

Supporting information

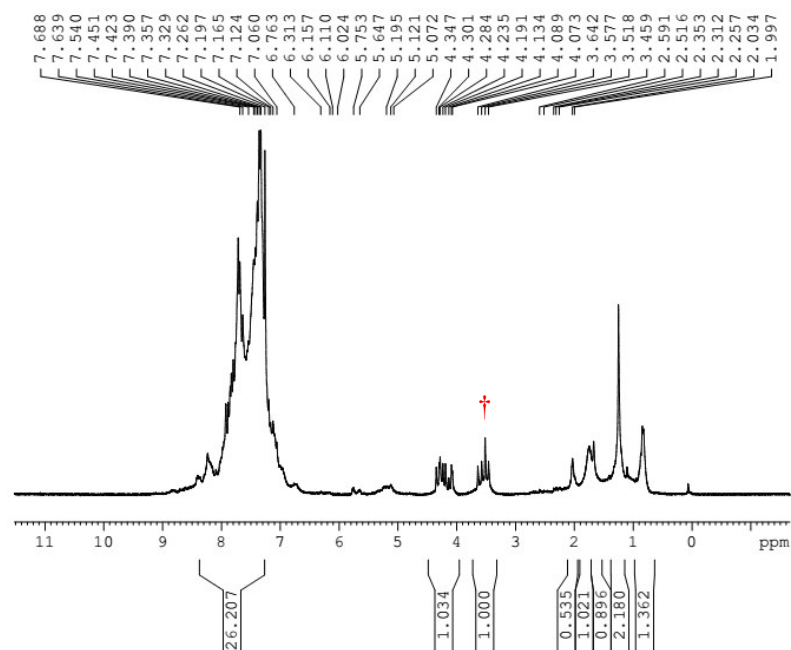
P, C- chelation versus P, P-coordination of unsymmetrical phosphorus ylides in palladacyclopropa[60]fullerene complexes; Synthetic, spectroscopic, and theoretical studies

Seyyed Javad Sabounchei,^{*,†} Marjan Hosseinzadeh,[†] Ali Hashemi,[†] Sadegh Salehzadeh,[†] and Farahnaz Maleki[†]

