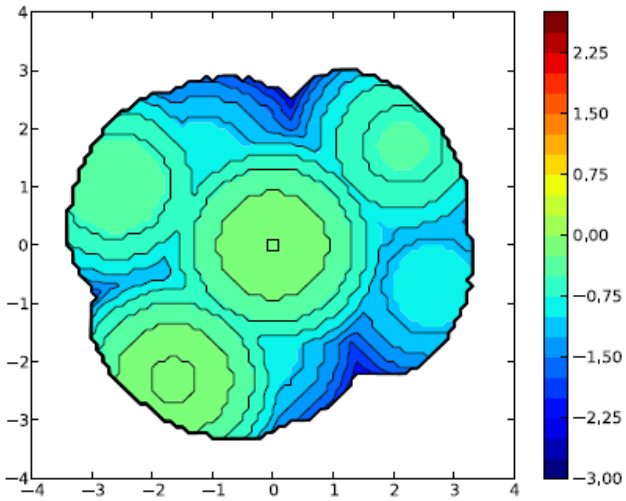
N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
116.367	63.168	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
64.816	35.184	99.967

The $\%V_{Bur}$ of *PCy₃* is: **35.2**

Steric map of PCy_3 in the complex $[PdCl_2(IPr)\{PCy_3\}]$ (2b)



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%V_{Bur} of IPr in the complex [$PdCl_2$(IPr){P(*o*-tolyl)$_3$}] (2c)

Number of atoms : 29
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 28 29

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C	4.86400	93.57400 -1.31700	C	6.23900	94.88500 2.29100	C	1.62900	93.70800 -0.37000
C	5.35100	95.76900 -1.05600	C	6.82900	92.54300 2.62900	C	2.74200	93.76500 -4.05700
C	4.03300	95.67800 -1.23800	C	7.86200	94.82500 -3.21100	C	2.39800	95.16900 -4.58400
C	7.25200	94.18800 -0.81300	C	8.14900	96.36800 -3.36300	C	2.55400	92.72800 -5.16500
C	7.59200	93.78100 0.48900	C	8.61700	94.05000 -4.25400	C	2.11300	94.18300 0.97700
C	8.92900	93.58800 0.75100	C	2.39200	93.80600 -1.53900	C	1.52100	95.56000 1.29900
C	9.86200	93.78100 -0.17100	C	1.91600	93.47800 -2.79400	C	1.76700	93.20200 2.14100
C	9.54900	94.22600 -1.45000	C	0.61400	92.95700 -2.87800	N	5.86000	94.47800 -1.08900
C	8.20300	94.39300 -1.79500	C	-0.13100	92.81000 -1.73500	N	3.73500	94.32100 -1.40400
C	6.55200	93.59800 1.59000	C	0.32500	93.19900 -0.50500			

Atoms and radius in the parameter file

H	1.29	N3	1.81	P	2.11
C2	1.99	N	1.81	S	2.10
C3	1.99	O	1.78	Cl	2.05
C	1.99	F	1.72	Br	2.16
N2	1.81	Si	2.45		

Coordinates scaled to put the metal at the origin

C	-0.16802	2.08568 0.17812	C	1.20698	3.39668 3.78612	C	-3.40302	2.21968 1.12512
C	0.31898	4.28068 0.43912	C	1.79698	1.05468 4.12412	C	-2.29002	2.27668 -2.56188
C	-0.99902	4.18968 0.25712	C	2.82998	3.33668 -1.71588	C	-2.63402	3.68068 -3.08888
C	2.21998	2.69968 0.68212	C	3.11698	4.87968 -1.86788	C	-2.47802	1.23968 -3.66988
C	2.55998	2.29268 1.98412	C	3.58498	2.56168 -2.75888	C	-2.91902	2.69468 2.47212
C	3.89698	2.09968 2.24612	C	-2.64002	2.31768 -0.04388	C	-3.51102	4.07168 2.79412
C	4.82998	2.29268 1.32412	C	-3.11602	1.98968 -1.29888	C	-3.26502	1.71368 3.63612
C	4.51698	2.73768 0.04512	C	-4.41802	1.46868 -1.38288	N	0.82798	2.98968 0.40612
C	3.17098	2.90468 -0.29988	C	-5.16302	1.32168 -0.23988	N	-1.29702	2.83268 0.09112
C	1.51998	2.10968 3.08512	C	-4.70702	1.71068 0.99012	XX	0.00000	0.00000 0.00000

Results : Volumes in Angs^3

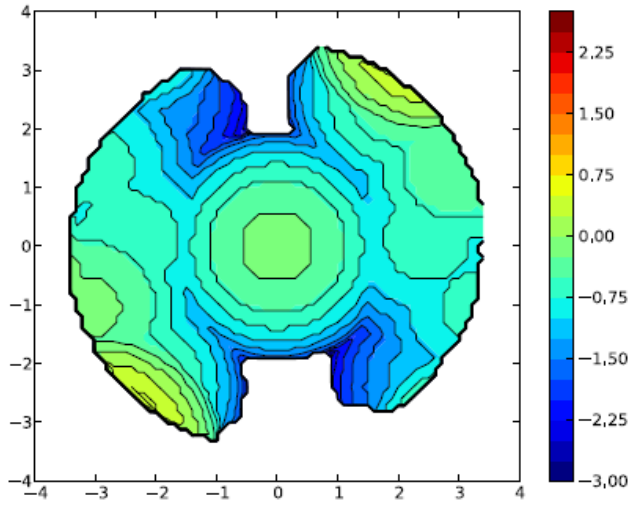
N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
120.563	58.972	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
67.153	32.847	99.967

The %V_{Bur} of your *IPr* is: **32.8**

Steric map of IPr in the complex [$PdCl_2$(IPr){P(*o*-tolyl)$_3$}] (2c)



%V_{Bur} of P(*o*-tolyl)$_3$ in the complex [PdCl$_2$(IPr){P(*o*-tolyl)$_3$}] (2c)

Number of atoms : 22
Atom that is coordinated : 22
Atoms that define the axis : 3
ID of these atoms : 1 8 15

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C 5.09900 88.10900 -0.56700	C 7.98400 87.70000 -2.11400	C 2.85800 88.51500 -4.82000
C 5.72100 88.15900 0.70500	C 9.38300 87.61700 -2.14200	C 3.58700 87.92700 -5.78400
C 5.30900 87.24600 1.67300	C 10.19500 88.76100 -2.13700	C 4.93700 87.71400 -5.57800
C 4.33600 86.27400 1.39700	C 9.60600 89.98000 -2.14700	C 5.52600 88.13900 -4.40600
C 3.73300 86.22600 0.15400	C 8.21100 90.10900 -2.08900	C 2.52600 89.58900 -2.55100
C 4.10700 87.13300 -0.81400	C 7.19700 86.40200 -2.05000	P 5.59000 89.28700 -1.86700
C 6.83100 89.13400 1.04100	C 4.76900 88.71300 -3.39600	
C 7.37900 88.96200 -2.07300	C 3.39900 88.93600 -3.58200	

