Palladium(II) complexes with chelating N-phosphanyl acyclic diaminocarbenes: synthesis, characterization and catalytic activity in Suzuki couplings

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Supporting Information

Crystallographic parameters of the compounds **2a**-**2d** and **3c** p. 2

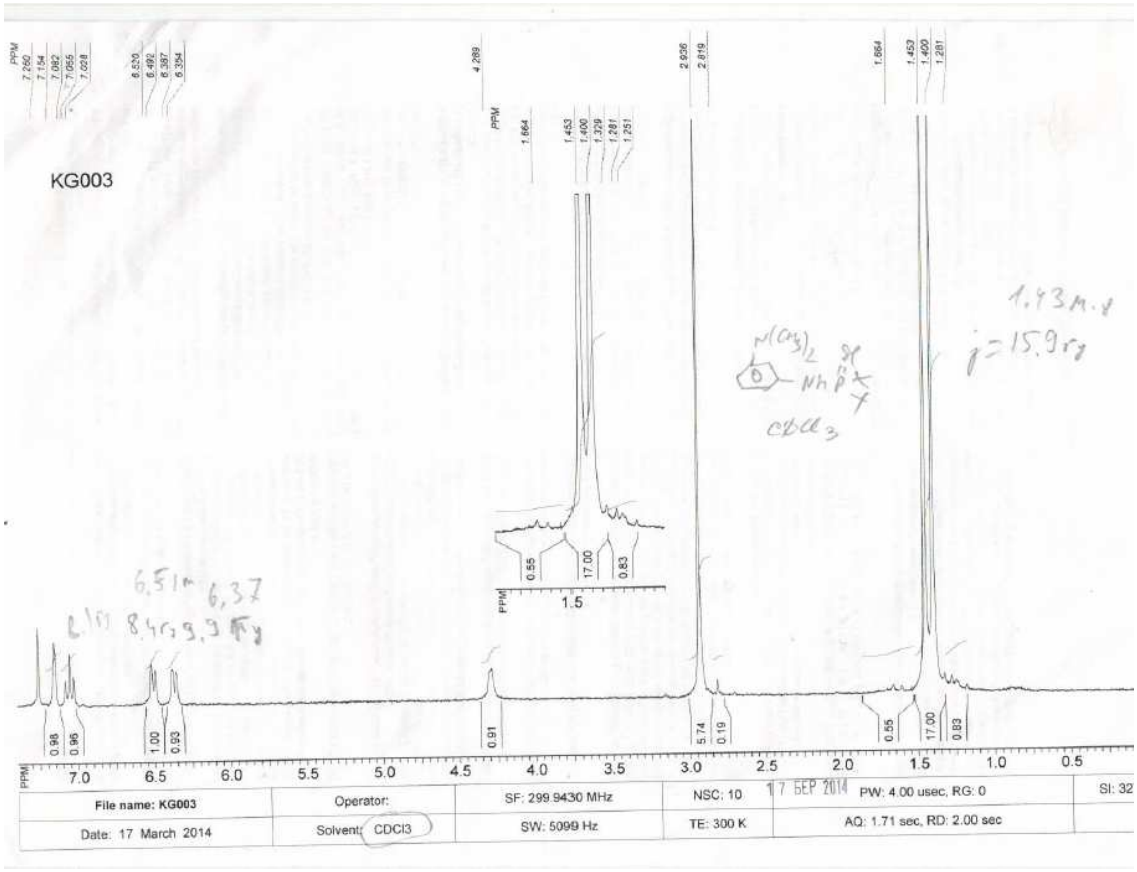
Copies of spectra of new compounds pp. 3-24

Table S1. Main crystallographic parameters of the compounds **2a**-**2d** and **3c**.

Compound	**2a**	**2b**	**2c**	**2d**	**3c**
Cell Parameters					
a[Å]	10.126(1)	10.249(1)	15.5317(3)	12.6614(3)	8.2299(2)
b[Å]	13.713(2)	12.257(2)	10.2561(2)	15.7007(3)	16.7796(3)
c[Å]	17.539(1)	19.524(3)	33.1968(6)	16.8900(4)	9.6743(2)
α[°]	90	90	90	90	90
β[°]	90	90	92.109(1)	90	103.954(1)
γ[°]	90	90	90	90	90
V[Å^3]	2435.6(5)	2452.7(6)	5284.5(2)	3357.6(1)	1296.54(5)
Z	4	4	4	4	2
D[g·cm^{-3}]	1.434	1.462	1.449	1.418	1.424
Crystal system	Orthorhombic	Orthorhombic	Monoclinic	Orthorhombic	Monoclinic
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_1/n$	$P2_12_12_1$	$P2_1$
μ[cm^{-1}]	1.056	1.051	0.984	0.802	0.999
F(000)	1088	1120	2392	1480	576
Indexes	$12 \geq h \geq -11$ $15 \geq k \geq -16$ $21 \geq l \geq -19$	$10 \geq h \geq -12$ $13 \geq k \geq -15$ $24 \geq l \geq -19$	$16 \geq h \geq -19$ $12 \geq k \geq -12$ $37 \geq l \geq -41$	$14 \geq h \geq -15$ $17 \geq k \geq -19$ $21 \geq l \geq -18$	$10 \geq h \geq -10$ $21 \geq k \geq -19$ $12 \geq l \geq -11$
θ_{max} [°]	26.3	26.4	26.4	26.4	26.6
No. of reflections:					
collected	14061	24875	42280	15793	15750
independent	4854	5027	10769	6840	5091
in refinement ($I \geq 3\sigma(I)$)	4053	3839	8616	6167	4950
R(int)	0.054	0.092	0.045	0.032	0.026
No. of refined parameters	245	254	550	362	263
Obsd./var.	16.5	15.1	15.7	17.0	18.8
Final *R* indices					
R_1(F)	0.033	0.072	0.033	0.027	0.016
R_w(F)	0.027	0.055	0.039	0.022	0.017
GOF	1.033	1.037	1.068	1.111	1.103

Weighting coefficients	0.614 -0.699 0.135 -0.278	3.39 -1.67 2.76	1.54 0.489 1.26	0.206 -0.678 -0.102 -0.249	1.26 -0.440 1.32 -0.128 0.412
Largest peak/hole [$e \cdot cm^{-3}$]	0.55/-0.85	1.70/-2.09	0.51/-0.80	0.61/-0.56	0.31/-0.45
CCDC deposition number	1039693	1039694	1039696	1039695	1039692

P,P-Di-tert-butyl-N-(3-dimethylaminophenyl)phosphinoselenoic amide



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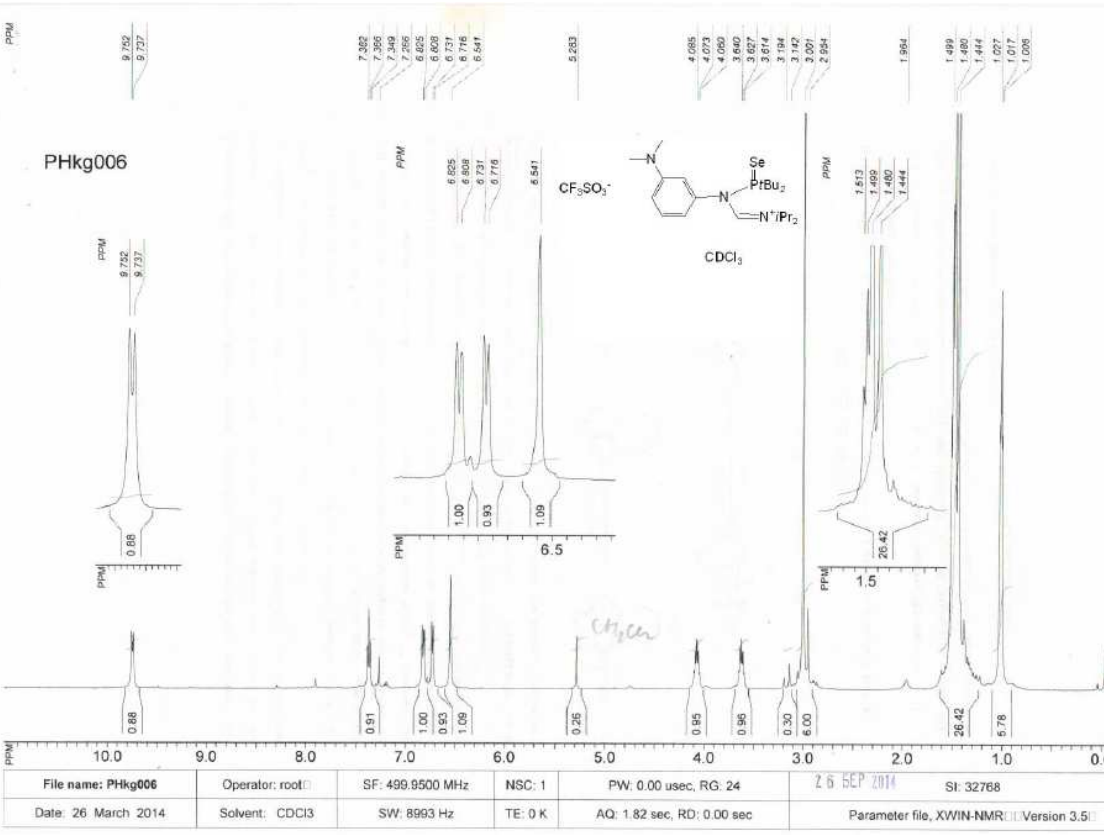