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60-m-Pd

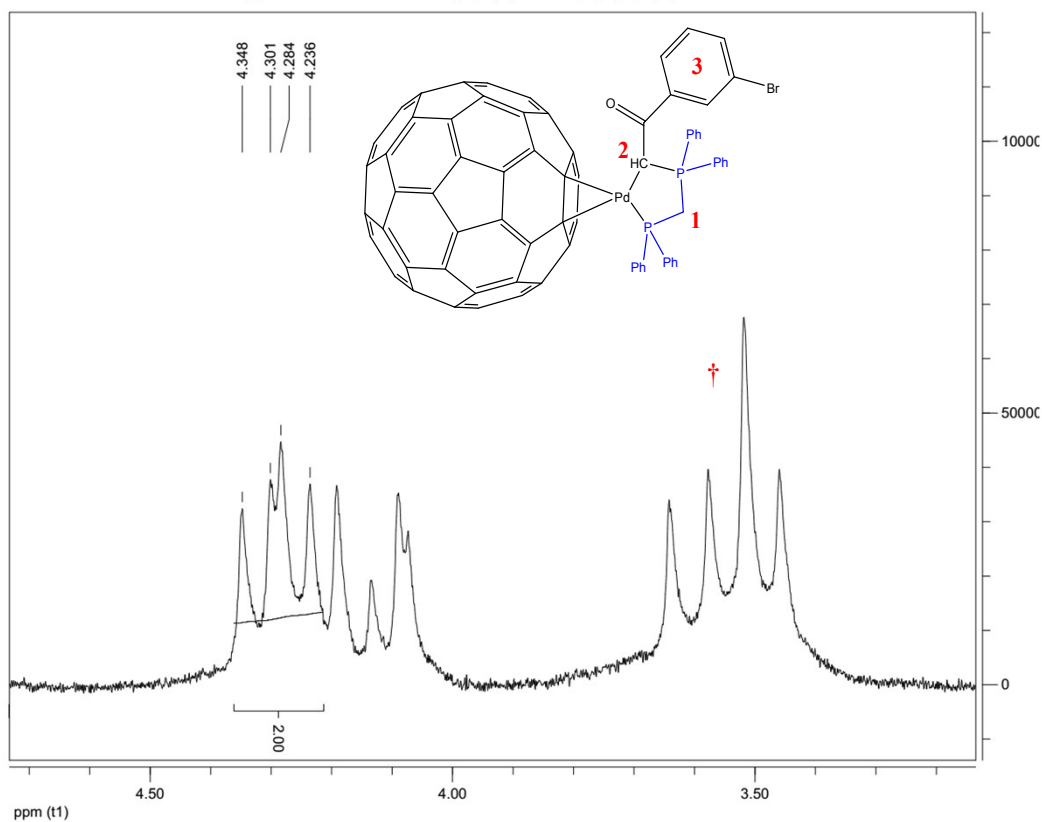


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EXPNO 220
PROCNO 1

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TD 16384
SOLVENT CDCl3
NS 50
DS 0
SWH 4496.403 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 256
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 3.0000000 sec

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PL1 3.00 dB
SFO1 250.1315008 MHz