Atoms and radius in the parameter file

H 1.29	N3 1.81	P 2.11
C2 1.99	N 1.81	S 2.10
C3 1.99	O 1.78	Cl 2.05
C 1.99	F 1.72	Br 2.16
N2 1.81	Si 2.45	

Coordinates scaled to put the metal at the origin

C -0.03045 -3.18337 0.88000	C 2.85455 -3.59237 -0.66700	C -2.27145 -2.77737 -3.37300
C 0.59155 -3.13337 2.15200	C 4.25355 -3.67537 -0.69500	C -1.54245 -3.36537 -4.33700
C 0.17955 -4.04637 3.12000	C 5.06555 -2.53137 -0.69000	C -0.19245 -3.57837 -4.13100
C -0.79345 -5.01837 2.84400	C 4.47655 -1.31237 -0.70000	C 0.39655 -3.15337 -2.95900
C -1.39645 -5.06637 1.60100	C 3.08155 -1.18337 -0.64200	C -2.60345 -1.70337 -1.10400
C -1.02245 -4.15937 0.63300	C 2.06755 -4.89037 -0.60300	P 0.46055 -2.00537 -0.42000
C 1.70155 -2.15837 2.48800	C -0.36045 -2.57937 -1.94900	XX 0.00000 0.00000 0.00000
C 2.24955 -2.33037 -0.62600	C -1.73045 -2.35637 -2.13500	

Results : Volumes in Angs^3

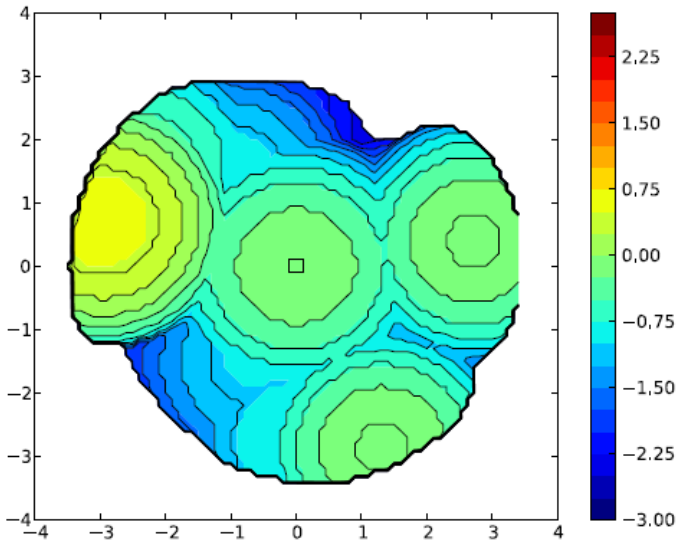
N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
109.594	69.941	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
61.043	38.957	99.967

The %V_Bur of *P(o-tolyl)$_3$* is: **39.0**

Steric map of P(*o*-tolyl)$_3$ in the complex [PdCl$_2$(IPr){P(*o*-tolyl)$_3$}] (2c)



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$\%V_{Bur}$ of IPr in the complex $[PdCl_2(IPr)\{P(1\text{-}Ad)_2(^nBu)\}]$ (2d)

Number of atoms : 29
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 28 29

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C 33.64000 -52.00100 -22.72600	C 30.86400 -54.34700 -19.69200	C 36.83500 -50.82400 -23.05600
C 32.63400 -50.32500 -21.62800	C 30.27000 -51.90800 -19.45900	C 35.56000 -52.83600 -20.05400
C 33.95900 -50.14400 -21.47500	C 31.27400 -50.80300 -24.94500	C 35.90100 -54.30800 -19.64200
C 31.20100 -52.05200 -22.71900	C 30.83400 -49.40000 -24.52500	C 35.64200 -51.93500 -18.83800
C 30.57800 -52.81800 -21.76900	C 30.97500 -51.04900 -26.42600	C 36.36500 -49.73400 -24.01300
C 29.38700 -53.52100 -22.17400	C 35.99800 -51.45400 -22.13000	C 36.51400 -48.35500 -23.36600
C 28.90700 -53.40200 -23.44500	C 36.48200 -52.33900 -21.16500	C 37.05000 -49.73200 -25.36700
C 29.53000 -52.52600 -24.34100	C 37.83600 -52.65200 -21.17600	N 32.46200 -51.46600 -22.38600
C 30.66000 -51.84200 -24.01300	C 38.67600 -52.10600 -22.13500	N 34.60100 -51.18000 -22.17600
C 31.03500 -52.93200 -20.32800	C 38.18200 -51.16900 -23.05400	

Atoms and radius in the parameter file

H 1.29	N3 1.81	P 2.11
C2 1.99	N 1.81	S 2.10
C3 1.99	O 1.78	Cl 2.05
C 1.99	F 1.72	Br 2.16
N2 1.81	Si 2.45	

Coordinates scaled to put the metal at the origin

C -0.27847 1.74012 1.14212	C -3.05447 -0.60588 4.17612	C 2.91653 2.91712 0.81212
C -1.28447 3.41612 2.24012	C -3.64847 1.83312 4.40912	C 1.64153 0.90512 3.81412
C 0.04053 3.59712 2.39312	C -2.64447 2.93812 -1.07688	C 1.98253 -0.56688 4.22612
C -2.71747 1.68912 1.14912	C -3.08447 4.34112 -0.65688	C 1.72353 1.80612 5.03012
C -3.34047 0.92312 2.09912	C -2.94347 2.69212 -2.55788	C 2.44653 4.00712 -0.14488
C -4.53147 0.22012 1.69412	C 2.07953 2.28712 1.73812	C 2.59553 5.38612 0.50212
C -5.01147 0.33912 0.42312	C 2.56353 1.40212 2.70312	C 3.13153 4.00912 -1.49888
C -4.38847 1.21512 -0.47288	C 3.91753 1.08912 2.69212	N -1.45647 2.27512 1.48212
C -3.25847 1.89912 -0.14488	C 4.75753 1.63512 1.73312	N 0.68253 2.56112 1.69212
C -2.88347 0.80912 3.54012	C 4.26353 2.57212 0.81412	XX 0.00000 0.00000 0.00000

Results : Volumes in Angs^3

N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
119.878	59.657	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
66.771	33.229	99.967