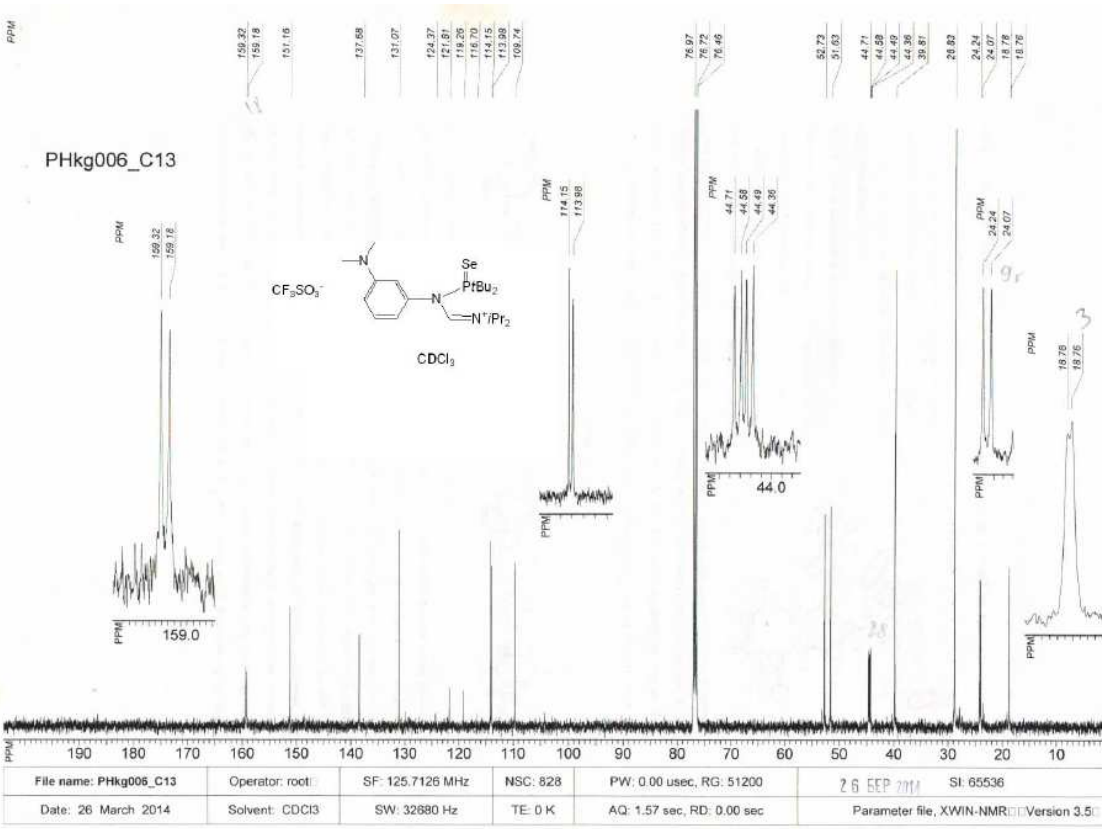

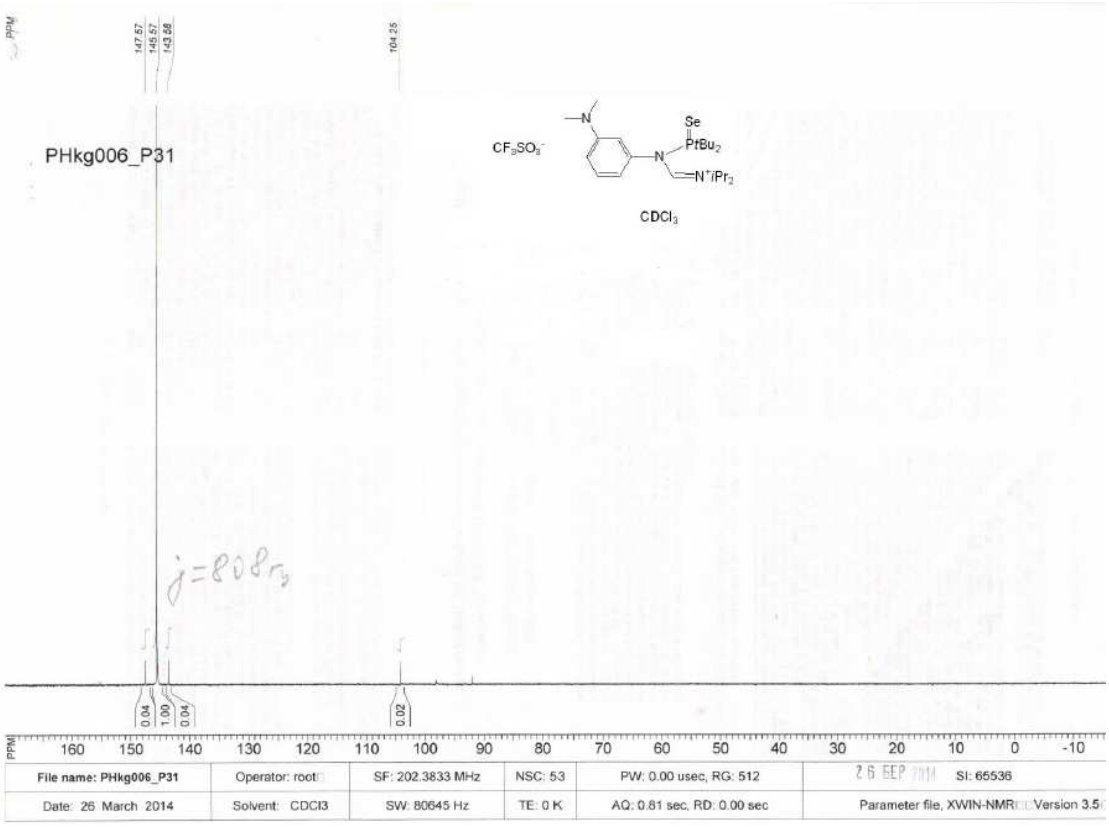
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Parameter file, XWIN-NMR Version 3.5

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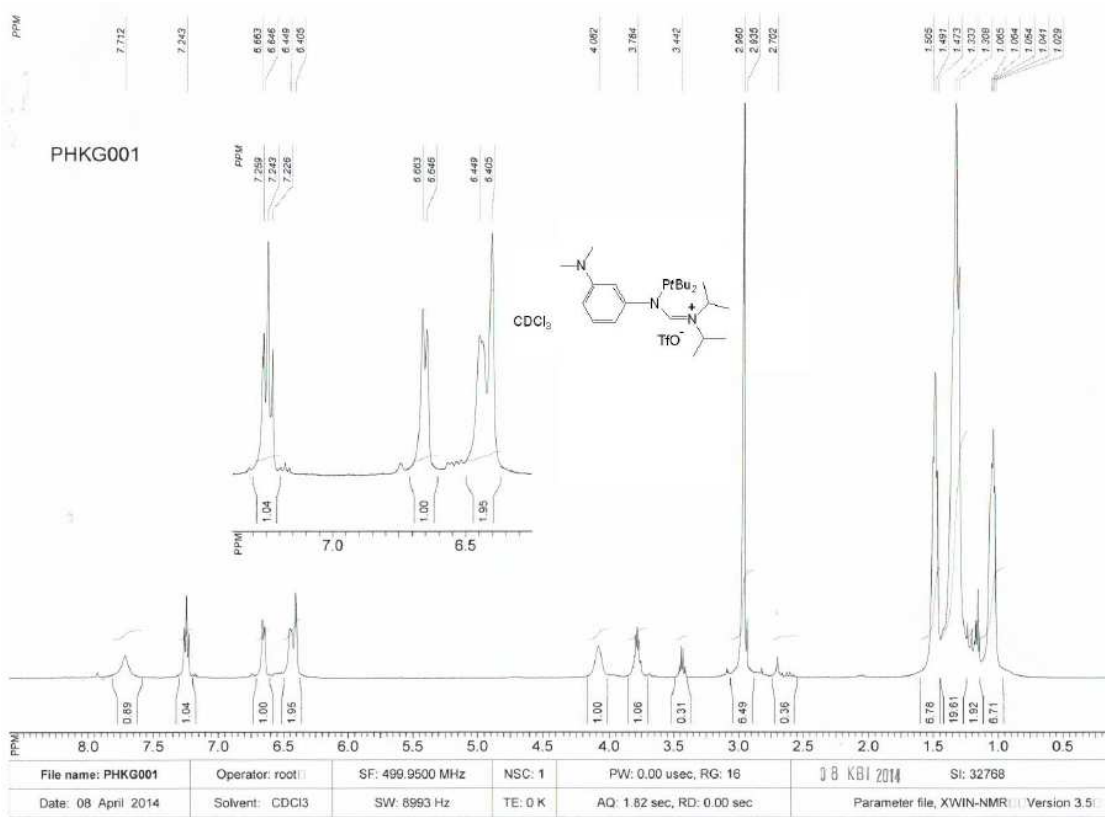

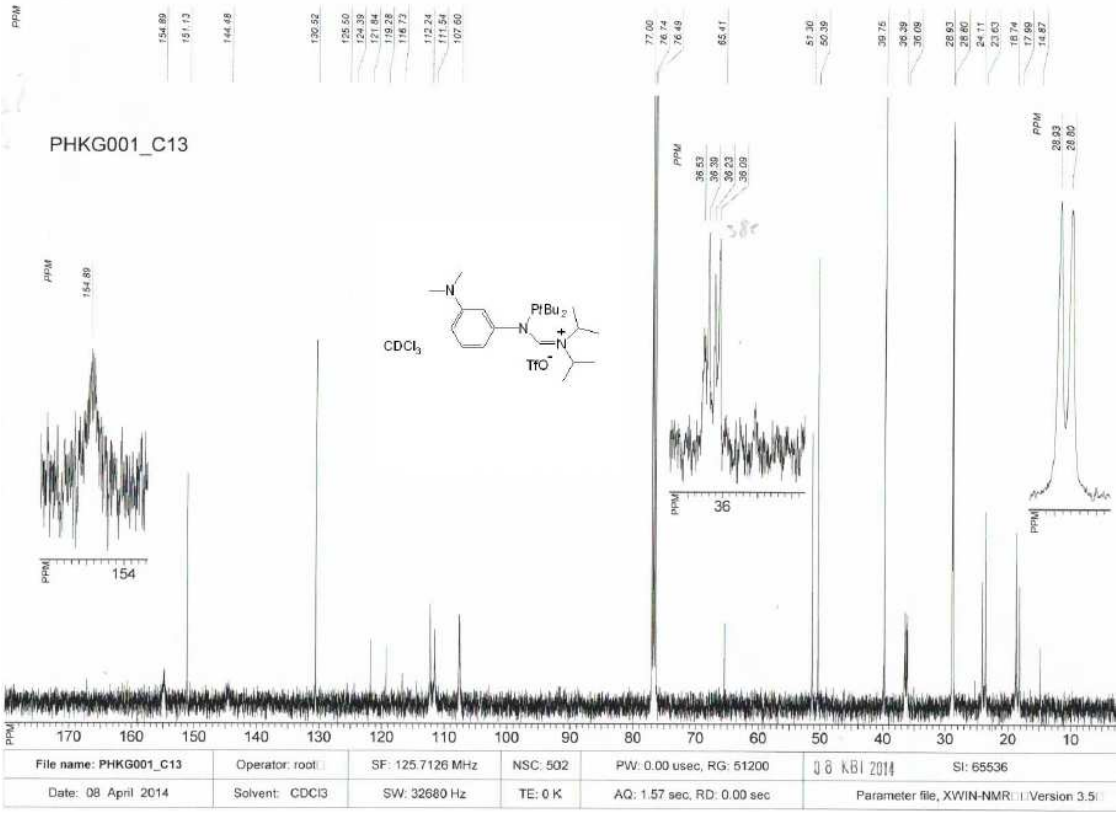

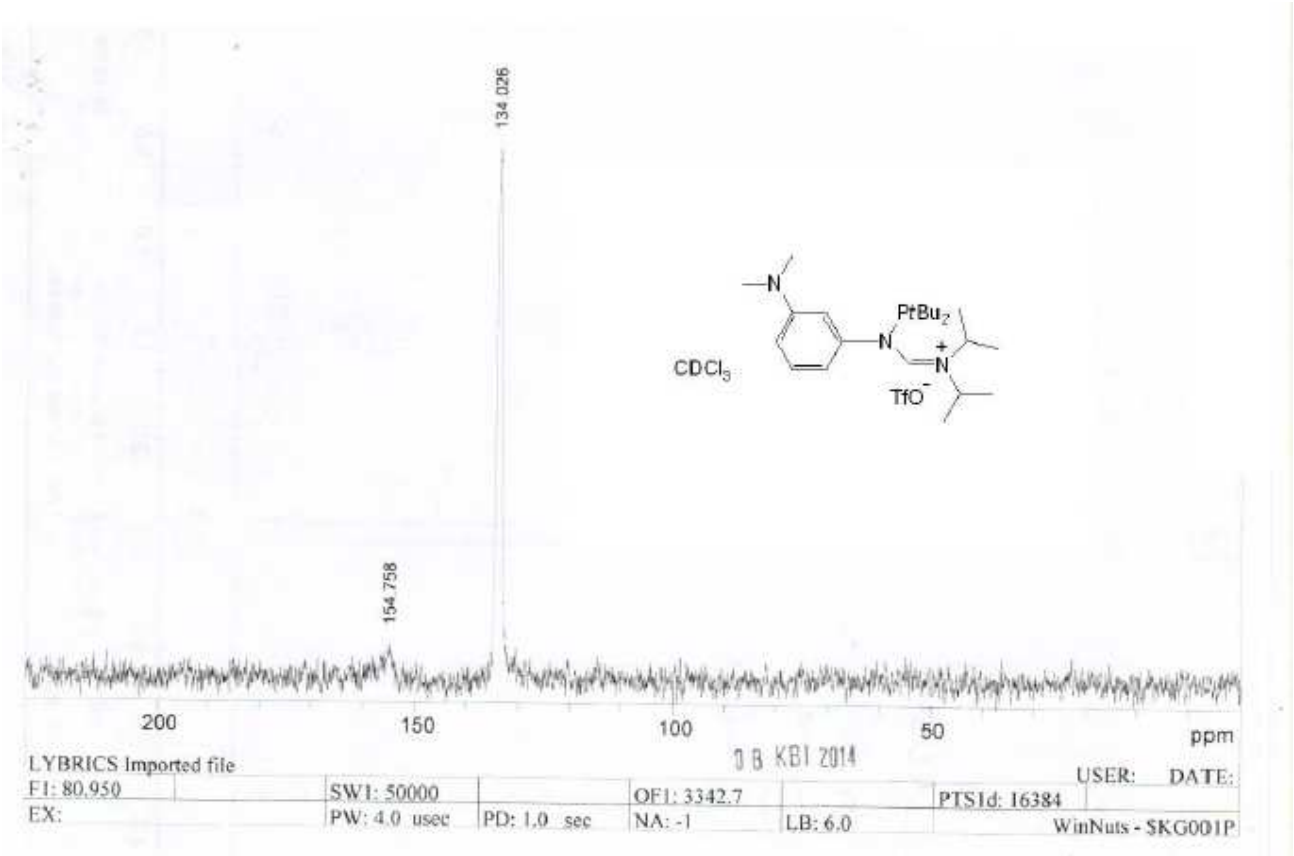
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50
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08 KBI 2014
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DATE:
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LB: 6.0
WinNuts - SKG001P