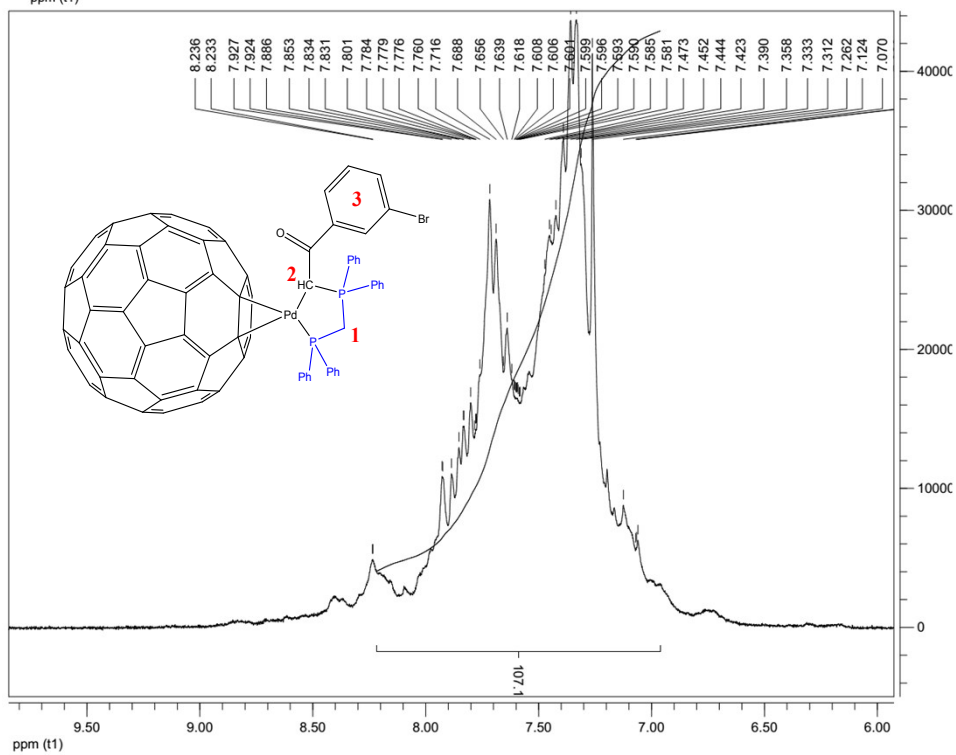
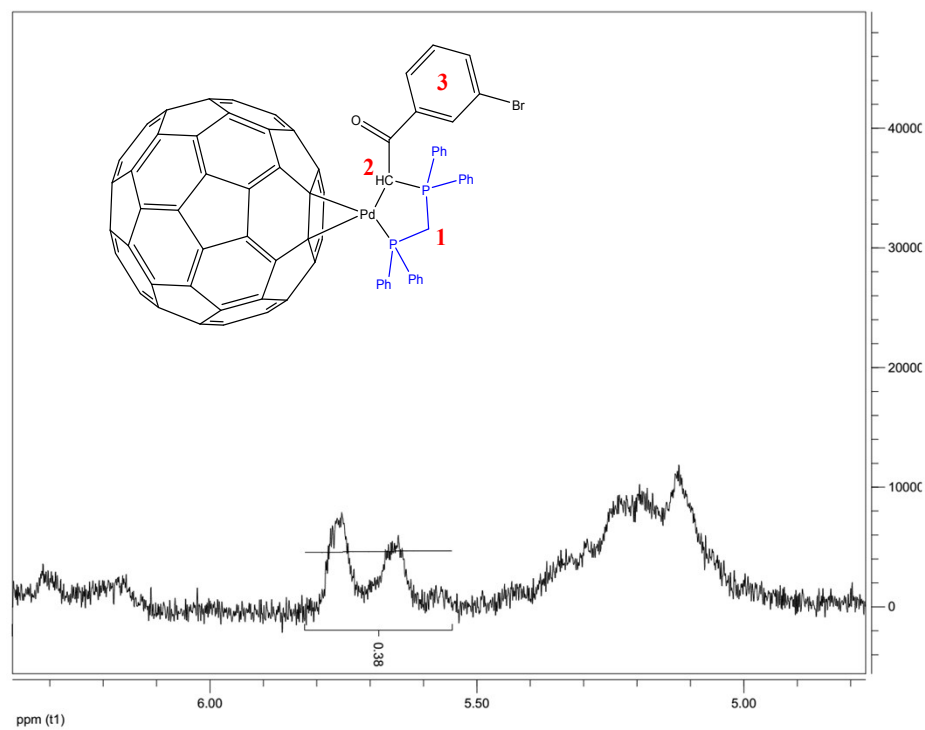
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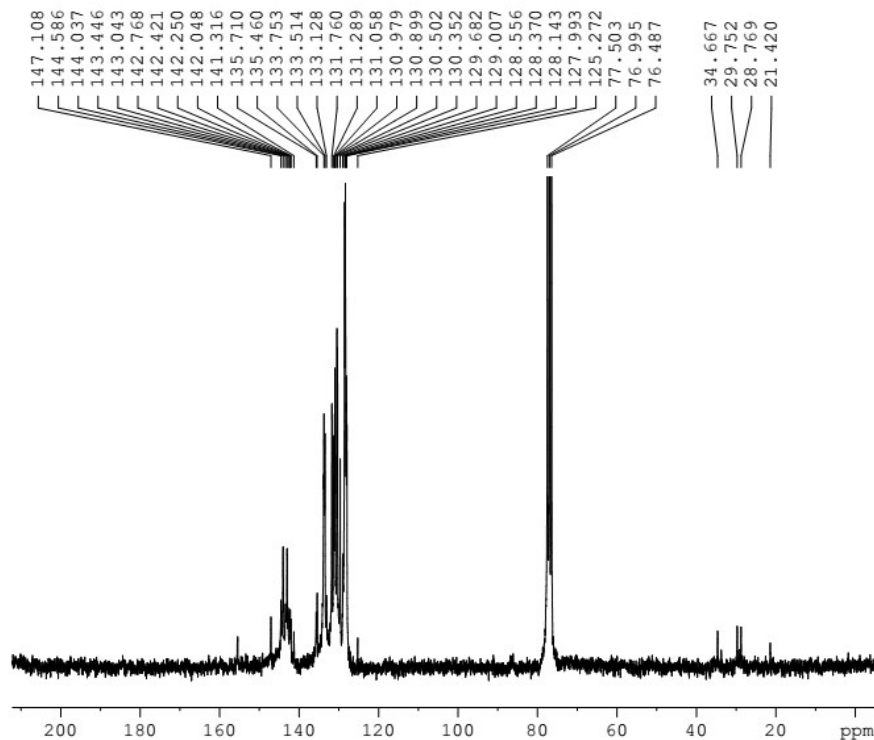
¹H NMR of (1)