The $\%V_{Bur}$ of your *IPr* is: **33.2**

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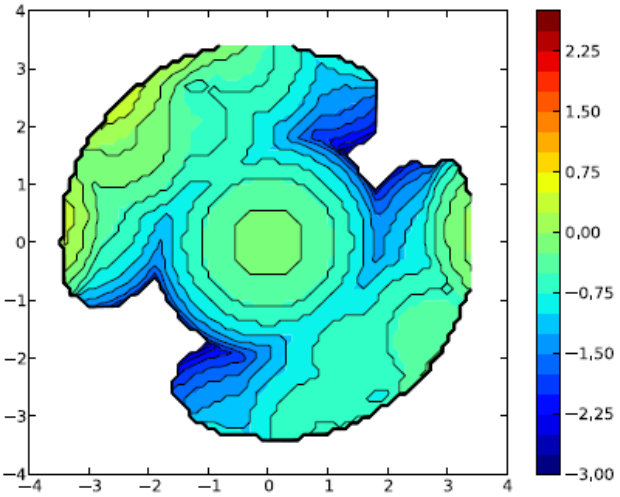
Steric map of IPr in the complex [$PdCl_2$(IPr){P(1-Ad)$_2$(^{n}Bu)}] (2d)



%V_{Bur} of P(1-Ad)$_2$(^{n}Bu) in the complex [$PdCl_2$(IPr){P(1-Ad)$_2$(^{n}Bu)}] (2d)

Number of atoms : 25
Atom that is coordinated : 25
Atoms that define the axis : 3
ID of these atoms : 1 11 21

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C 36.16200 -55.33200 -26.23800	C 39.10000 -55.72700 -26.47700	C 31.03000 -57.92400 -27.06900
C 35.92800 -54.59900 -27.57900	C 33.11800 -56.01700 -26.25200	C 31.98700 -56.50400 -25.29000
C 37.23500 -54.43600 -28.33700	C 33.38900 -57.13400 -27.25600	C 34.87300 -57.00500 -24.17500
C 37.86000 -55.84600 -28.63800	C 32.10200 -57.44600 -28.03200	C 36.03000 -56.90900 -23.14200
C 38.09600 -56.53700 -27.34200	C 31.58700 -56.22400 -28.77000	C 35.90900 -58.02100 -22.07600
C 36.80800 -56.69400 -26.56300	C 31.22800 -55.16100 -27.75800	C 37.03900 -58.02800 -21.07800
C 37.16400 -54.51300 -25.42500	C 32.52600 -54.78900 -26.97900	P 34.59000 -55.51000 -25.21100
C 38.48800 -54.34600 -26.18800	C 30.22200 -55.59900 -26.80800	
C 38.23400 -53.64000 -27.48700	C 30.69900 -56.81900 -26.06600	

Atoms and radius in the parameter file

H 1.29	N3 1.81	P 2.11
C2 1.99	N 1.81	S 2.10
C3 1.99	O 1.78	Cl 2.05
C 1.99	F 1.72	Br 2.16
N2 1.81	Si 2.45	

Coordinates scaled to put the metal at the origin

C 1.94953 -1.61996 -2.04426	C 4.02153 0.07204 -3.29326	C -3.99047 -1.88696 -2.61426
C 1.71553 -0.88696 -3.38526	C 4.88753 -2.01496 -2.28326	C -3.51347 -3.10696 -1.87226
C 3.02253 -0.72396 -4.14326	C -1.09447 -2.30496 -2.05826	C -3.18247 -4.21196 -2.87526
C 3.64753 -2.13396 -4.44426	C -0.82347 -3.42196 -3.06226	C -2.22547 -2.79196 -1.09626
C 3.88353 -2.82496 -3.14826	C -2.11047 -3.73396 -3.83826	C 0.66053 -3.29296 0.01874
C 2.59553 -2.98196 -2.36926	C -2.62547 -2.51196 -4.57626	C 1.81753 -3.19696 1.05174
C 2.95153 -0.80096 -1.23126	C -2.98447 -1.44896 -3.56426	C 1.69653 -4.30896 2.11774
C 4.27553 -0.63396 -1.99426	C -1.68647 -1.07696 -2.78526	C 2.82653 -4.31596 3.11574

P 0.37753 -1.79796 -1.01726 XX 0.00000 0.00000 0.00000

Results : Volumes in Angs^3

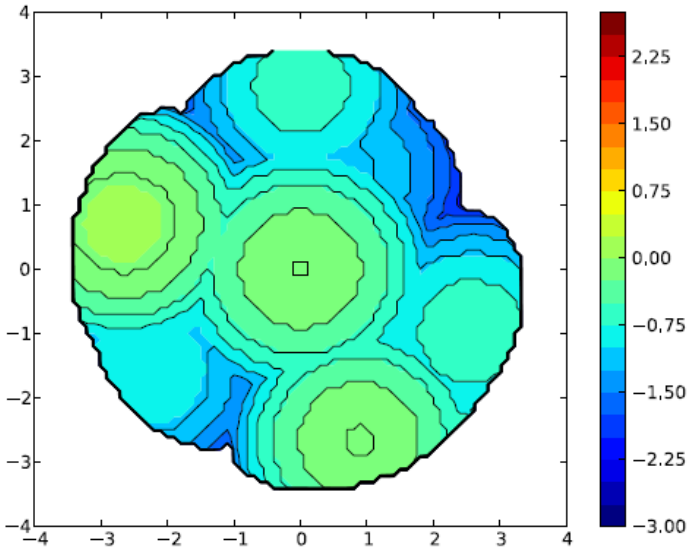
N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
112.694	66.841	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
62.770	37.230	99.967

The $\%V_{Bur}$ of *P(1-Ad)$_2$(^{n}Bu)* is: **37.2**

Steric map of P(1-Ad)$_2$(^{n}Bu) in the complex [PdCl$_2$(IPr){P(1-Ad)$_2$(^{n}Bu)}] (2d)



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%V_{Bur} of IPr in the complex [$PdCl_2$(IPr){PCy_2(*o*-biphenyl)}] (2e)

Number of atoms : 29
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 28 29

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C	-39.80152	-49.83545	74.11914	C	-35.99912	-47.00196	72.90656	C	-42.46197	-50.37678	72.16213
C	-39.48735	-47.60674	74.14079	C	-35.45581	-49.32563	72.15288	C	-42.77617	-49.21929	75.80434
C	-40.69742	-47.83274	73.63158	C	-39.00773	-49.28685	77.31137	C	-43.52409	-47.88385	75.81817
C	-37.67944	-49.03971	75.13805	C	-39.29553	-47.84393	77.74631	C	-43.14937	-50.02185	77.03665
C	-36.48215	-48.92130	74.43201	C	-39.01454	-50.20342	78.54939	C	-41.58137	-50.17034	70.95295
C	-35.31306	-49.16516	75.13802	C	-42.16214	-49.86871	73.41856	C	-42.16124	-49.02454	70.10977
C	-35.32333	-49.49326	76.45969	C	-43.03696	-49.93626	74.50047	C	-41.40327	-51.42461	70.12345
C	-36.51945	-49.56887	77.14661	C	-44.22182	-50.63299	74.30505	N	-38.93789	-48.83934	74.45015
C	-37.72186	-49.32829	76.51093	C	-44.52666	-51.19836	73.10535	N	-40.88726	-49.20694	73.64140
C	-36.41723	-48.48219	72.98848	C	-43.66885	-51.06478	72.03018				