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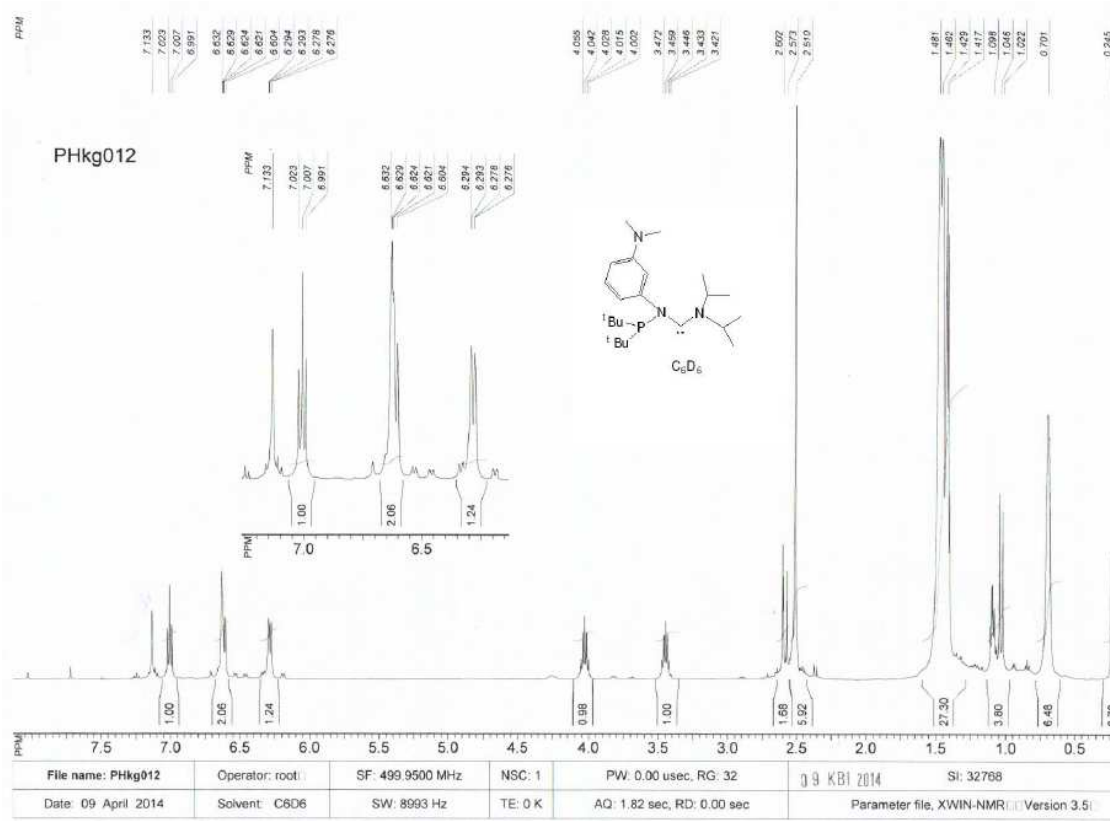