* n-Hexane

† dppm oxide



¹H NMR of (1)



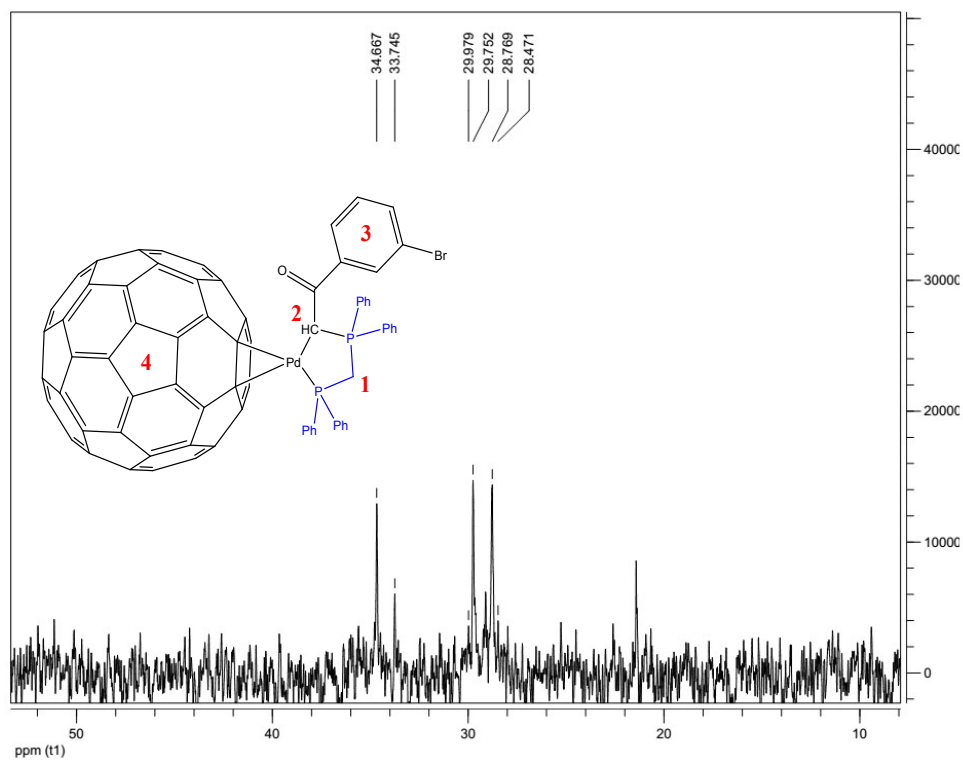
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TD 65536
SOLVENT CDCl3
NS 10000
DS 0
SWH 13812.154 Hz
FIDRES 0.210757 Hz
AQ 2.3724532 sec
RG 32768
DW 36.200 usec
DE 6.00 usec
TE 300.0 K
D1 3.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