Atoms and radius in the parameter file

H	1.29	N3	1.81	P	2.11
C2	1.99	N	1.81	S	2.10
C3	1.99	O	1.78	Cl	2.05
C	1.99	F	1.72	Br	2.16
N2	1.81	Si	2.45	I	2.31

Coordinates scaled to put the metal at the origin

C	-0.28332	2.07236	-0.18717	C	3.51908	4.90585	-1.39975	C	-2.94377	1.53103	-2.14418
C	0.03085	4.30107	-0.16552	C	4.06239	2.58218	-2.15343	C	-3.25797	2.68852	1.49803
C	-1.17922	4.07507	-0.67473	C	0.51047	2.62096	3.00506	C	-4.00589	4.02396	1.51186
C	1.83876	2.86810	0.83174	C	0.22267	4.06388	3.44000	C	-3.63117	1.88596	2.73034
C	3.03605	2.98651	0.12570	C	0.50366	1.70439	4.24308	C	-2.06317	1.73747	-3.35336
C	4.20514	2.74265	0.83171	C	-2.64394	2.03910	-0.88775	C	-2.64304	2.88327	-4.19654
C	4.19487	2.41455	2.15338	C	-3.51876	1.97155	0.19416	C	-1.88507	0.48320	-4.18286
C	2.99875	2.33894	2.84030	C	-4.70362	1.27482	-0.00126	N	0.58031	3.06847	0.14384
C	1.79634	2.57952	2.20462	C	-5.00846	0.70945	-1.20096	N	-1.36906	2.70087	-0.66491
C	3.10097	3.42562	-1.31783	C	-4.15065	0.84303	-2.27613	XX	0.00000	0.00000	0.00000

Results : Volumes in Angs^3

N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
119.051	60.484	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
66.311	33.689	99.967

The %V_{Bur} of *IPr* is: **33.7**

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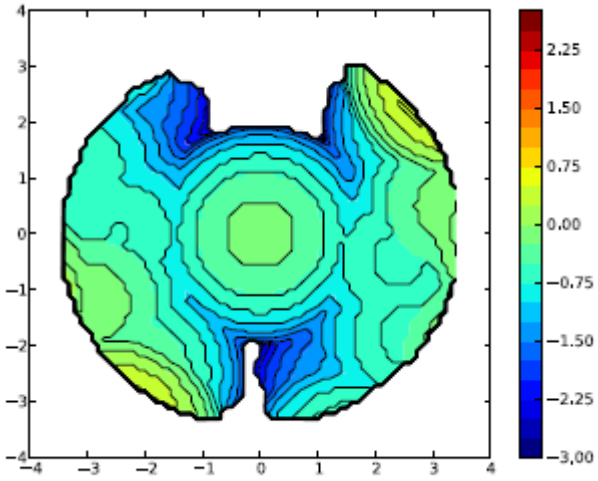
Steric map of IPr in the complex [$PdCl_2$(IPr){PCy_2(*o*-biphenyl)}] (2e)



%V_{Bur} of P(Cy)$_2$(*o*-biphenyl) in the complex [$PdCl_2$(IPr){PCy_2(*o*-biphenyl)}] (2e)

Number of atoms : 25
Atom that is coordinated : 25
Atoms that define the axis : 3
ID of these atoms : 1 7 13

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C -55.35469 -23.98032 81.03696	C -50.02273 -23.53634 80.60962	C -57.59245 -24.58891 78.81068
C -55.30685 -25.50879 81.17204	C -50.65397 -22.19631 80.24024	C -58.05544 -23.30886 79.03008
C -56.15339 -25.96150 82.35652	C -52.17753 -22.21217 80.41765	C -59.18775 -23.07970 79.79003
C -55.68915 -25.29906 83.63511	C -55.11768 -24.39275 78.12517	C -59.88820 -24.12384 80.33322
C -55.67613 -23.78766 83.51414	C -56.42953 -24.86870 77.92445	C -59.45148 -25.40177 80.09215
C -54.82131 -23.34039 82.32347	C -56.69089 -25.65612 76.80779	C -58.32118 -25.64517 79.34927
C -52.77708 -23.36687 79.59216	C -55.74184 -25.95381 75.86884	P -54.62379 -23.26750 79.50251
C -52.15467 -24.70376 79.99716	C -54.46706 -25.47236 76.04203	
C -50.64656 -24.66553 79.82151	C -54.15643 -24.71804 77.15119	

Atoms and radius in the parameter file

H 1.29	N3 1.81	P 2.11
C2 1.99	N 1.81	S 2.10
C3 1.99	O 1.78	Cl 2.05
C 1.99	F 1.72	Br 2.16
N2 1.81	Si 2.45	I 2.31

Coordinates scaled to put the metal at the origin

C -0.09372 -2.69779 1.78726	C 5.23824 -2.25381 1.35992	C -2.33148 -3.30638 -0.43902
C -0.04588 -4.22626 1.92234	C 4.60700 -0.91378 0.99054	C -2.79447 -2.02633 -0.21962
C -0.89242 -4.67897 3.10682	C 3.08344 -0.92964 1.16795	C -3.92678 -1.79717 0.54033
C -0.42818 -4.01653 4.38541	C 0.14329 -3.11022 -1.12453	C -4.62723 -2.84131 1.08352
C -0.41516 -2.50513 4.26444	C -1.16856 -3.58617 -1.32525	C -4.19051 -4.11924 0.84245
C 0.43966 -2.05786 3.07377	C -1.42992 -4.37359 -2.44191	C -3.06021 -4.36264 0.09957
C 2.48389 -2.08434 0.34246	C -0.48087 -4.67128 -3.38086	P 0.63718 -1.98497 0.25281
C 3.10630 -3.42123 0.74746	C 0.79391 -4.18983 -3.20767	XX 0.00000 0.00000 0.0000
C 4.61441 -3.38300 0.57181	C 1.10454 -3.43551 -2.09851	

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Results : Volumes in Angs^3

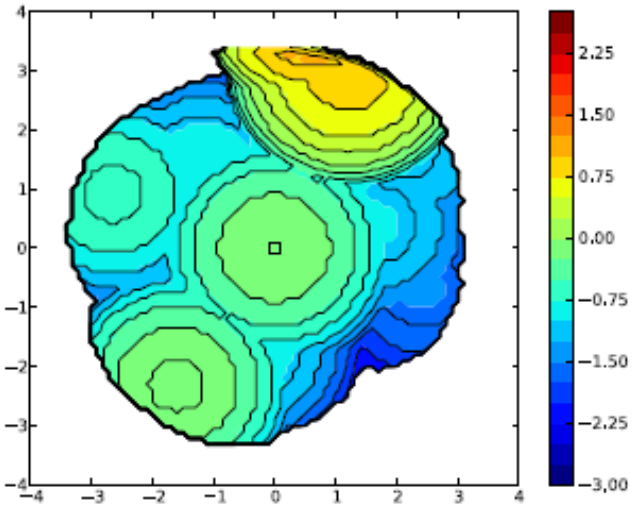
N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
111.235	68.300	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
61.957	38.043	99.967