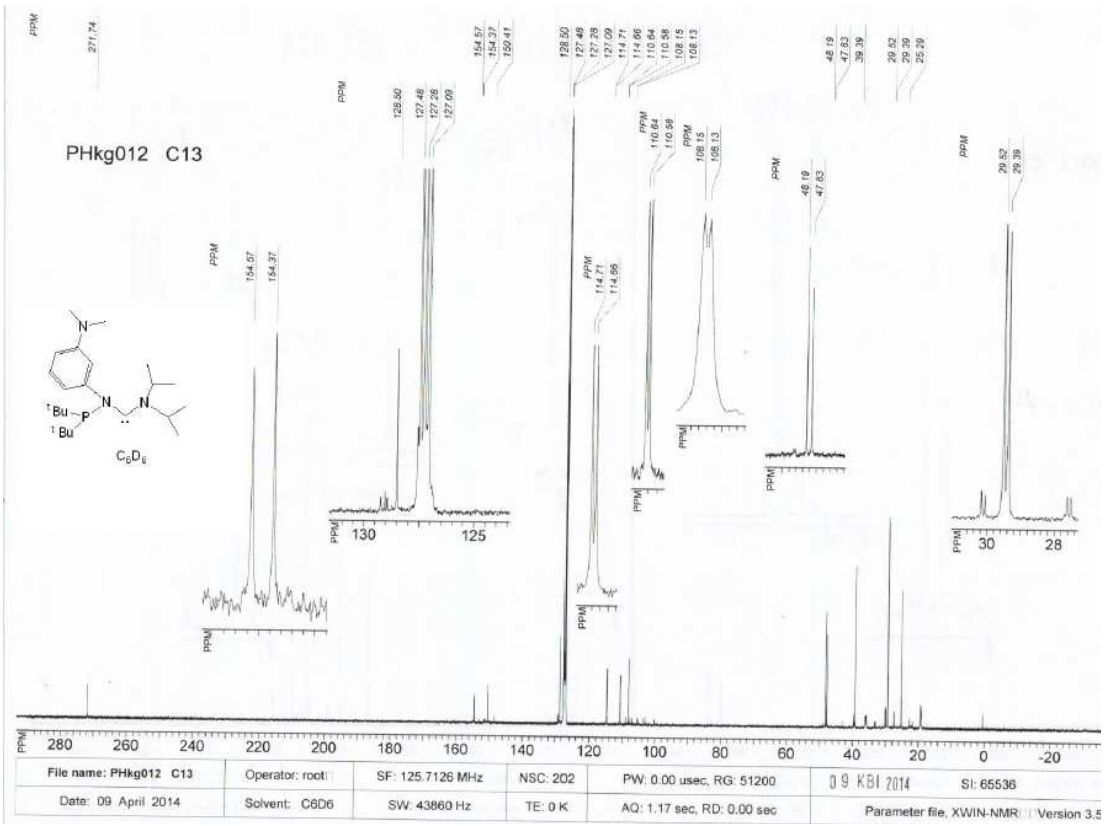

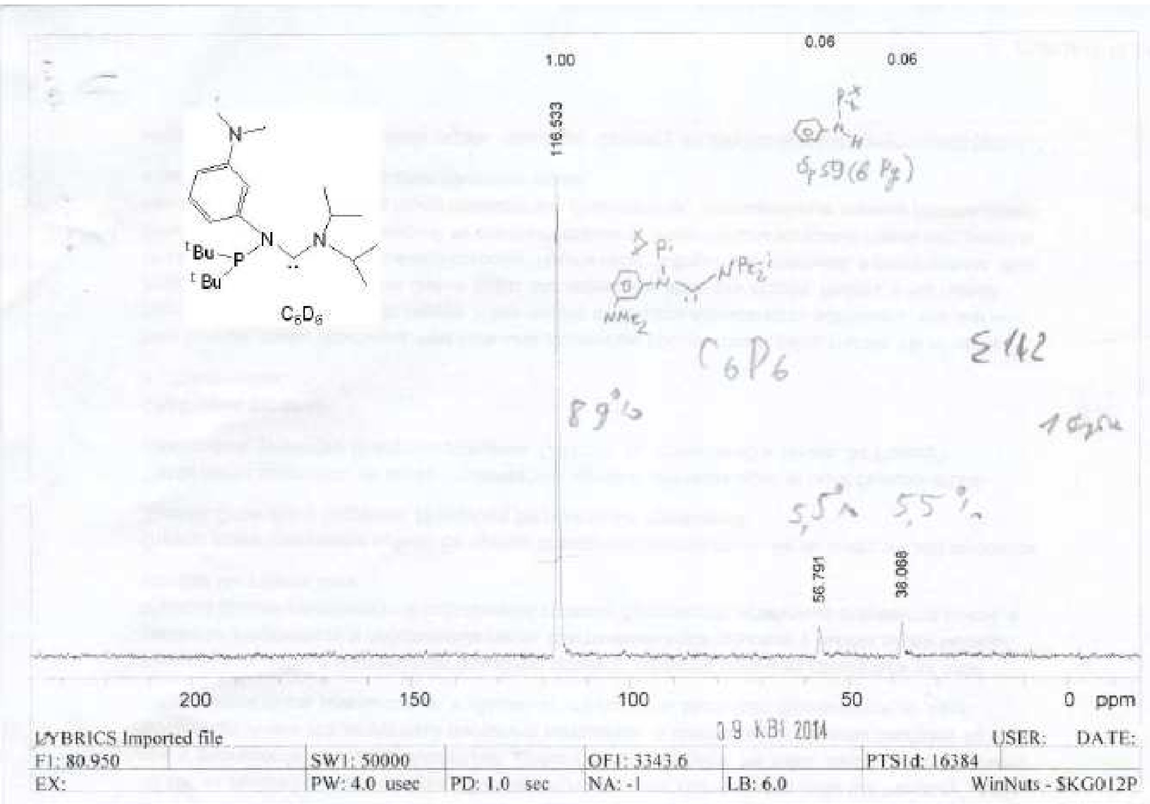

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38.068
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150
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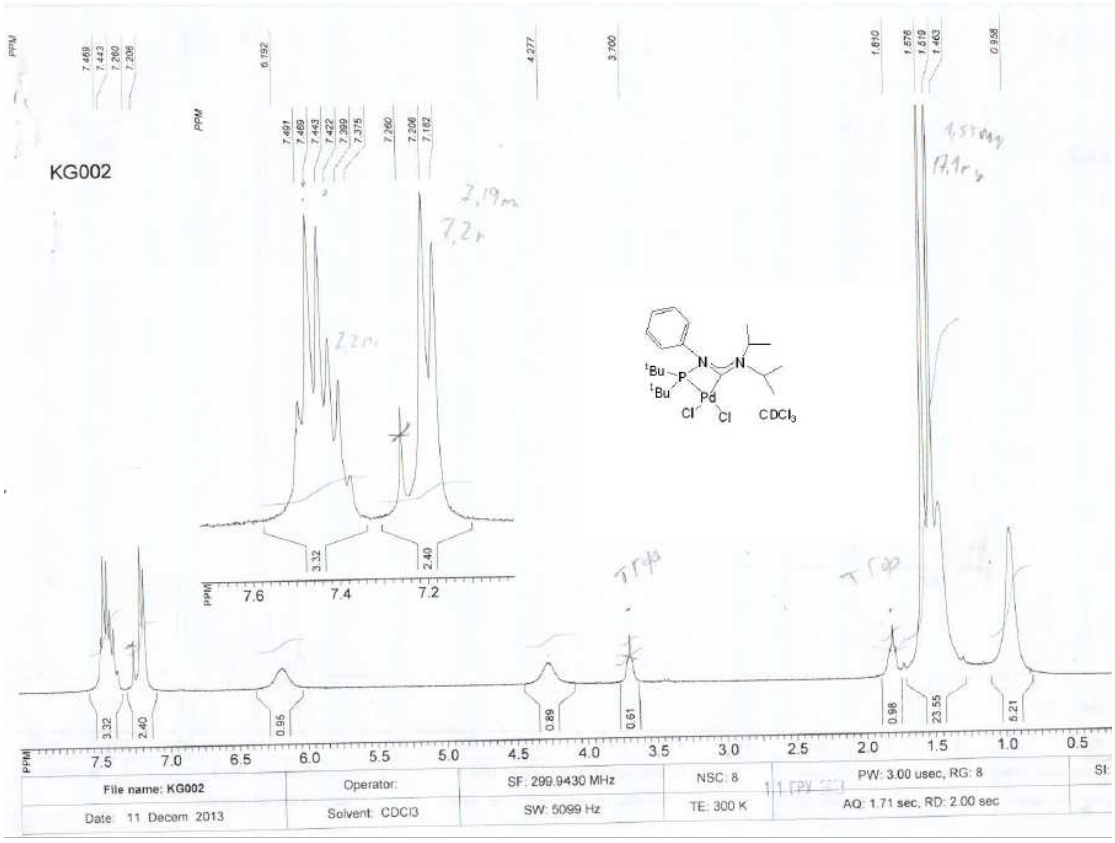
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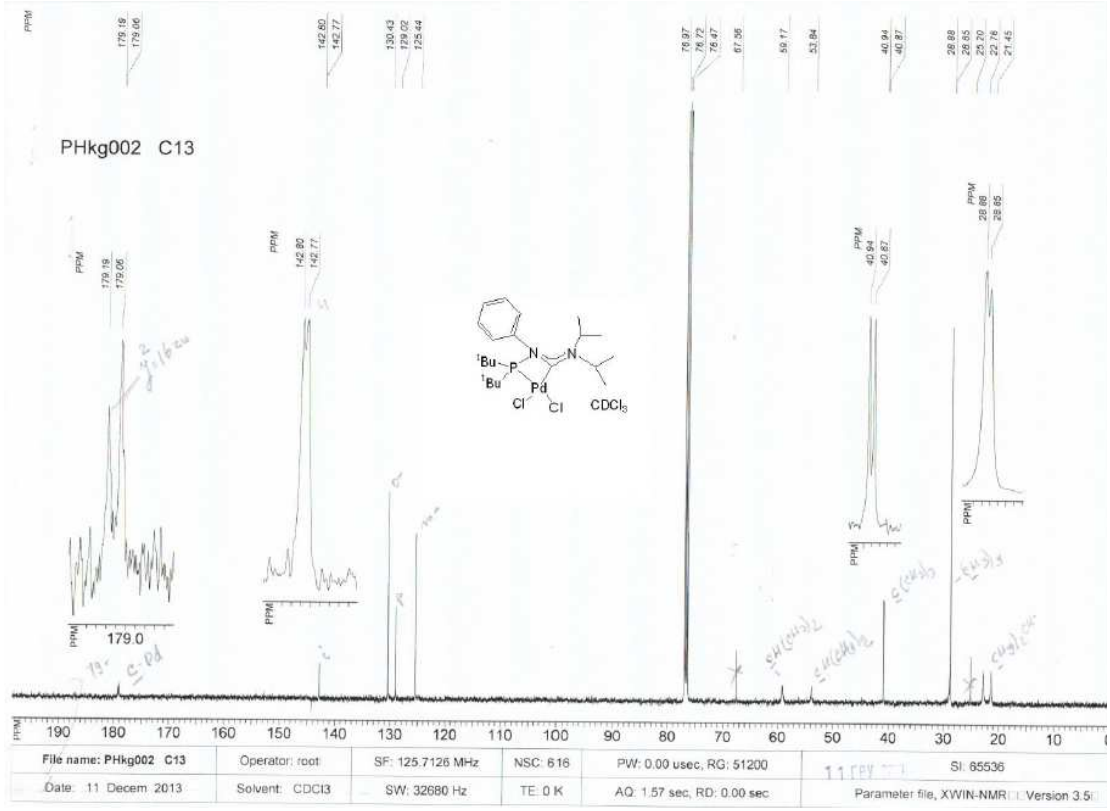
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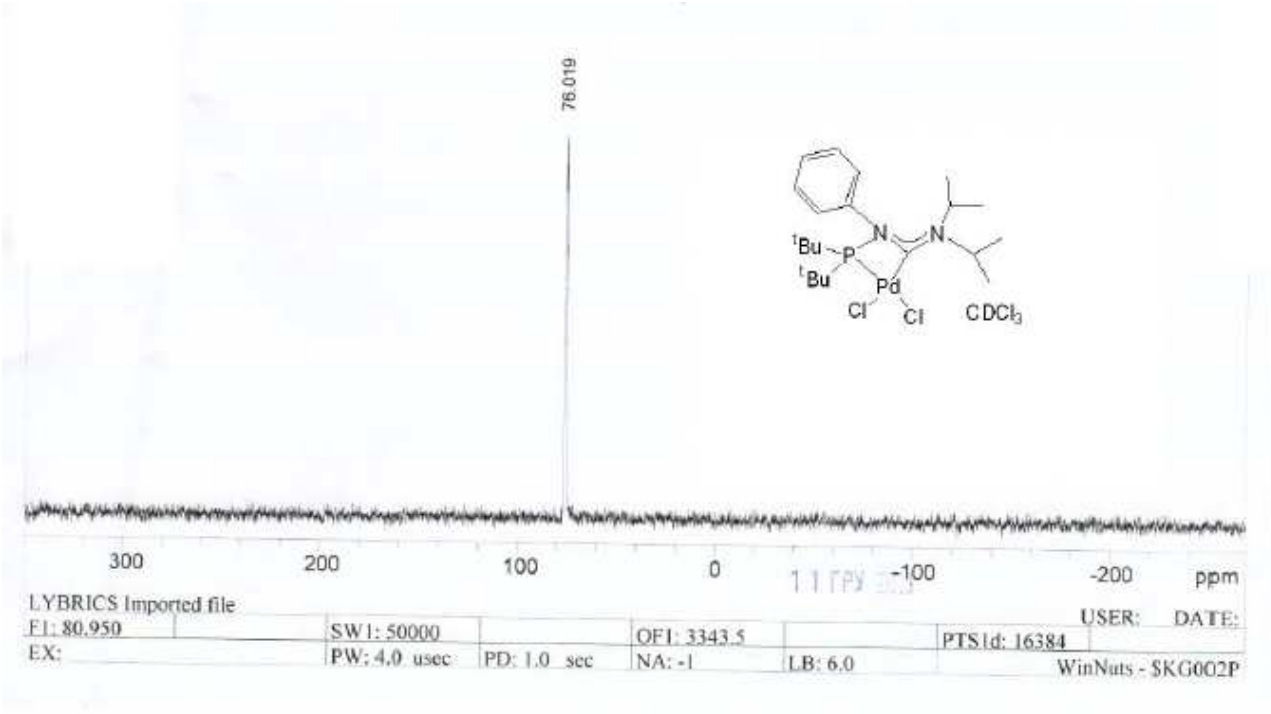
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Pd
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Cl
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200
100
0
-100
-200
ppm
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PTS1d: 16384
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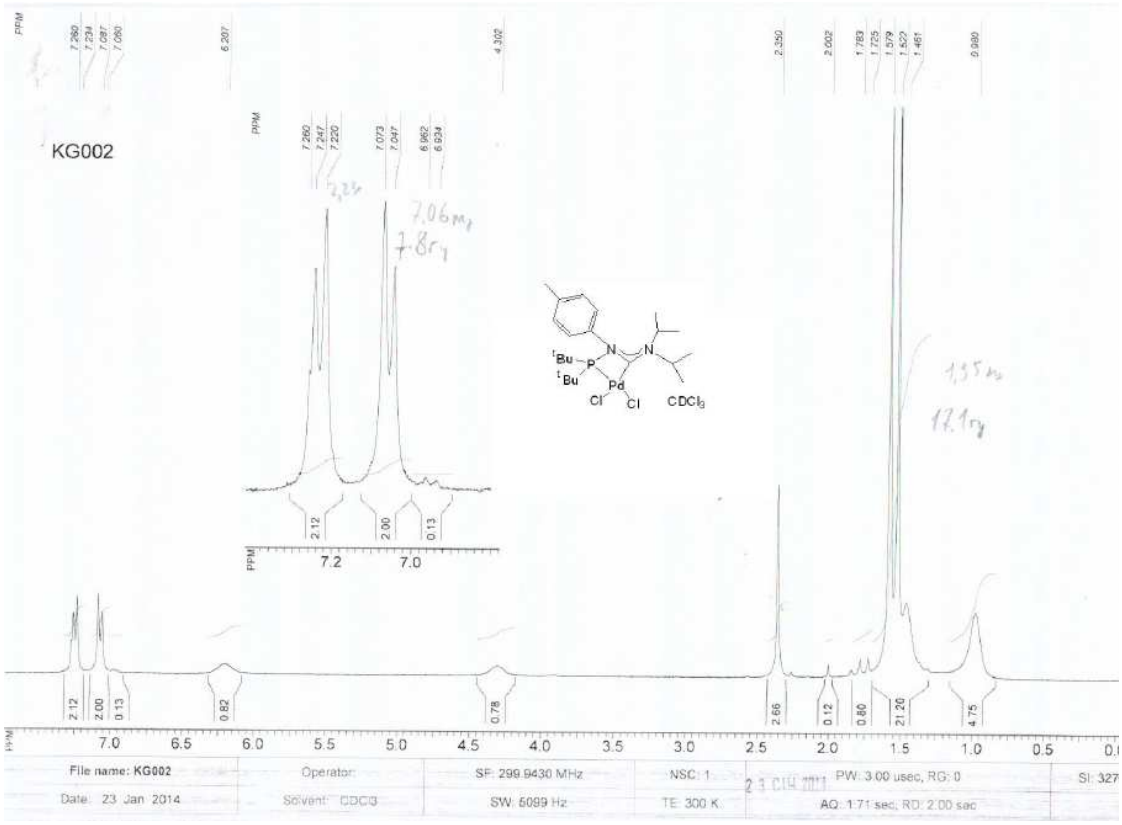
WinNuts - SKG002P