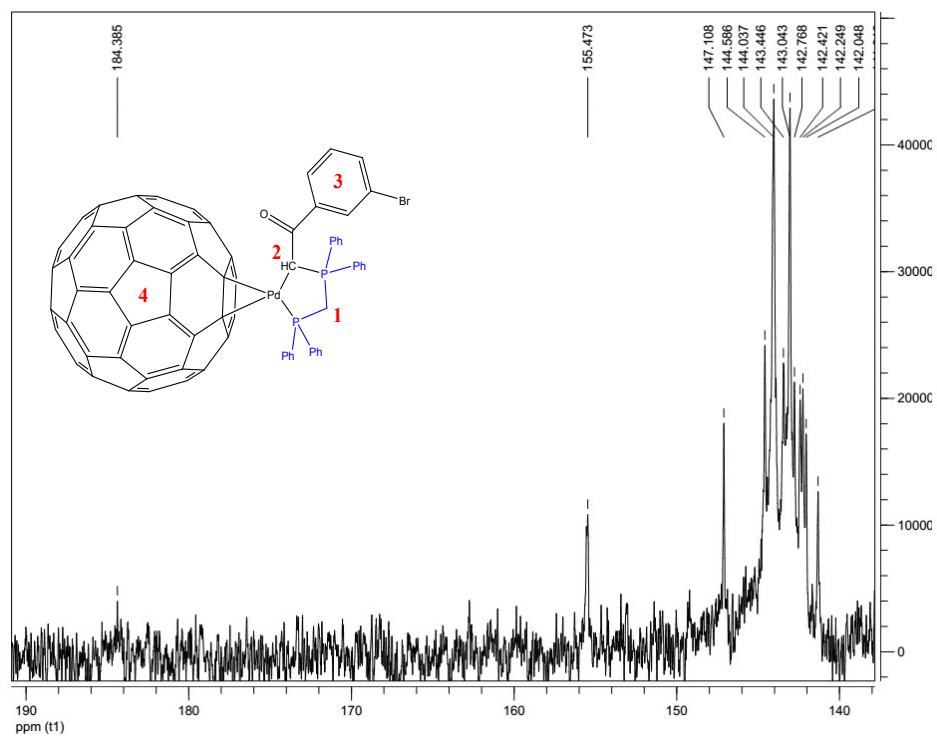
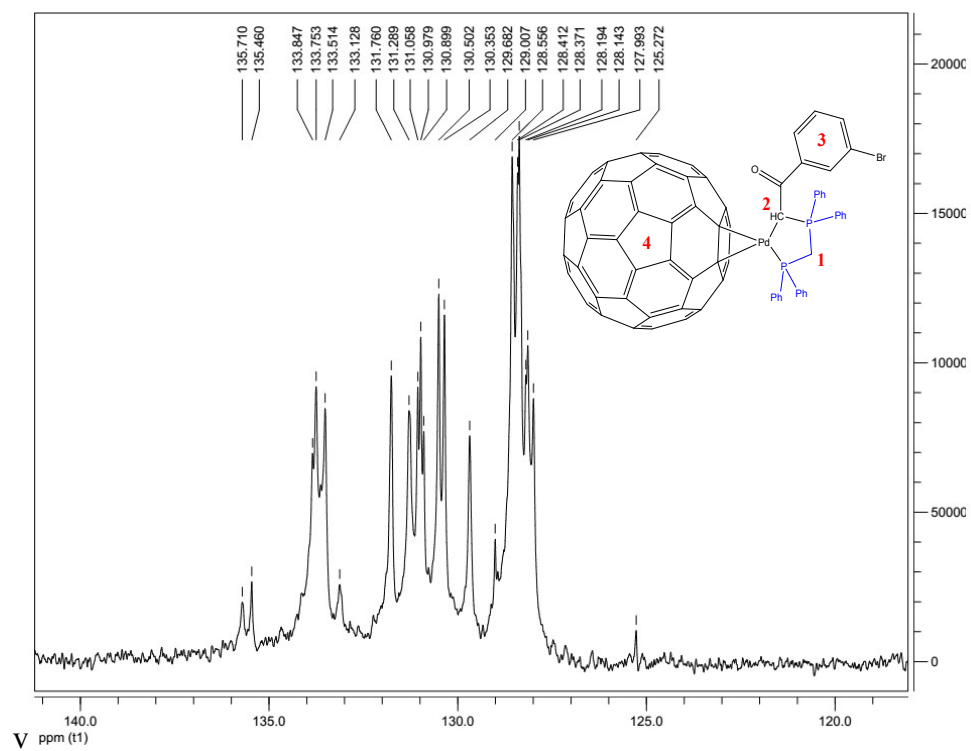
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NUC1 13C
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SFO1 62.9018430 MHz

----- CHANNEL f2 -----
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NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 21.50 dB
PL13 23.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952390 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

 ^{13}C NMR of (1)

* n-Hexane



¹³C NMR of (1)