The $\%V_{Bur}$ of *PCy_2(o-biphenyl)* is: **38.0**

Steric map of PCy_2(*o*-biphenyl) in the complex [$PdCl_2$(IPr){PCy_2(*o*-biphenyl)}] (2e)



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%V_{Bur} of IPr in the complex [$PdCl_2$(IPr)(XPhos)] (2f)

Number of atoms : 29
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 28 29

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C	-51.95100	30.63500	12.43200	C	-49.90900	32.61500	16.11700	C	-55.11800	31.16100	12.68000
C	-50.91600	32.59300	12.75600	C	-50.78400	30.41000	16.93800	C	-53.43500	32.10600	9.32500
C	-52.15400	32.87100	12.32900	C	-48.90400	30.00300	10.98500	C	-53.49300	33.61400	9.13700
C	-49.63800	30.54500	13.36500	C	-48.49500	31.37800	10.44300	C	-53.60100	31.42000	7.97100
C	-49.47700	30.55200	14.76000	C	-48.13900	28.90500	10.24400	C	-54.78700	31.13200	14.16400
C	-48.34200	29.92500	15.27200	C	-54.16700	31.47800	11.70800	C	-54.84000	32.55800	14.74000
C	-47.43800	29.30800	14.43300	C	-54.47300	31.64900	10.35800	C	-55.68100	30.21500	14.98800
C	-47.62400	29.30900	13.06800	C	-55.80800	31.43200	9.97200	N	-50.80000	31.22600	12.82100
C	-48.72100	29.94100	12.48400	C	-56.75000	31.08000	10.89600	N	-52.78900	31.64500	12.13000
C	-50.45000	31.25200	15.69600	C	-56.42100	30.94700	12.22200				

Atoms and radius in the parameter file

H	1.29	N3	1.81	P	2.11
C2	1.99	N	1.81	S	2.10
C3	1.99	O	1.78	Cl	2.05
C	1.99	F	1.72	Br	2.16
N2	1.81	Si	2.45		

Coordinates scaled to put the metal at the origin

C	0.40236	2.05806	0.11184	C	2.44436	4.03806	3.79684	C	-2.76464	2.58406	0.35984
C	1.43736	4.01606	0.43584	C	1.56936	1.83306	4.61784	C	-1.08164	3.52906	-2.99516
C	0.19936	4.29406	0.00884	C	3.44936	1.42606	-1.33516	C	-1.13964	5.03706	-3.18316
C	2.71536	1.96806	1.04484	C	3.85836	2.80106	-1.87716	C	-1.24764	2.84306	-4.34916
C	2.87636	1.97506	2.43984	C	4.21436	0.32806	-2.07616	C	-2.43364	2.55506	1.84384
C	4.01136	1.34806	2.95184	C	-1.81364	2.90106	-0.61216	C	-2.48664	3.98106	2.41984
C	4.91536	0.73106	2.11284	C	-2.11964	3.07206	-1.96216	C	-3.32764	1.63806	2.66784
C	4.72936	0.73206	0.74784	C	-3.45464	2.85506	-2.34816	N	1.55336	2.64906	0.50084
C	3.63236	1.36406	0.16384	C	-4.39664	2.50306	-1.42416	N	-0.43564	3.06806	-0.19016
C	1.90336	2.67506	3.37584	C	-4.06764	2.37006	-0.09816	XX	0.00000	0.00000	0.00000

Results : Volumes in Angs^3

N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
118.768	60.767	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
66.153	33.847	99.967

The %V_{Bur} of *IPr* is: **33.8**

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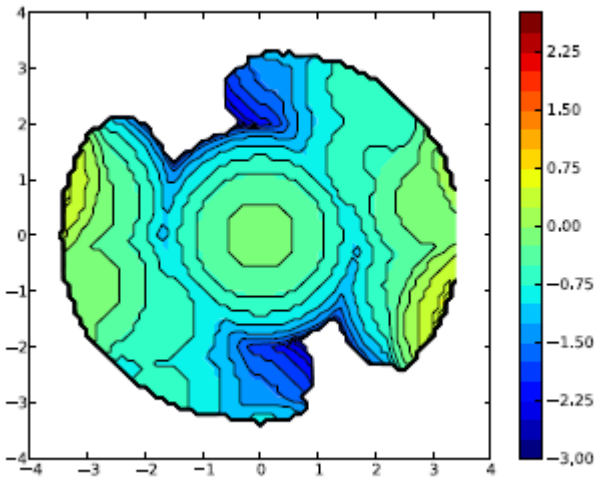
Steric map of IPr in the complex [$PdCl_2$(IPr)(XPhos)] (2f)



%V_{Bur} of XPhos in the complex [$PdCl_2$(IPr)(XPhos)] (2f)

Number of atoms : 34
Atom that is coordinated : 34
Atoms that define the axis : 3
ID of these atoms : 1 7 13

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C	-54.64900	26.10400	12.07300	C	-52.16700	25.63000	10.42700	C	-54.51500	26.71400	7.94600
C	-55.34900	27.33200	11.46400	C	-52.76900	24.81000	9.43800	C	-55.54900	27.81300	7.83100
C	-56.87400	27.13300	11.42700	C	-51.92800	24.24700	8.45300	C	-53.92800	26.42100	6.56700
C	-57.41000	26.85700	12.82100	C	-50.56600	24.46800	8.42100	C	-58.44900	23.60700	8.78600
C	-56.69800	25.67900	13.47200	C	-49.98700	25.32200	9.34600	C	-59.22300	24.34600	9.88400
C	-55.17600	25.87400	13.50400	C	-50.78700	25.89800	10.31300	C	-59.04000	23.89600	7.41400
C	-52.08400	25.33200	13.30600	C	-54.24300	24.52000	9.26900	C	-53.88500	22.21300	10.35500
C	-52.27900	23.82500	13.09200	C	-55.06400	25.43100	8.56600	C	-54.55700	21.60200	11.60000
C	-51.82600	23.03200	14.33500	C	-56.41100	25.09000	8.39100	C	-53.53700	21.11400	9.35000
C	-50.38100	23.35400	14.68600	C	-56.95100	23.90900	8.88300	P	-52.82700	26.37300	11.97000
C	-50.17100	24.86500	14.83700	C	-56.10900	23.02100	9.50500				
C	-50.61300	25.64000	13.59200	C	-54.75800	23.29000	9.69600				