Complex 2b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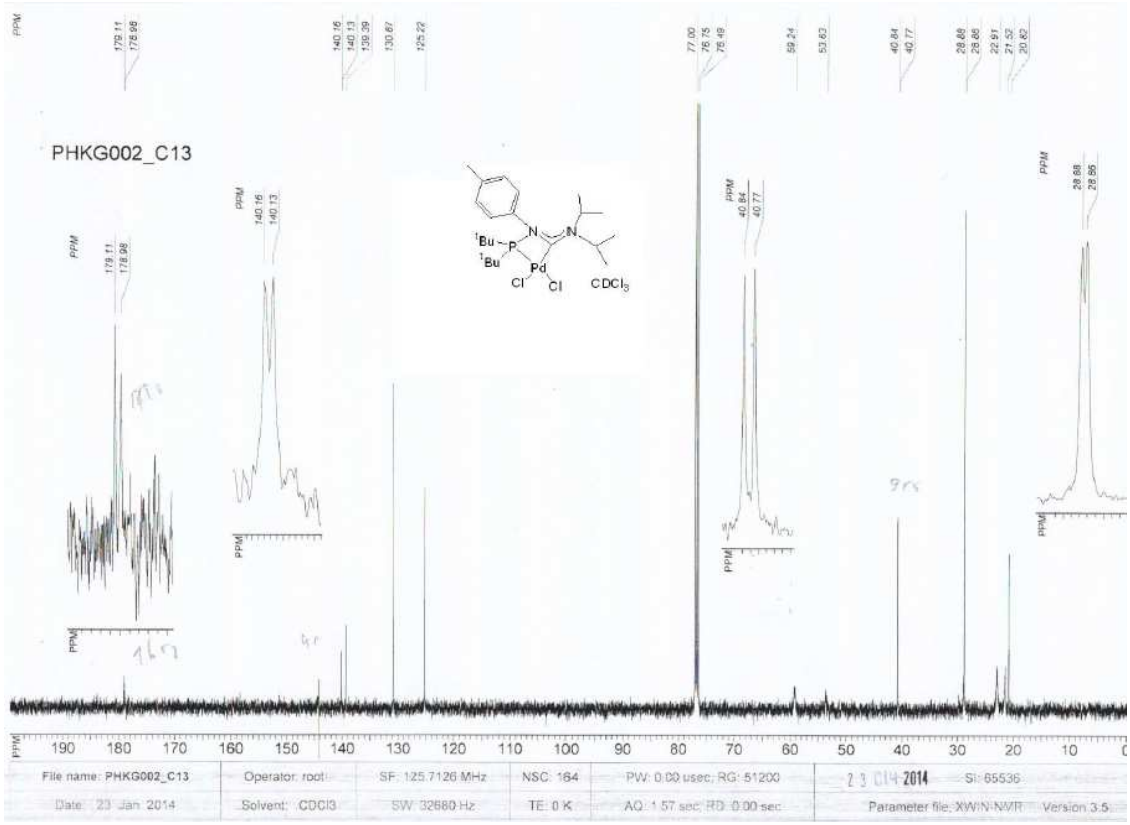
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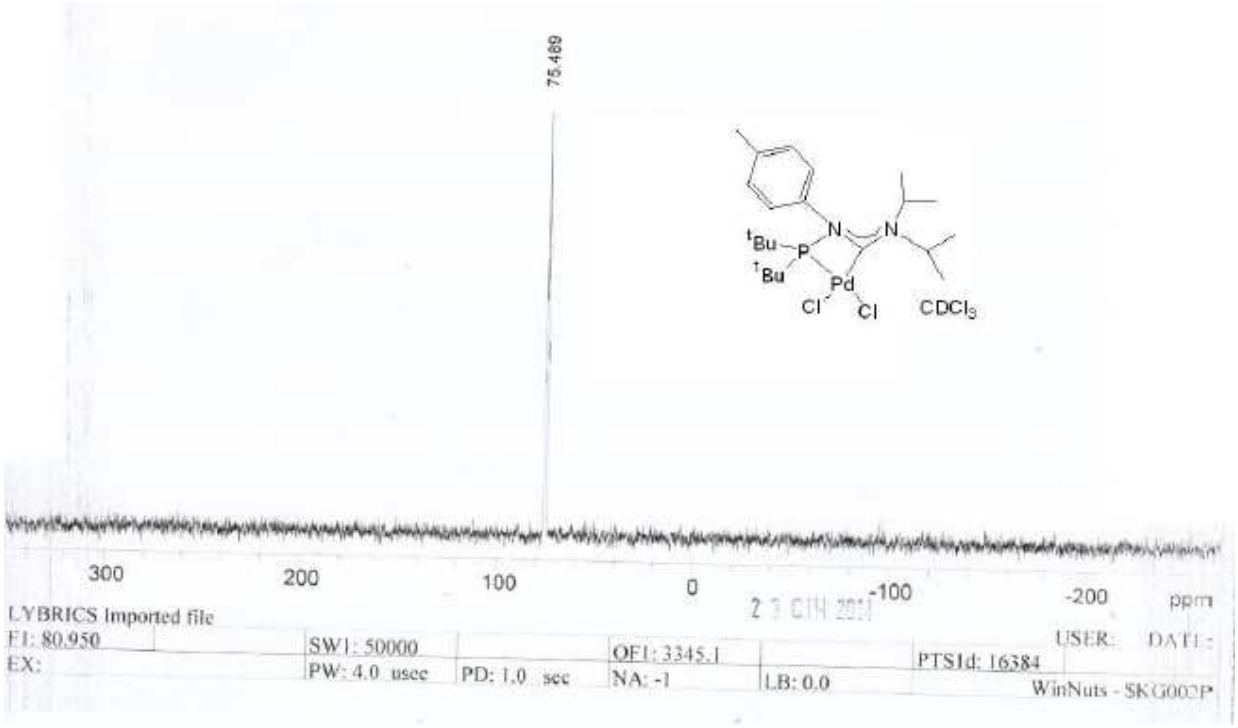
Version 3.5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P
N
N
Pd
Cl
Cl
CDCl3
300
200
100
0
-100
-200
ppm
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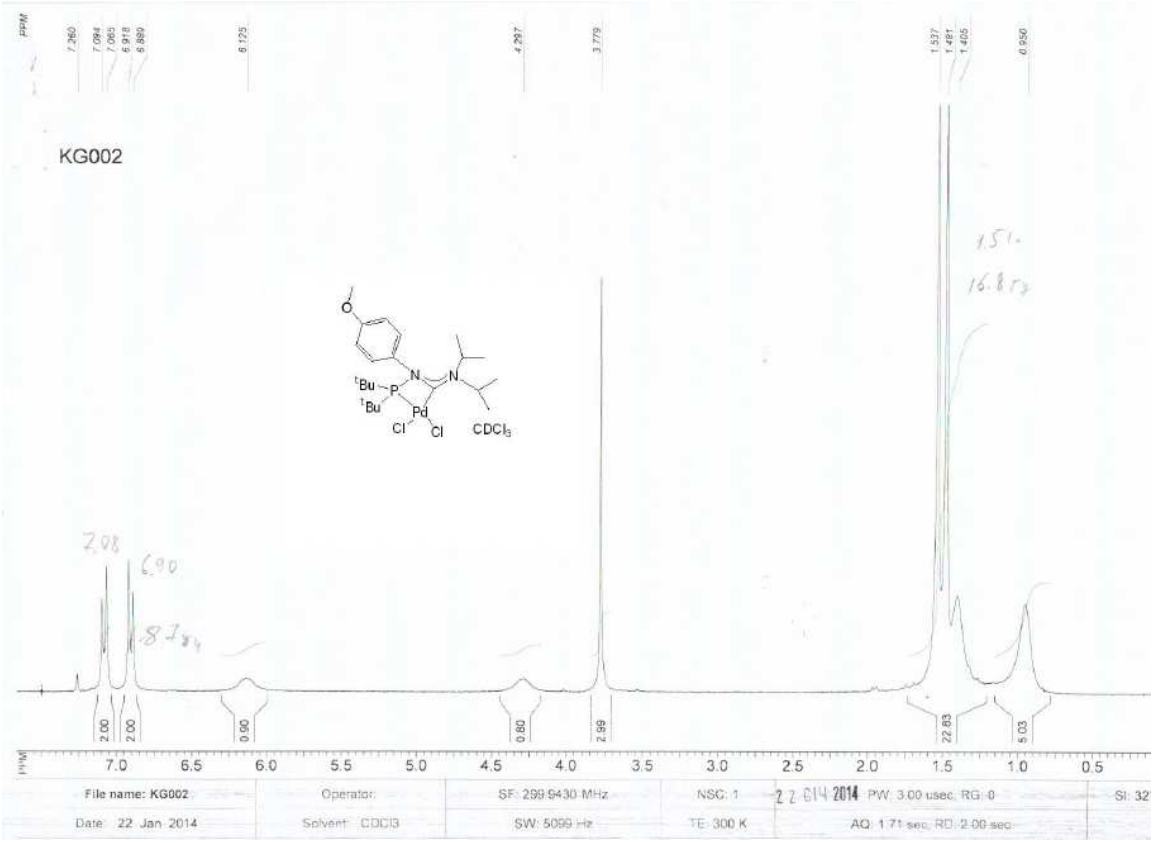
Complex 2c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2.00
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0.80
2.99
22.83
5.03
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
1.5
1.0
0.5
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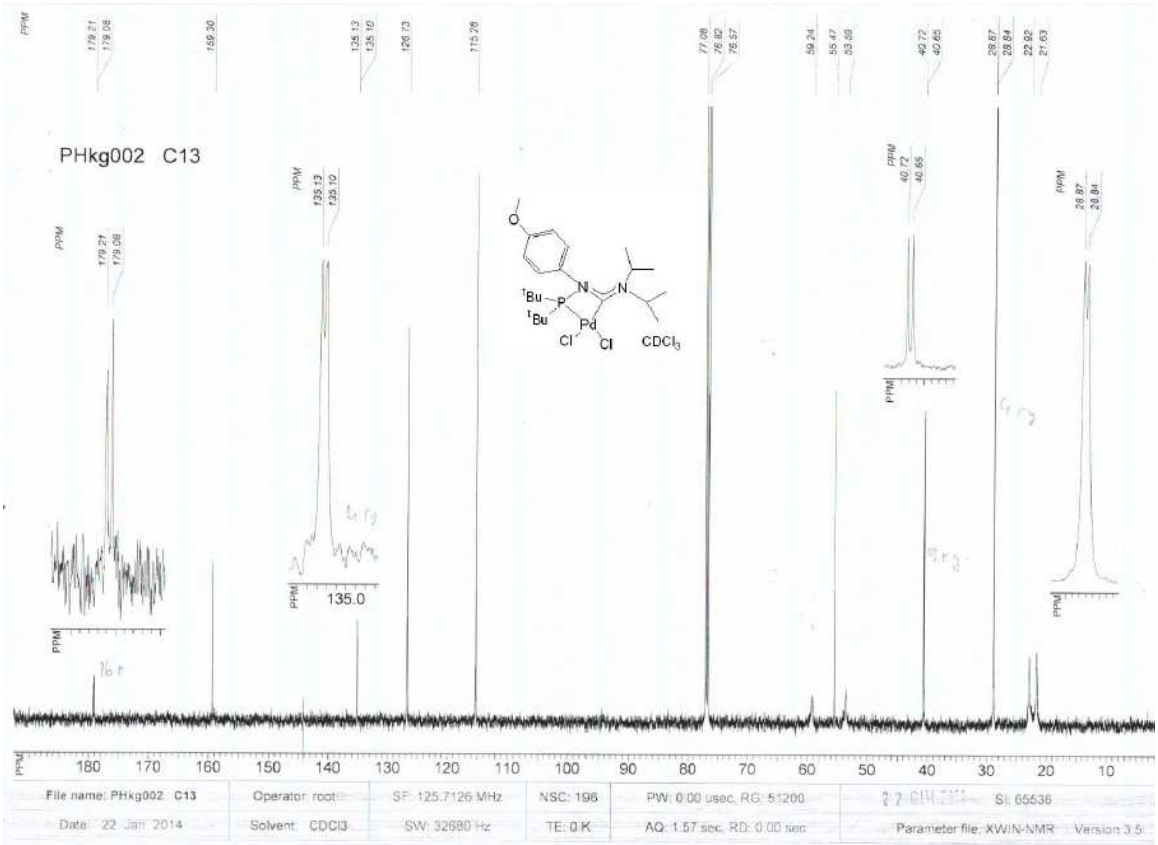
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59.24
55.47
55.08
40.72
40.65
28.87
28.84
22.82
21.63
135.0