Hosseinzadeh-60-m-pd



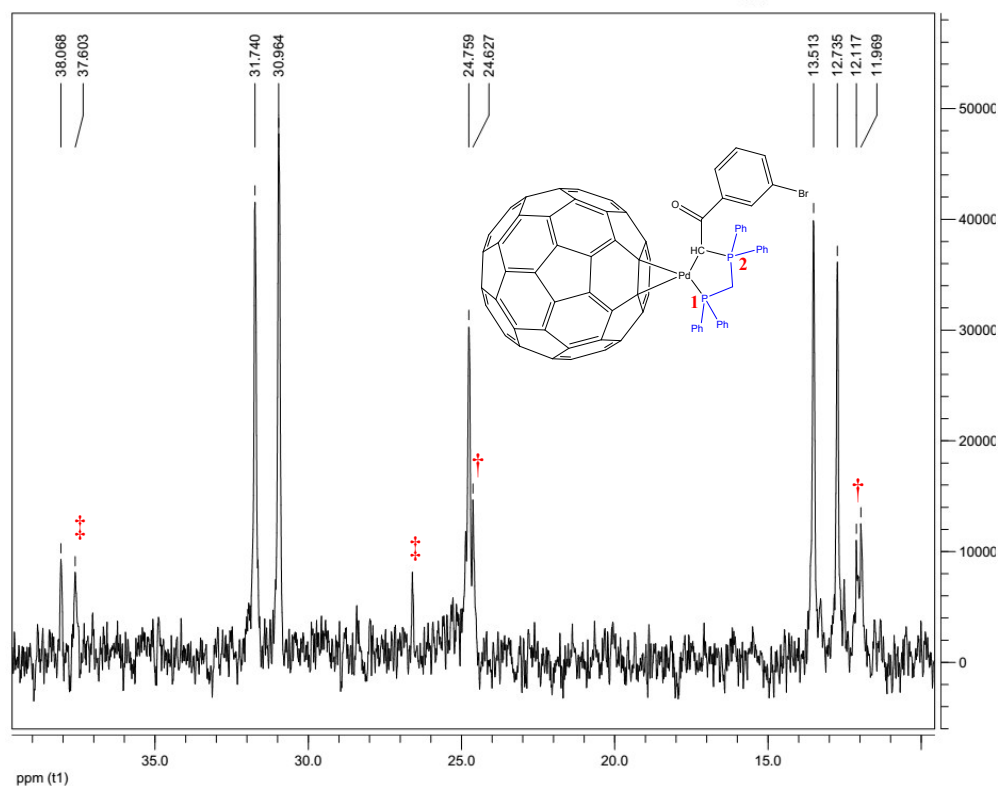
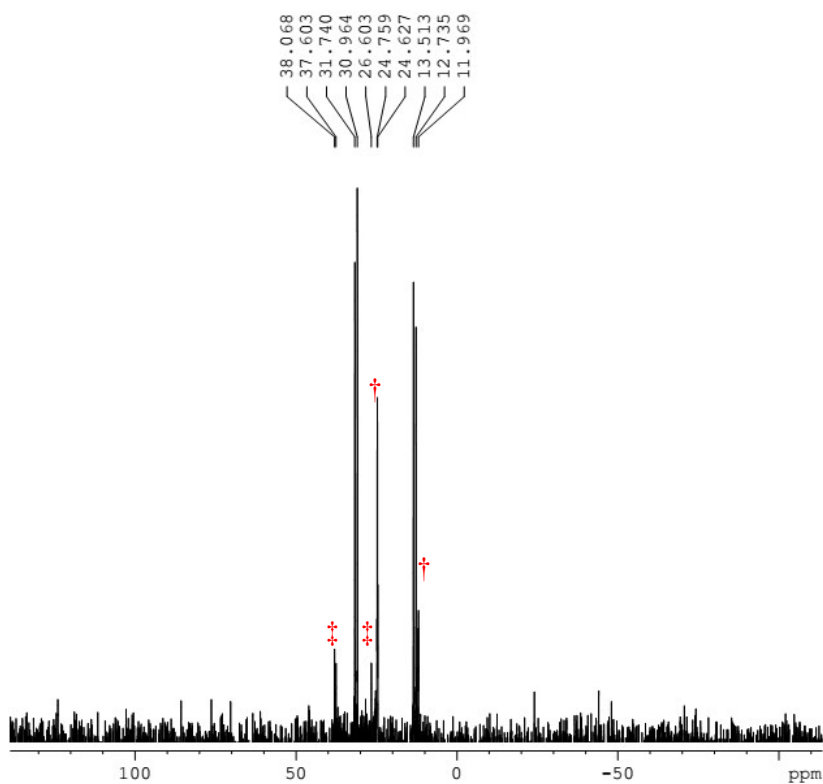
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PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 20
DS 0
SWH 40650.406 Hz
FIDRES 0.620276 Hz
AQ 0.8061428 sec
RG 22800
DW 12.300 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