Atoms and radius in the parameter file

H	1.29	N3	1.81	P	2.11
C2	1.99	N	1.81	S	2.10
C3	1.99	O	1.78	Cl	2.05
C	1.99	F	1.72	Br	2.16
N2	1.81	Si	2.45		

Coordinates scaled to put the metal at the origin

C	-2.24142	-2.32405	-0.00110	C	0.32358	-3.09605	1.23190	C	0.24058	-2.79805	-1.64710
C	-2.94142	-1.09605	-0.61010	C	0.12858	-4.60305	1.01790	C	-0.36142	-3.61805	-2.63610
C	-4.46642	-1.29505	-0.64710	C	0.58158	-5.39605	2.26090	C	0.47958	-4.18105	-3.62110
C	-5.00242	-1.57105	0.74690	C	2.02658	-5.07405	2.61190	C	1.84158	-3.96005	-3.65310
C	-4.29042	-2.74905	1.39790	C	2.23658	-3.56305	2.76290	C	2.42058	-3.10605	-2.72810
C	-2.76842	-2.55405	1.42990	C	1.79458	-2.78805	1.51790	C	1.62058	-2.53005	-1.76110

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C	-1.83542	-3.90805	-2.80510	C	-2.10742	-1.71405	-4.12810	C	-1.47742	-6.21505	-1.71910
C	-2.65642	-2.99705	-3.50810	C	-3.14142	-0.61505	-4.24310	C	-2.14942	-6.82605	-0.47410
C	-4.00342	-3.33805	-3.68310	C	-1.52042	-2.00705	-5.50710	C	-1.12942	-7.31405	-2.72410
C	-4.54342	-4.51905	-3.19110	C	-6.04142	-4.82105	-3.28810	P	-0.41942	-2.05505	-0.10410
C	-3.70142	-5.40705	-2.56910	C	-6.81542	-4.08205	-2.19010	XX	0.00000	0.00000	0.00000
C	-2.35042	-5.13805	-2.37810	C	-6.63242	-4.53205	-4.66010				

Results : Volumes in Angs^3

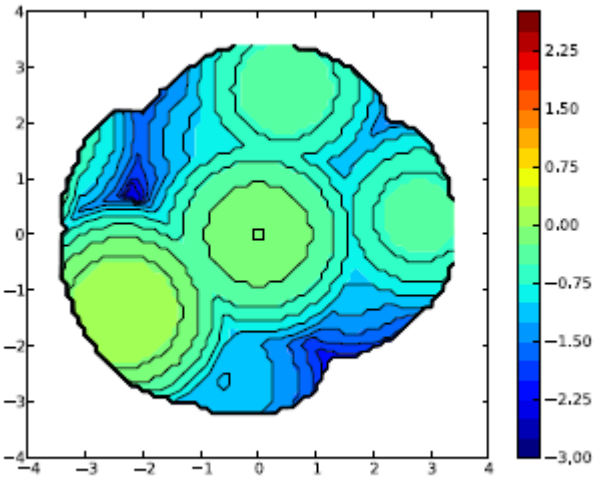
N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
114.484	65.050	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
63.767	36.233	99.967

The $\%V_{Bur}$ of XPhos is: **36.2**

Steric map of XPhos in the complex [$PdCl_2$(IPr)(XPhos)] (2f)



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%V_{Bur} of IPr in the complex [$PdCl_2$(IPr)(SPhos)] (2g)

Number of atoms : 29
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 28 29

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C	23.18300	82.64000	11.32200	C	21.14000	82.20000	7.27100	C	26.22200	83.80800	10.47400
C	22.11200	84.60300	11.63000	C	20.89100	84.51300	8.25300	C	25.32000	83.06900	14.14700
C	23.41600	84.83400	11.81700	C	20.24400	82.49700	13.51700	C	25.86200	81.82800	14.88800
C	20.71000	82.65100	11.01000	C	19.84900	81.33300	14.42300	C	25.36500	84.28900	15.04100
C	20.35000	82.51300	9.66800	C	19.60800	83.79100	14.05200	C	25.52800	83.99100	9.14800
C	19.11400	81.93800	9.40100	C	25.50700	83.54000	11.65700	C	26.34400	83.49000	7.95800
C	18.26800	81.54000	10.41600	C	26.10500	83.34500	12.89700	C	25.11500	85.45400	8.87700
C	18.64200	81.71600	11.72900	C	27.52800	83.46300	12.91700	N	21.98000	83.26200	11.32800
C	19.87200	82.27100	12.06600	C	28.21300	83.75300	11.76000	N	24.06400	83.62600	11.59600
C	21.22700	83.03600	8.53900	C	27.59000	83.92800	10.57100				

Atoms and radius in the parameter file

H	1.29	N3	1.81	P	2.11
C2	1.99	N	1.81	S	2.10
C3	1.99	O	1.78	Cl	2.05
C	1.99	F	1.72	Br	2.16
N2	1.81	Si	2.45		

Coordinates scaled to put the metal at the origin

C	-0.40645	2.02975	0.35344	C	-2.44945	1.58975	-3.69756	C	2.63255	3.19775	-0.49456
C	-1.47745	3.99275	0.66144	C	-2.69845	3.90275	-2.71556	C	1.73055	2.45875	3.17844
C	-0.17345	4.22375	0.84844	C	-3.34545	1.88675	2.54844	C	2.27255	1.21775	3.91944
C	-2.87945	2.04075	0.04144	C	-3.74045	0.72275	3.45444	C	1.77555	3.67875	4.07244
C	-3.23945	1.90275	-1.30056	C	-3.98145	3.18075	3.08344	C	1.93855	3.38075	-1.82056
C	-4.47545	1.32775	-1.56756	C	1.91755	2.92975	0.68844	C	2.75455	2.87975	-3.01056
C	-5.32145	0.92975	-0.55256	C	2.51555	2.73475	1.92844	C	1.52555	4.84375	-2.09156
C	-4.94745	1.10575	0.76044	C	3.93855	2.85275	1.94844	N	-1.60945	2.65175	0.35944
C	-3.71745	1.66075	1.09744	C	4.62355	3.14275	0.79144	N	0.47455	3.01575	0.62744
C	-2.36245	2.42575	-2.42956	C	4.00055	3.31775	-0.39756	XX	0.00000	0.00000	0.00000

Results : Volumes in Angs^3

N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
121.493	58.042	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
67.671	32.329	99.967

The %V_{Bur} of *IPr* is: **32.3**

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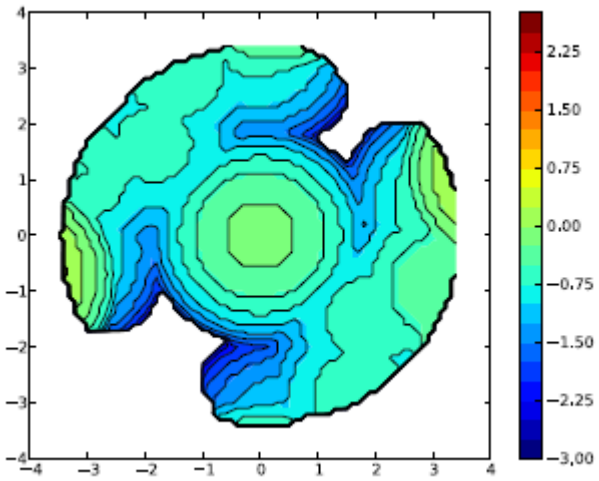
Steric map of IPr in the complex [$PdCl_2$(IPr)(SPhos)] (2g)