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160
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140
130
120
110
100
90
80
70
60
50
40
30
20
10
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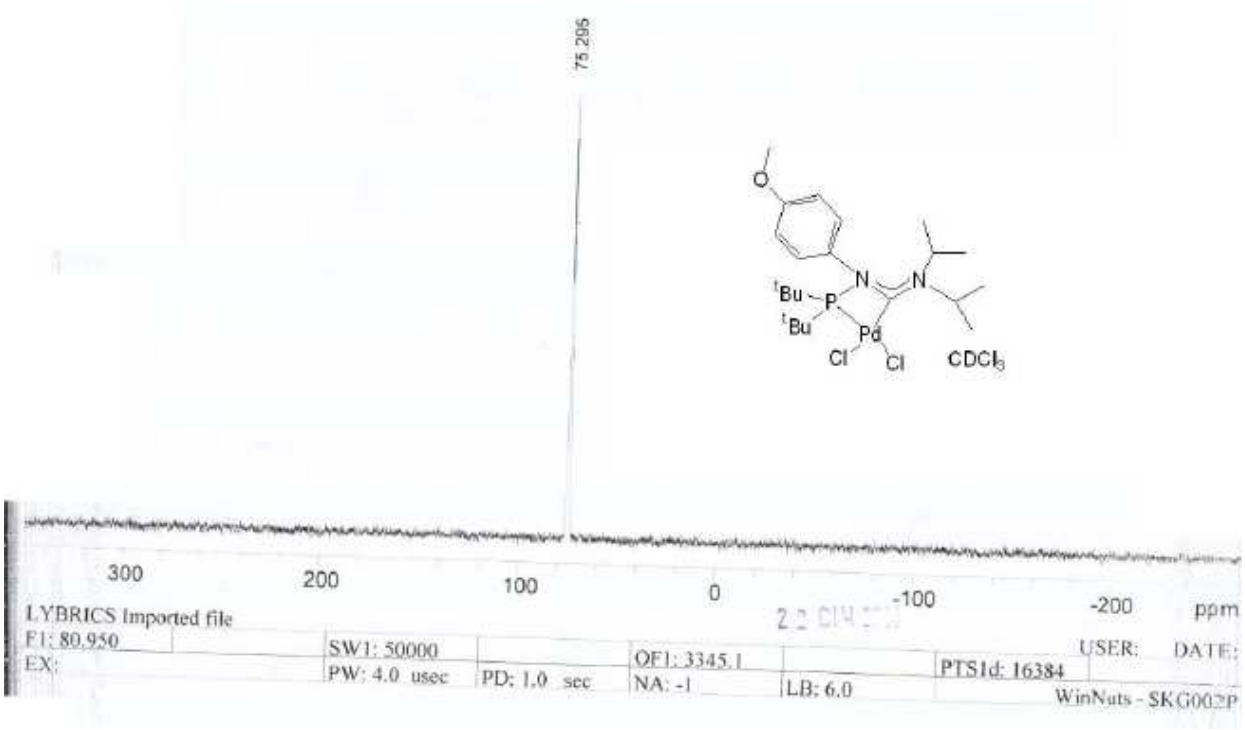
Version 3.5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0
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ppm
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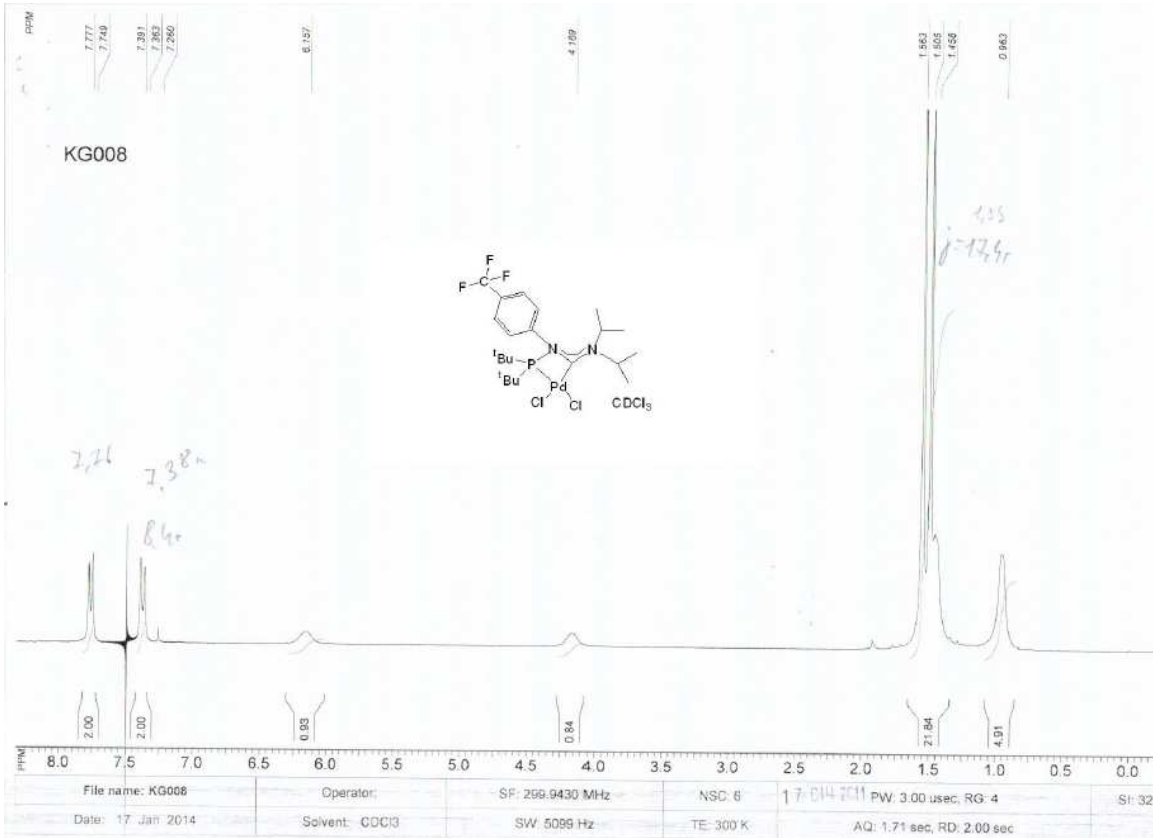
Complex 2d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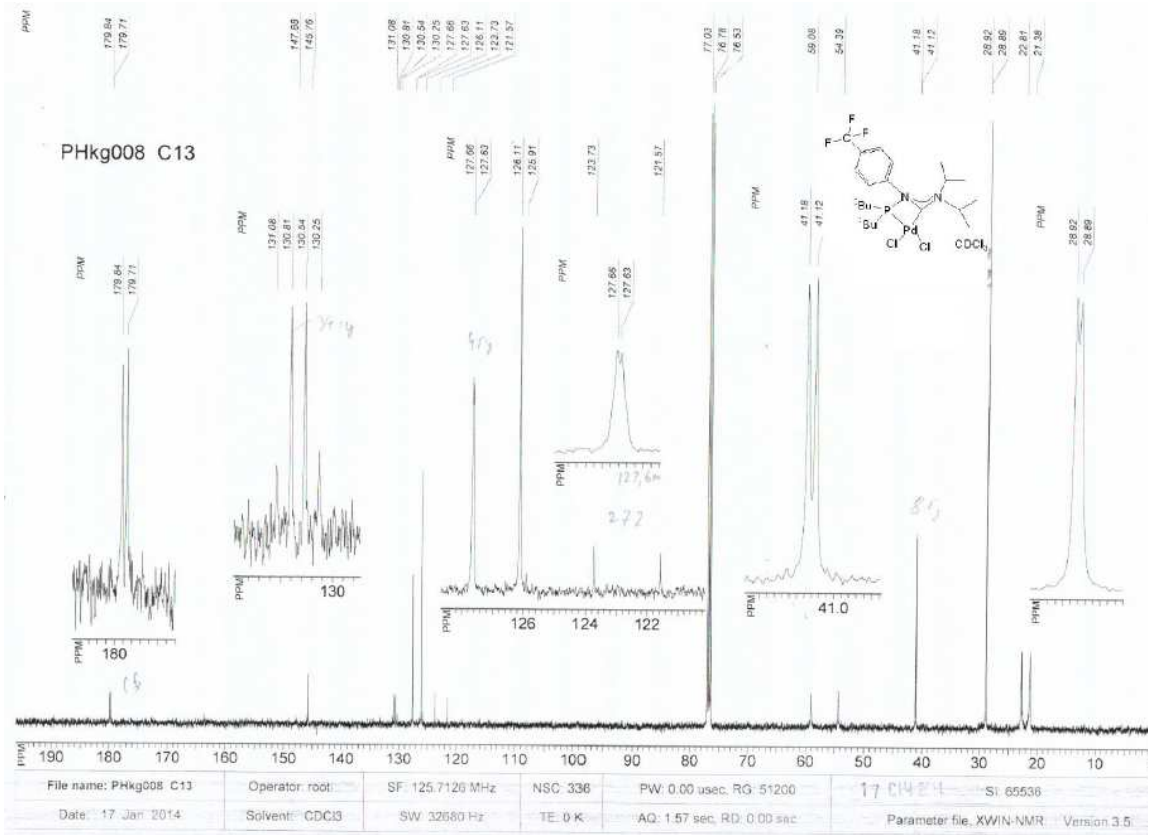
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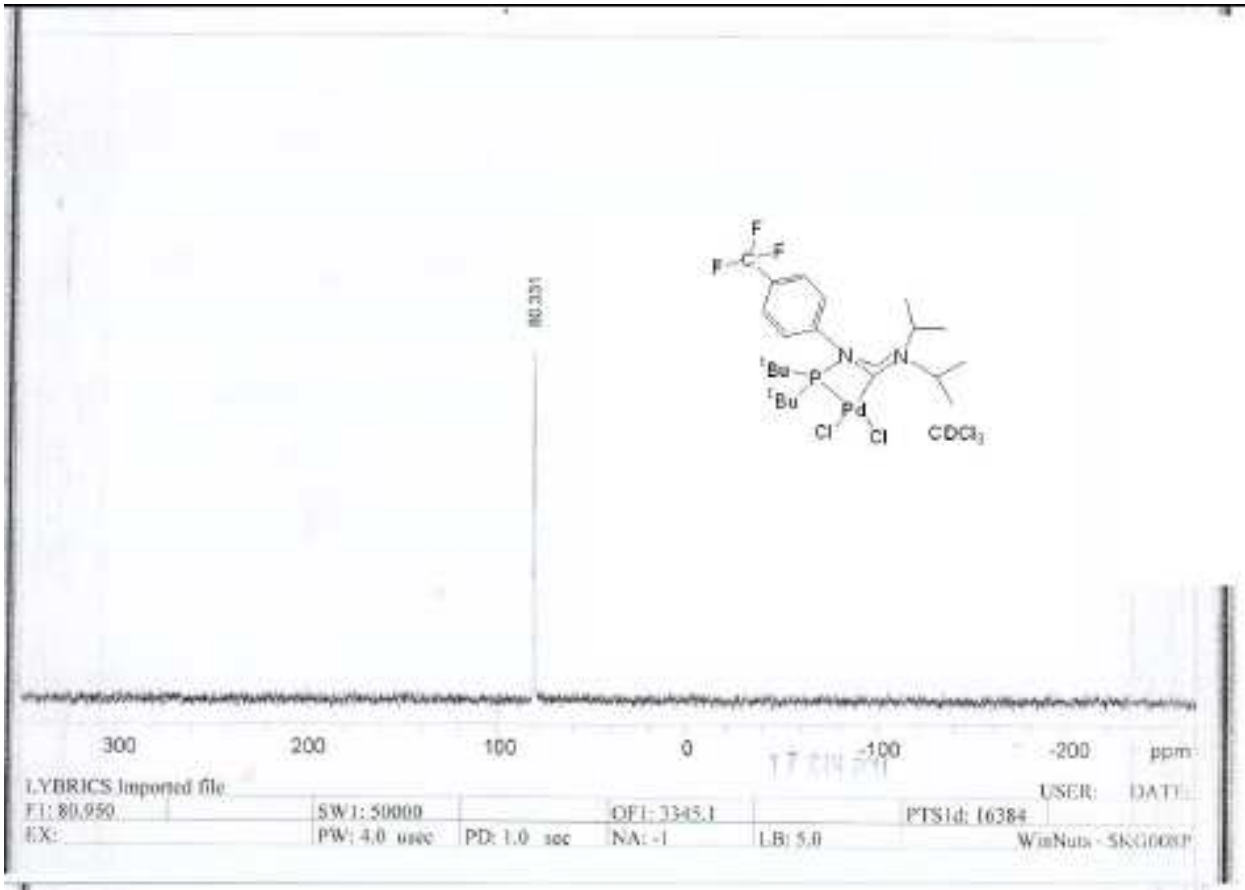
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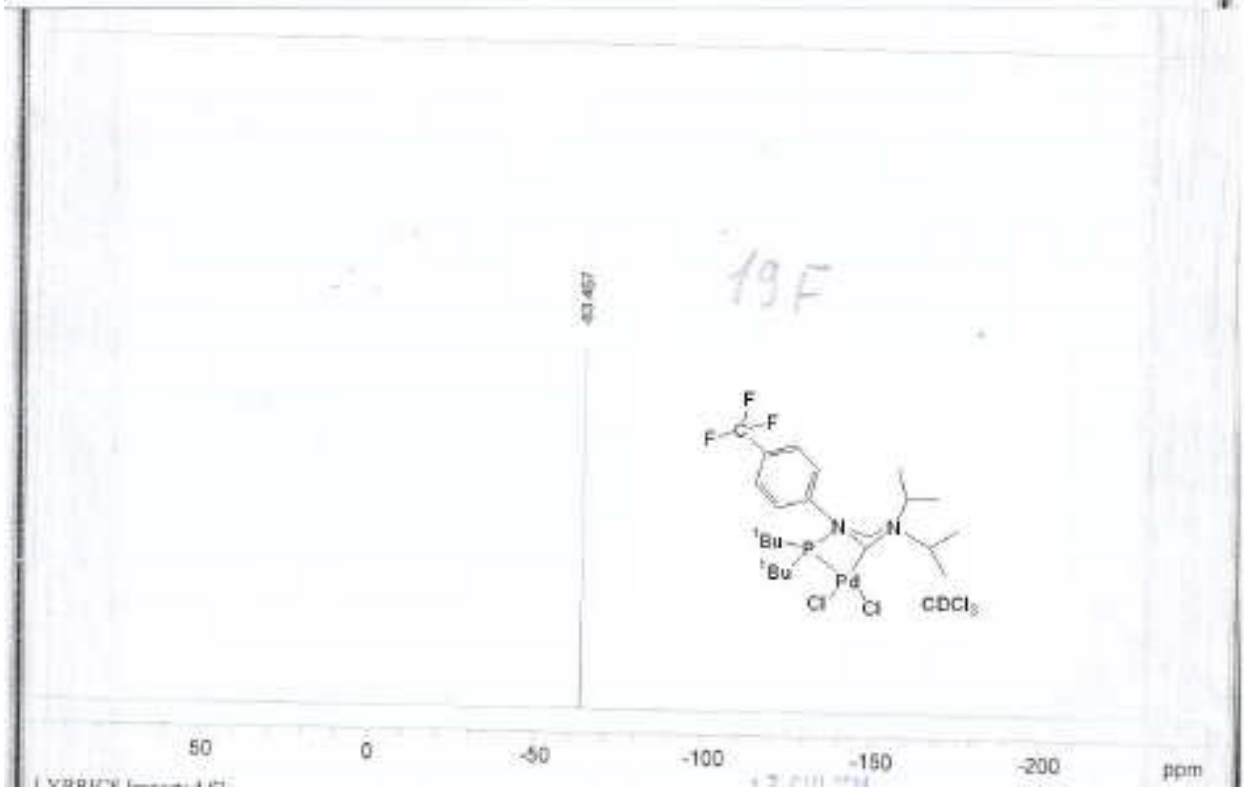
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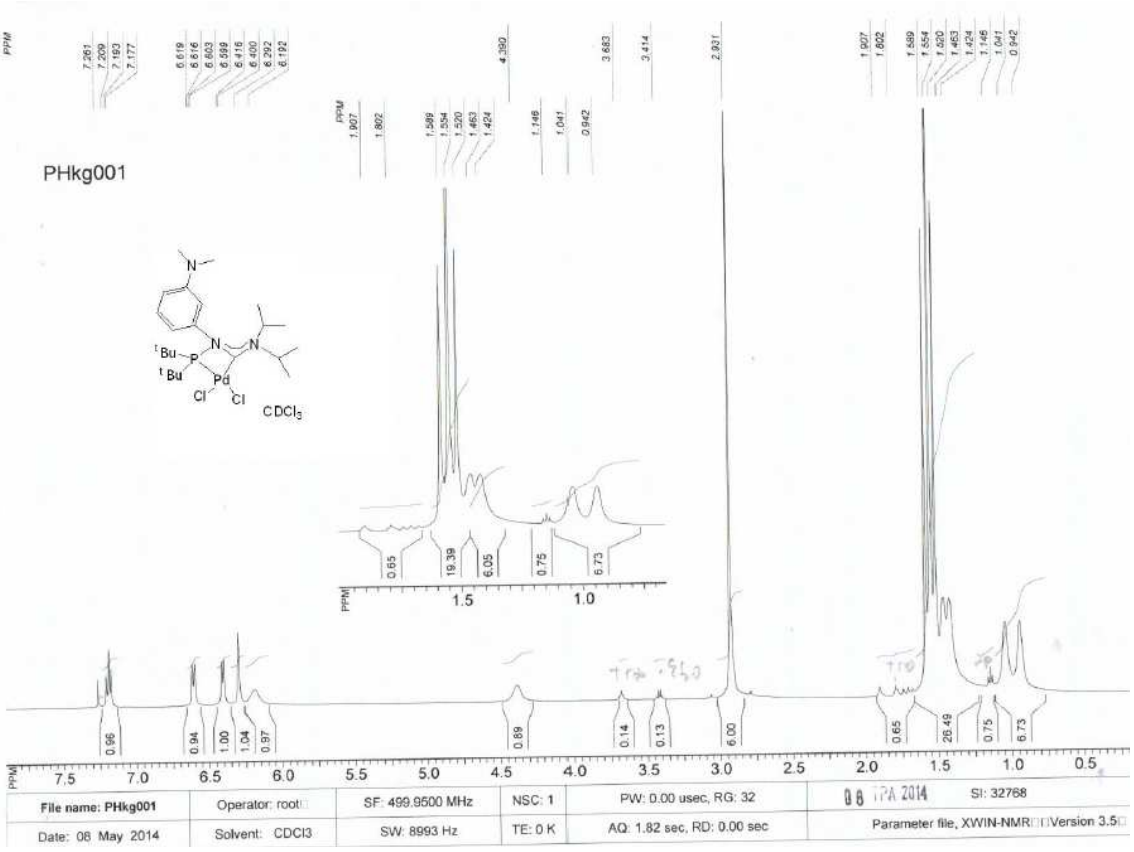