CHANNEL f1
NUC1 31P
P1 9.00 usec
PL1 5.00 dB
SFO1 101.2494047 MHz

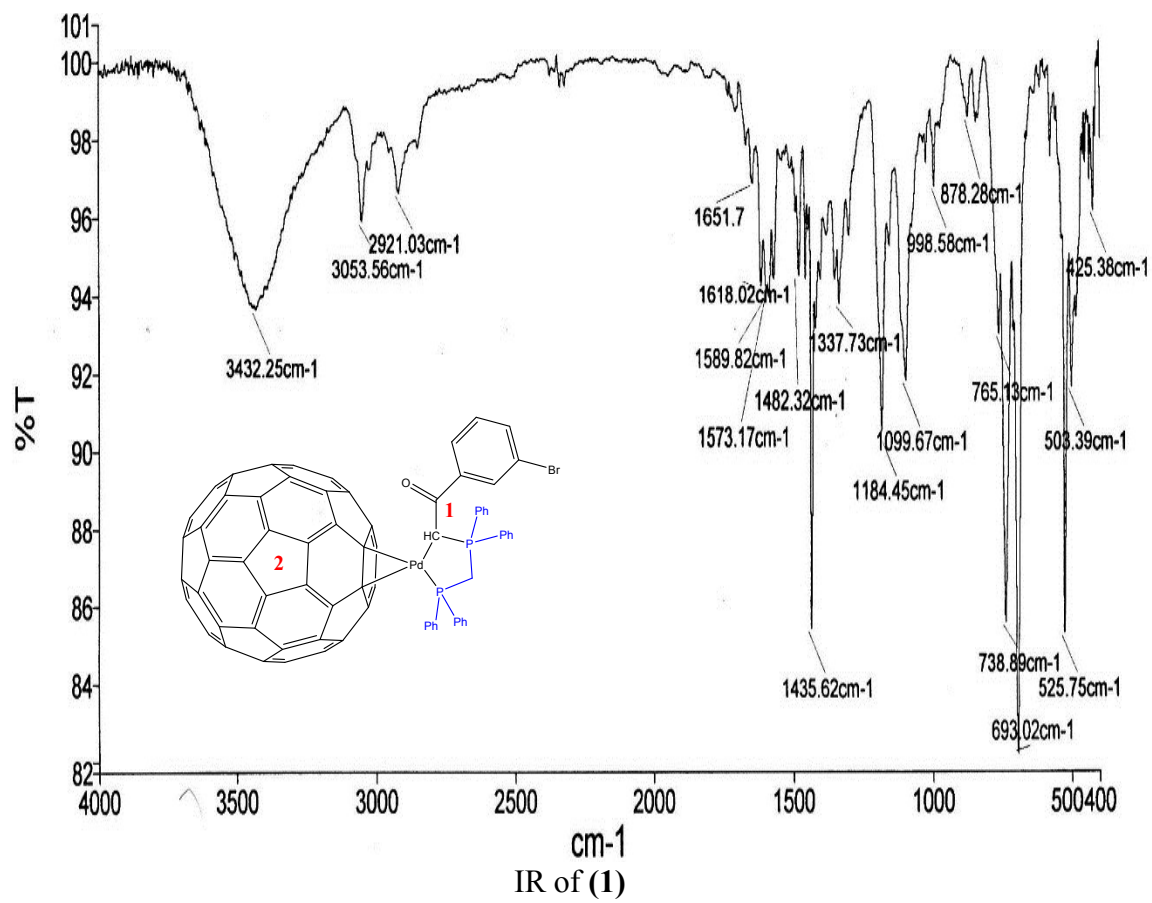
CHANNEL f2
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NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 21.50 dB
PL13 23.00 dB
SFO2 250.1310005 MHz