%V_{Bur} of SPhos in the complex [$PdCl_2$(IPr)(SPhos)] (2g)

Number of atoms : 29
Atom that is coordinated : 29
Atoms that define the axis : 3
ID of these atoms : 1 7 13

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C 24.10300 77.38600 12.30100	C 19.96400 78.13100 8.83300	C 22.29700 74.00200 8.25500
C 25.45300 77.81500 12.89000	C 21.33200 78.64400 9.27300	C 21.48000 74.52700 7.28000
C 25.68200 77.12000 14.23000	C 24.92100 77.78900 9.54100	C 21.74500 75.73700 6.67800
C 25.62900 75.60300 14.08000	C 24.87300 76.80100 8.54700	C 22.84900 76.48300 7.11600
C 24.31100 75.17200 13.49000	C 26.02900 76.53200 7.81200	C 24.11700 73.02800 10.20100
C 24.05200 75.86400 12.14900	C 27.22200 77.21100 8.02600	C 22.34400 78.30700 5.65100
C 21.96800 77.70800 10.29900	C 27.26600 78.19800 8.98000	O 24.35900 74.26600 9.52400
C 21.04200 77.57100 11.51600	C 26.13200 78.49100 9.72100	O 23.21900 77.67800 6.58400
C 19.68200 77.02700 11.06700	C 23.67300 76.01000 8.13400	P 23.65100 78.31800 10.77400
C 19.04500 77.91700 10.01100	C 23.42700 74.73800 8.65100	

Atoms and radius in the parameter file

H 1.29	N3 1.81	P 2.11
C2 1.99	N 1.81	S 2.10
C3 1.99	O 1.78	Cl 2.05
C 1.99	F 1.72	Br 2.16
N2 1.81	Si 2.45	

Coordinates scaled to put the metal at the origin

C 0.49139 -3.02366 1.34419	C -3.64761 -2.27866 -2.12381	C -1.31461 -6.40766 -2.70181
C 1.84139 -2.59466 1.93319	C -2.27961 -1.76566 -1.68381	C -2.13161 -5.88266 -3.67681
C 2.07039 -3.28966 3.27319	C 1.30939 -2.62066 -1.41581	C -1.86661 -4.67266 -4.27881
C 2.01739 -4.80666 3.12319	C 1.26139 -3.60866 -2.40981	C -0.76261 -3.92666 -3.84081
C 0.69939 -5.23766 2.53319	C 2.41739 -3.87766 -3.14481	C 0.50539 -7.38166 -0.75581
C 0.44039 -4.54566 1.19219	C 3.61039 -3.19866 -2.93081	C -1.26761 -2.10266 -5.30581
C -1.64361 -2.70166 -0.65781	C 3.65439 -2.21166 -1.97681	O 0.74739 -6.14366 -1.43281
C -2.56961 -2.83866 0.55919	C 2.52039 -1.91866 -1.23581	O -0.39261 -2.73166 -4.37281
C -3.92961 -3.38266 0.11019	C 0.06139 -4.39966 -2.82281	P 0.03939 -2.09166 -0.18281
C -4.56661 -2.49266 -0.94581	C -0.18461 -5.67166 -2.30581	XX 0.00000 0.00000 0.00000

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Results : Volumes in Angs^3

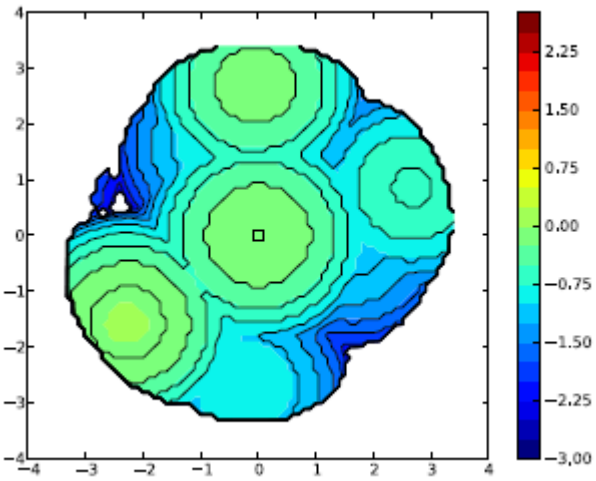
N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
115.621	63.913	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
64.401	35.599	99.967

The $\%V_{Bur}$ of *SPhos* is: **35.6**

Steric map of SPhos in the complex [$PdCl_2$(IPr)(SPhos)] (2g)



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%V_{Bur} of IPr [Pd(IPr)(SPhos)] (6)

Number of atoms : 29
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 28 29

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C	5.15500	39.13900 -62.43100	C	2.92800	42.41100 -65.44500	C	8.33100	38.78300 -63.36000
C	5.15100	41.36600 -61.85800	C	3.55600	39.98200 -65.90800	C	7.04000	37.90000 -59.83700
C	6.41600	40.94800 -61.75300	C	2.73900	39.70600 -59.96100	C	7.83800	38.24900 -58.58100
C	2.96400	40.29400 -62.43800	C	1.91300	40.29300 -58.85400	C	6.36200	36.54200 -59.66900
C	2.48200	40.63700 -63.68600	C	2.96300	38.19800 -59.76200	C	7.87900	39.59800 -64.56100
C	1.08800	40.55900 -63.86900	C	7.58100	38.74900 -62.19300	C	9.04600	40.31200 -65.22500
C	0.26400	40.17300 -62.83200	C	7.88900	37.94200 -61.08100	C	7.15000	38.67000 -65.54000
C	0.77900	39.91500 -61.58800	C	9.02100	37.13400 -61.19300	N	4.40100	40.26700 -62.24000
C	2.15300	39.97300 -61.35900	C	9.80300	37.14800 -62.34700	N	6.40800	39.60500 -62.09000
C	3.39200	41.08600 -64.82100	C	9.45700	37.95400 -63.41100			