Complex 2e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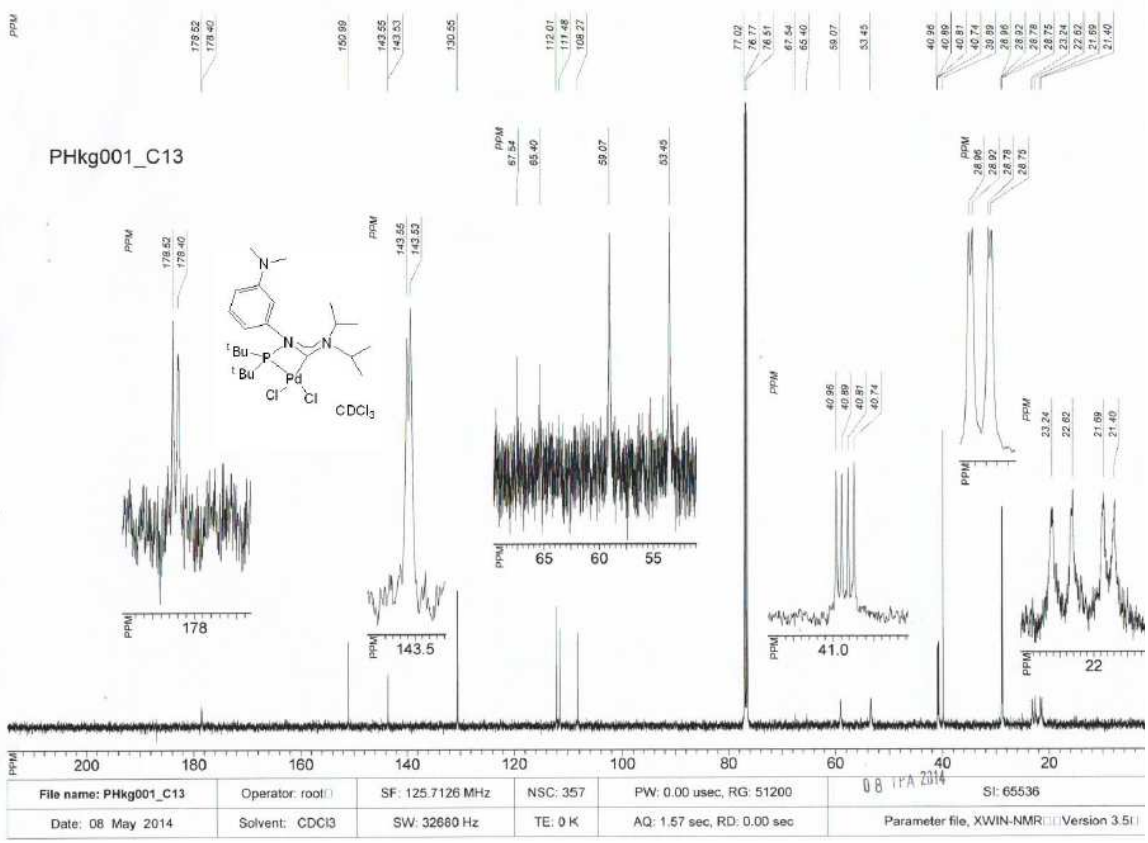
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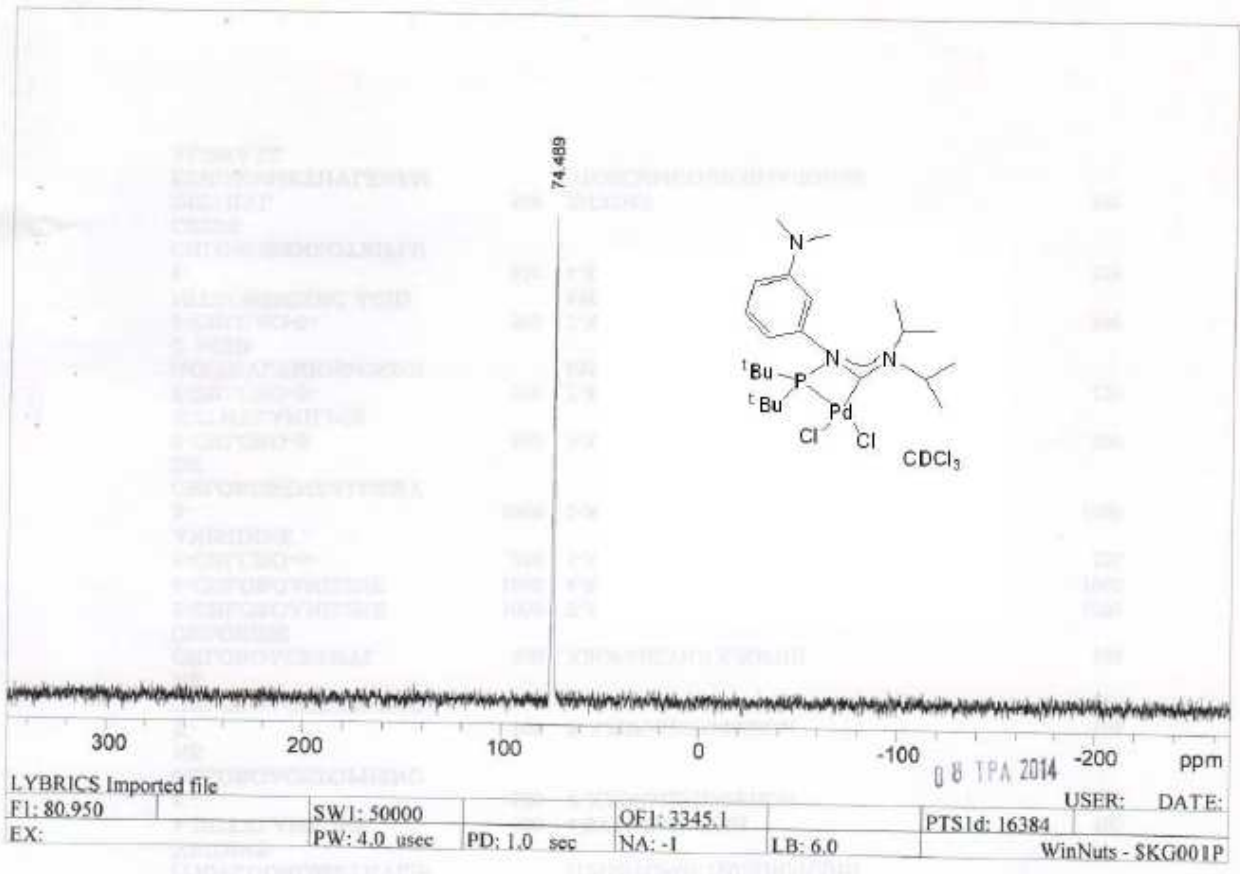
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ppm
08 TPA 2014
LYBRICS Imported file
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PTS1d: 16384
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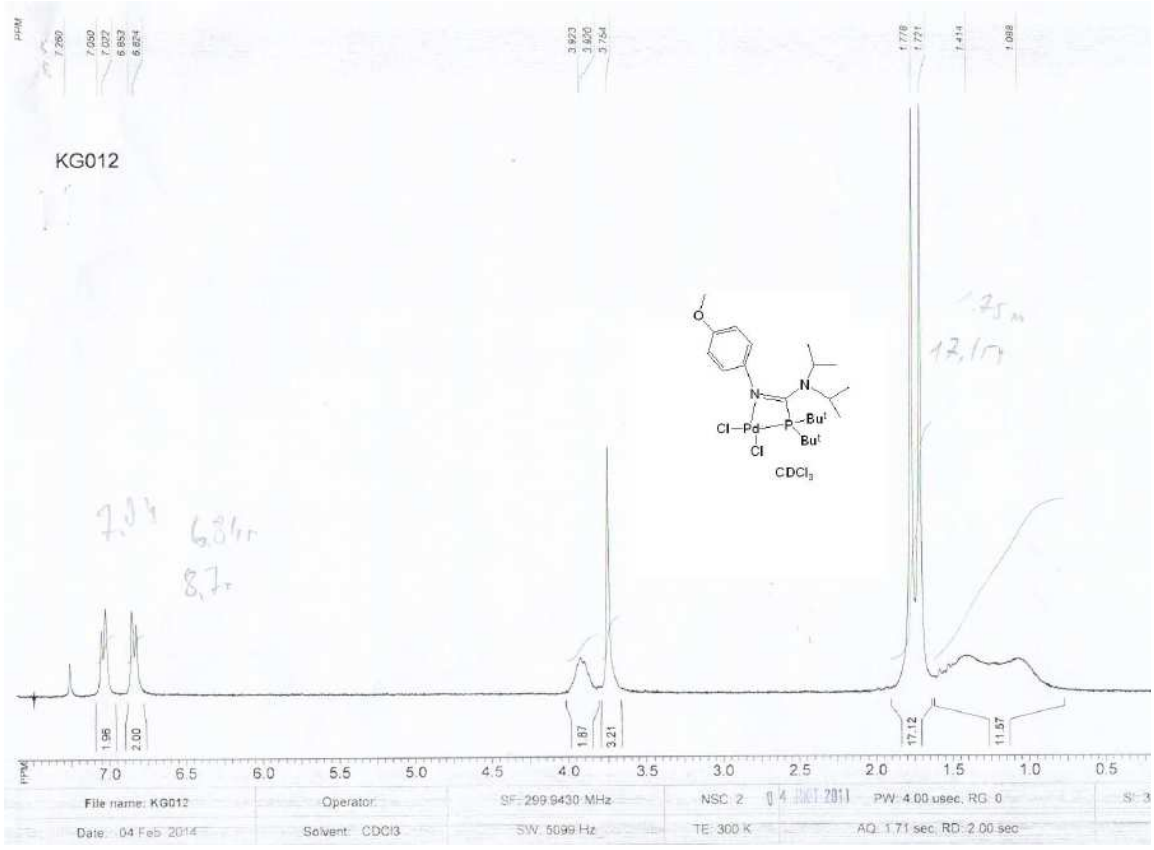
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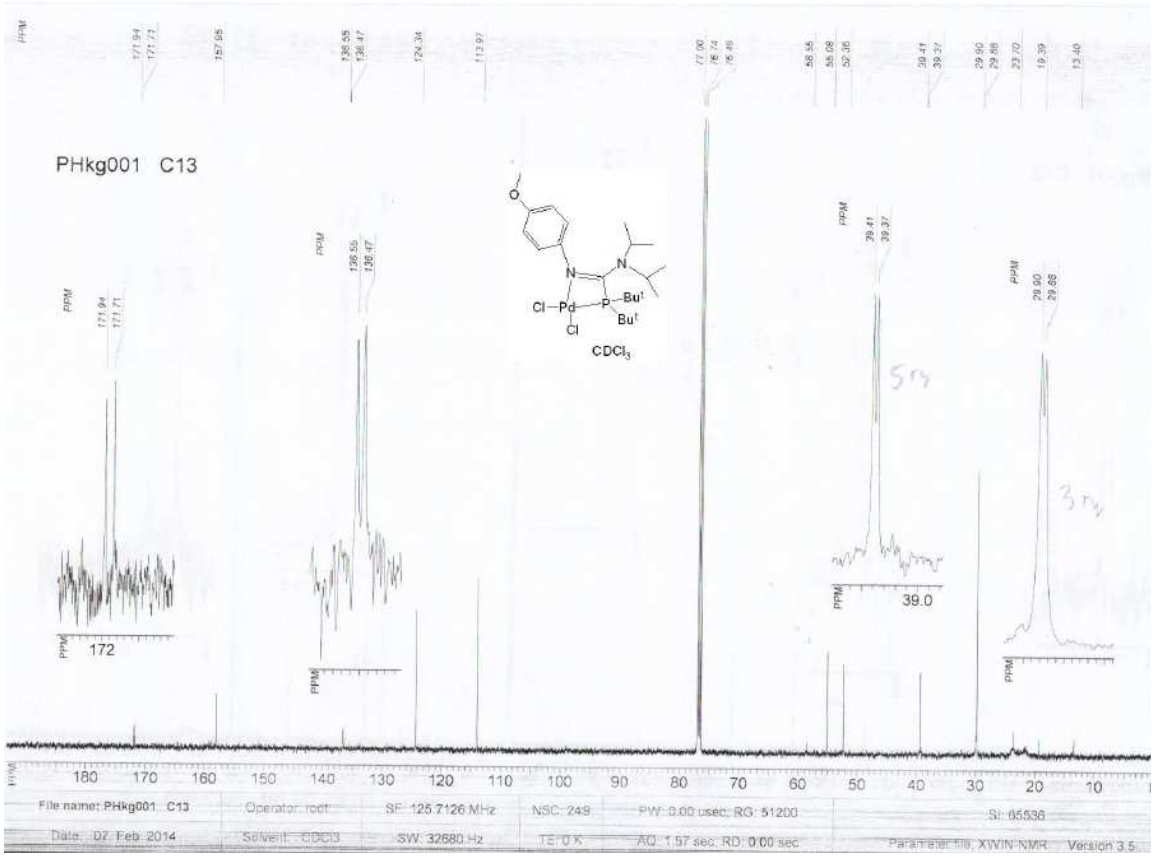
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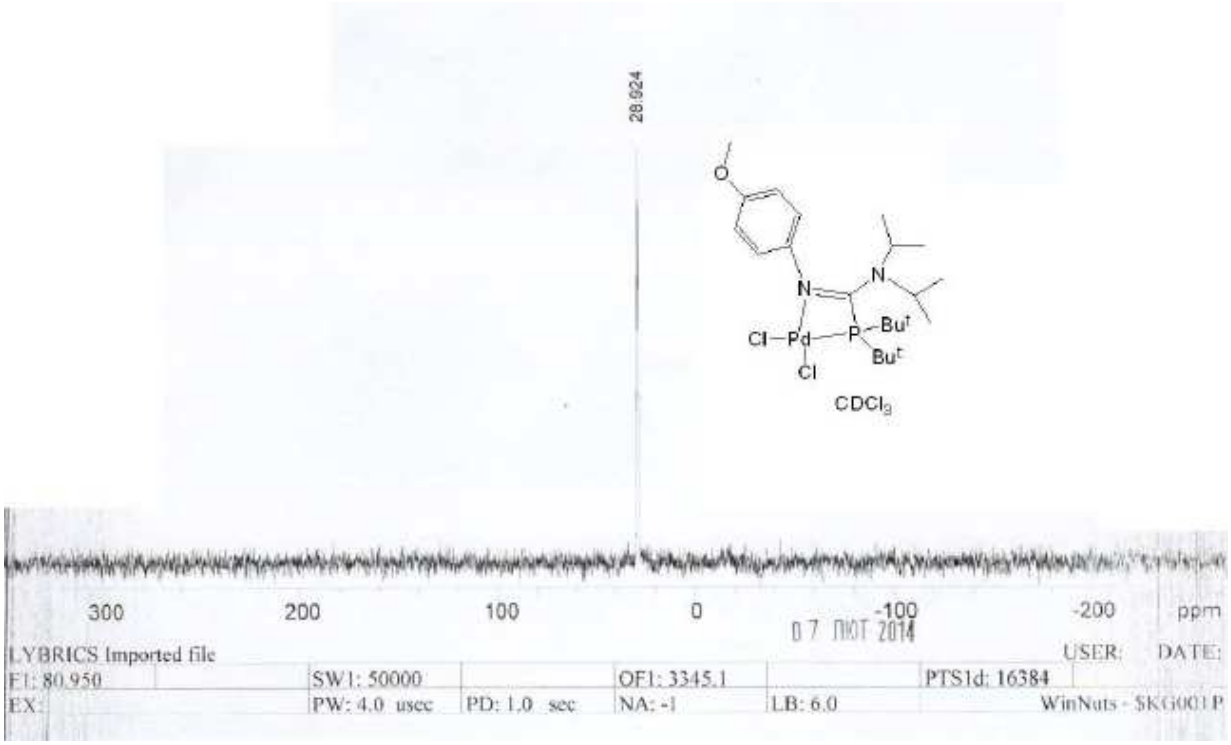
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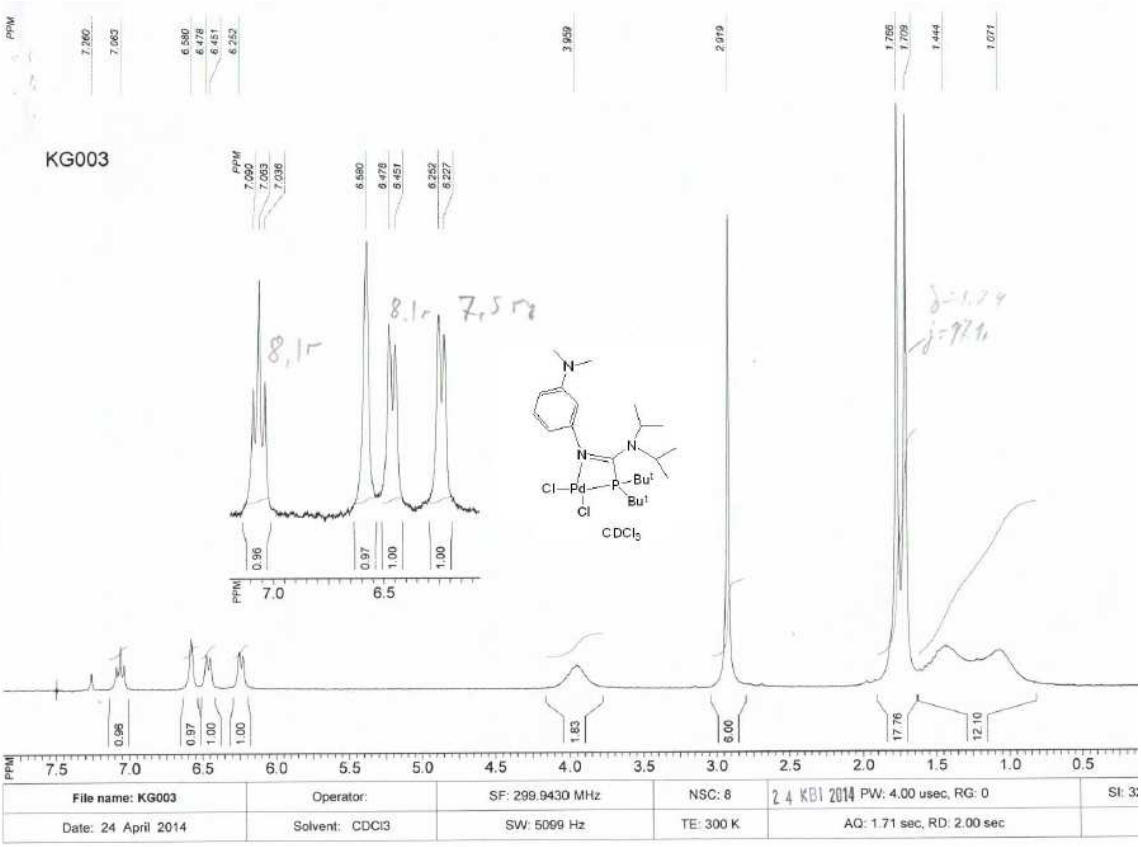
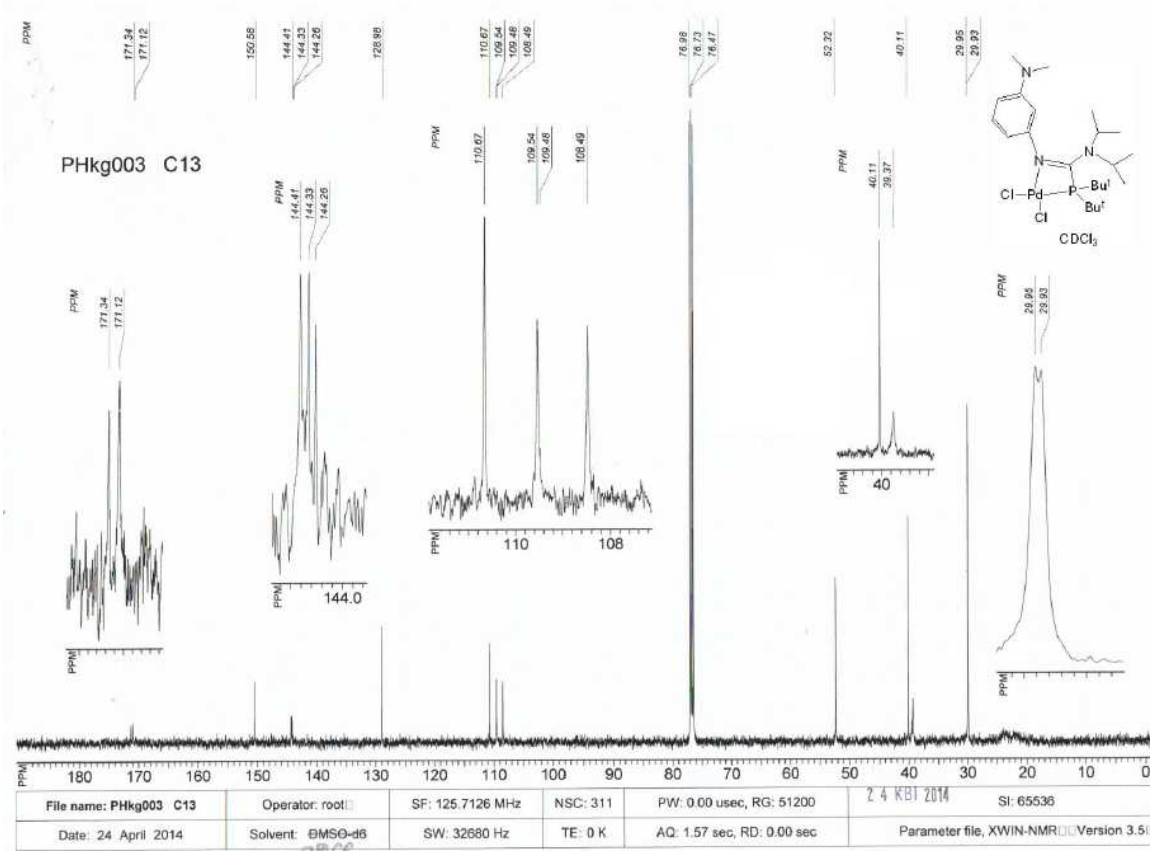
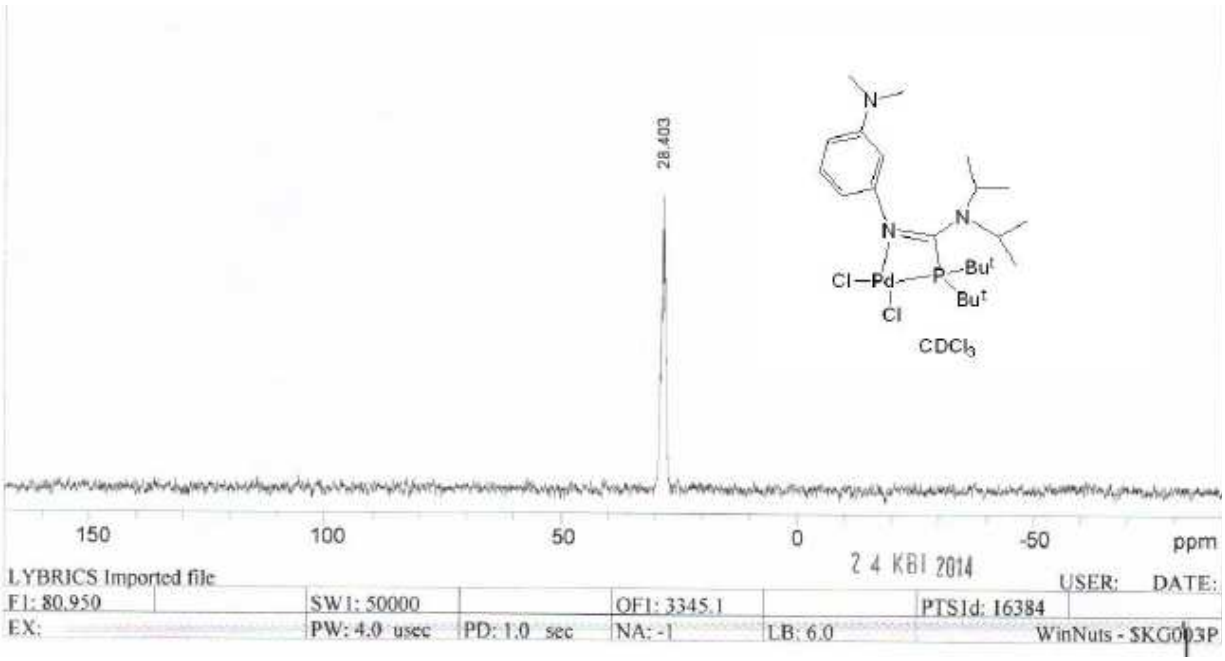
N
N
Cl—Pd—P
Bu^t
Bu^t
Cl
$CDCl_3$
300
200
100
0
-100
-200
ppm
07 ПЮТ 2014
LYBRICS Imported file
USER:
DATE:
F1: 80.950
SW1: 50000
OF1: 3345.1
PTS1d: 16384
EX:
PW: 4.0 usec
PD: 1.0 sec
NA: -1
LB: 6.0
WinNuts - SKG001P

Complex 3e


KG003
CDCl3
File name: KG003
Operator:
SF: 299.9430 MHz
NSC: 8
Date: 24 April 2014
Solvent: CDCl3
SW: 5099 Hz
TE: 300 K
AQ: 1.71 sec, RD: 2.00 sec


PHkg003 C13
CDCl3
File name: PHkg003 C13
Operator: root
SF: 125.7126 MHz
NSC: 311
PW: 0.00 usec, RG: 51200
Date: 24 April 2014
Solvent: DMSO-d6
SW: 32680 Hz
TE: 0 K
AQ: 1.57 sec, RD: 0.00 sec
Parameter file, XWIN-NMR Version 3.5


28.403
N
N
N
Cl—Pd
P
Bu^t
Bu^t
Cl
CDCl$_3$
150
100
50
0
-50
ppm
2 4 KBI 2014
LYBRICS Imported file
USER:
DATE:
F1: 80.950
SW1: 50000
OF1: 3345.1
PTS1d: 16384
EX:
PW: 4.0 usec
PD: 1.0 sec
NA: -1
LB: 6.0
WinNuts - $KG003P