Atoms and radius in the parameter file

H	1.29	N3	1.81	P	2.11
C2	1.99	N	1.81	S	2.10
C3	1.99	O	1.78	Cl	2.05
C	1.99	F	1.72	Br	2.16
N2	1.81	Si	2.45		

Coordinates scaled to put the metal at the origin

C	0.59779	1.90957 0.63732	C	-1.00121	2.75257 -2.83968	C	3.28079	1.01957 4.48732
C	0.59379	4.13657 1.21032	C	-1.81821	2.47657 3.10732	C	1.80479	-0.68743 3.39932
C	1.85879	3.71857 1.31532	C	-2.64421	3.06357 4.21432	C	3.32179	2.36857 -1.49268
C	-1.59321	3.06457 0.63032	C	-1.59421	0.96857 3.30632	C	4.48879	3.08257 -2.15668
C	-2.07521	3.40757 -0.61768	C	3.02379	1.51957 0.87532	C	2.59279	1.44057 -2.47168
C	-3.46921	3.32957 -0.80068	C	3.33179	0.71257 1.98732	N	-0.15621	3.03757 0.82832
C	-4.29321	2.94357 0.23632	C	4.46379	-0.09543 1.87532	N	1.85079	2.37557 0.97832
C	-3.77821	2.68557 1.48032	C	5.24579	-0.08143 0.72132	XX	0.00000	0.00000 0.00000
C	-2.40421	2.74357 1.70932	C	4.89979	0.72457 -0.34268			
C	-1.16521	3.85657 -1.75268	C	3.77379	1.55357 -0.29168			
C	-1.62921	5.18157 -2.37668	C	2.48279	0.67057 3.23132			

Results : Volumes in Angs^3

N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
100.743	78.791	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
56.114	43.886	99.967

The %V_{Bur} of *IPr* is: **43.9**

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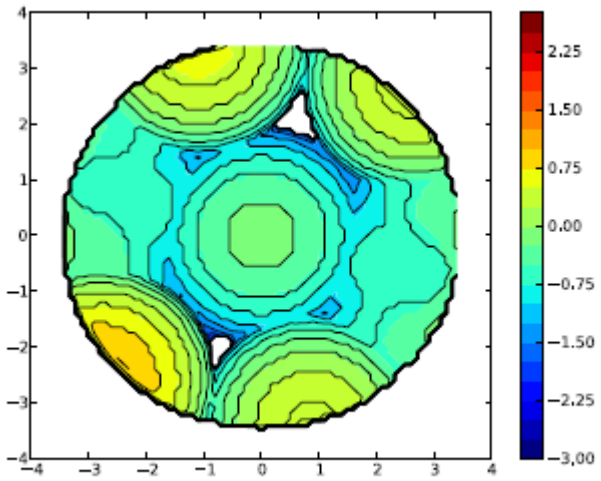
Steric map of IPr [Pd(IPr)(SPhos)] (6)



%V_{Bur} of SPhos of [Pd(IPr)(SPhos)] (6)

Number of atoms : 29
Atom that is coordinated : 29
Atoms that define the axis : 3
ID of these atoms : 1 7 13

Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.100
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

C	3.23500	34.05700 -62.90000	C	7.74200	32.79600 -62.62300	C	6.56600	31.60700 -67.01600
C	1.80300	34.28500 -63.38200	C	6.44300	33.60200 -62.48800	C	5.98000	30.48200 -66.44300
C	0.81800	33.40200 -62.60900	C	3.77600	35.15100 -65.51300	C	4.70600	30.52000 -65.93900
C	0.89800	33.64800 -61.12500	C	3.80700	34.17400 -66.52600	C	3.99400	31.71400 -65.97200
C	2.31000	33.45400 -60.59500	C	3.06900	34.36200 -67.67600	C	7.60200	33.92600 -68.22900
C	3.30500	34.30900 -61.38900	C	2.29200	35.48700 -67.88200	C	1.96000	30.62100 -65.37200
C	6.01000	34.14900 -63.84300	C	2.25100	36.46100 -66.91100	O	6.32100	33.95900 -67.57500
C	7.13700	35.01200 -64.43700	C	2.98900	36.31100 -65.75200	O	2.71200	31.83900 -65.52000
C	8.46200	34.22400 -64.56100	C	4.58400	32.87600 -66.48200	P	4.45800	35.15900 -63.78300
C	8.86700	33.64600 -63.20500	C	5.85400	32.79400 -67.03300			

Atoms and radius in the parameter file

H	1.29	N3	1.81	P	2.11
C2	1.99	N	1.81	S	2.10
C3	1.99	O	1.78	Cl	2.05
C	1.99	F	1.72	Br	2.16
N2	1.81	Si	2.45		

Coordinates scaled to put the metal at the origin

C	-1.54078	-3.01049 0.06649	C	1.66722	-3.46549 0.47849	C	-0.06978	-6.54749 -2.97251
C	-2.97278	-2.78249 -0.41551	C	-0.99978	-1.91649 -2.54651	C	-0.78178	-5.35349 -3.00551
C	-3.95778	-3.66549 0.35749	C	-0.96878	-2.89349 -3.55951	C	2.82622	-3.14149 -5.26251
C	-3.87778	-3.41949 1.84149	C	-1.70678	-2.70549 -4.70951	C	-2.81578	-6.44649 -2.40551
C	-2.46578	-3.61349 2.37149	C	-2.48378	-1.58049 -4.91551	O	1.54522	-3.10849 -4.60851
C	-1.47078	-2.75849 1.57749	C	-2.52478	-0.60649 -3.94451	O	-2.06378	-5.22849 -2.55351
C	1.23422	-2.91849 -0.87651	C	-1.78678	-0.75649 -2.78551	P	-0.31778	-1.90849 -0.81651
C	2.36122	-2.05549 -1.47051	C	-0.19178	-4.19149 -3.51551	XX	0.00000	0.00000 0.00000
C	3.68622	-2.84349 -1.59451	C	1.07822	-4.27349 -4.06651			
C	4.09122	-3.42149 -0.23851	C	1.79022	-5.46049 -4.04951			
C	2.96622	-4.27149 0.34349	C	1.20422	-6.58549 -3.47651			

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Results : Volumes in Angs^3

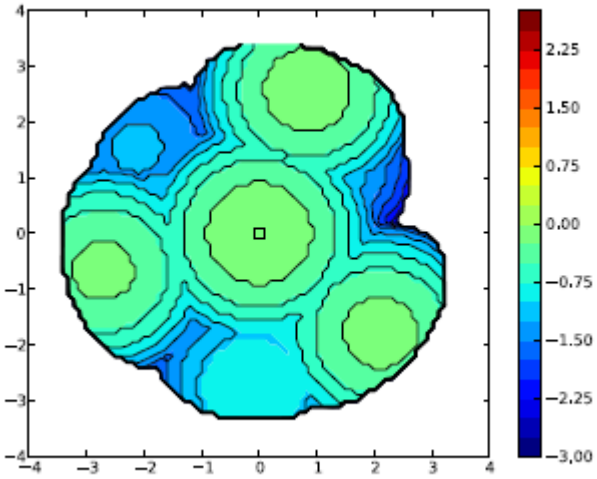
N of voxels examined : 1436277
Volume of voxel : 0.125E-03

V Free	V Buried	V Total	V Exact
114.350	65.184	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
63.693	36.307	99.967

The $\%V_{Bur}$ of *SPhos* is: **36.3**

Steric map of SPhos of [Pd(IPr)(SPhos)] (6)



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