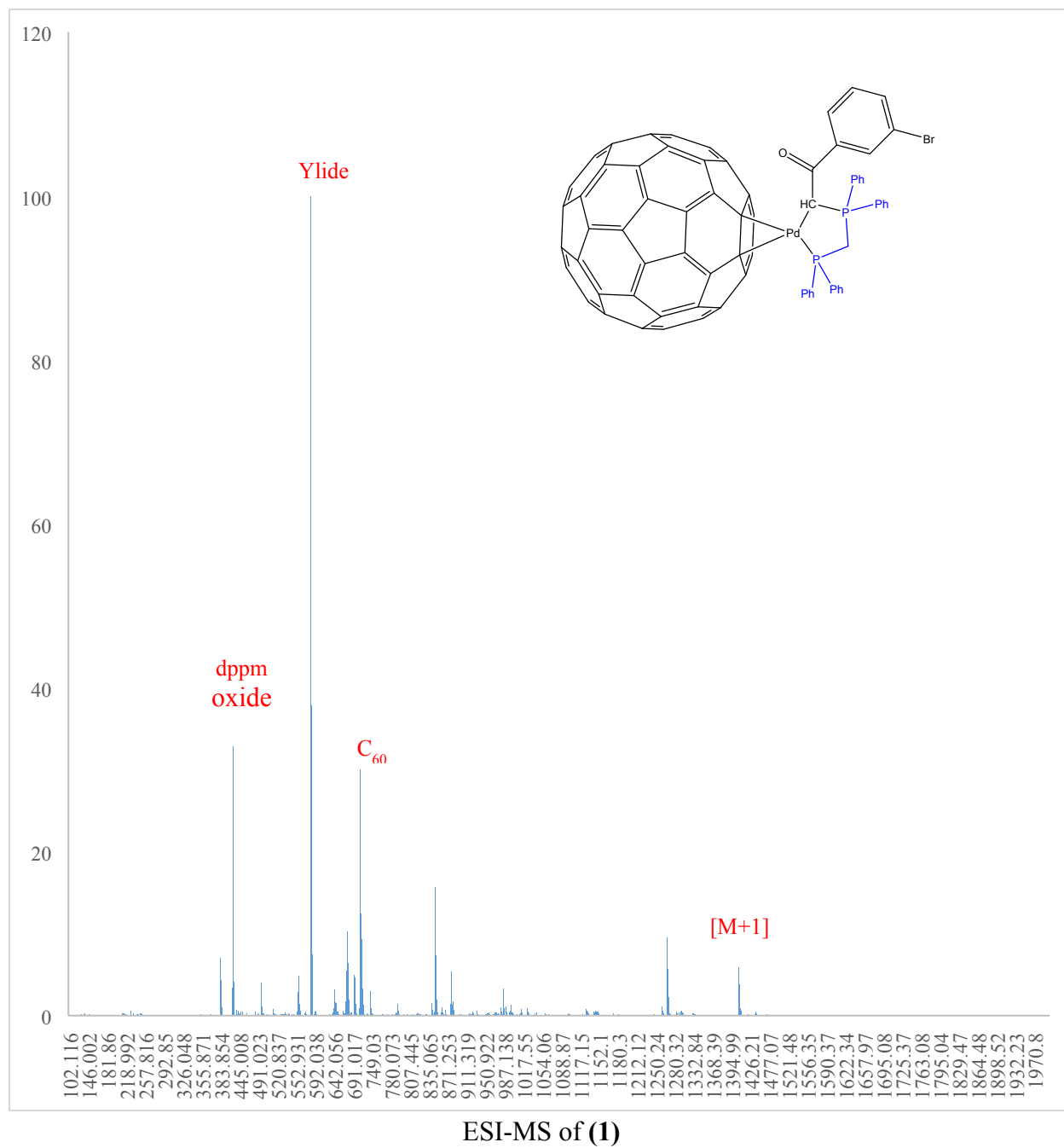
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PC 1.40

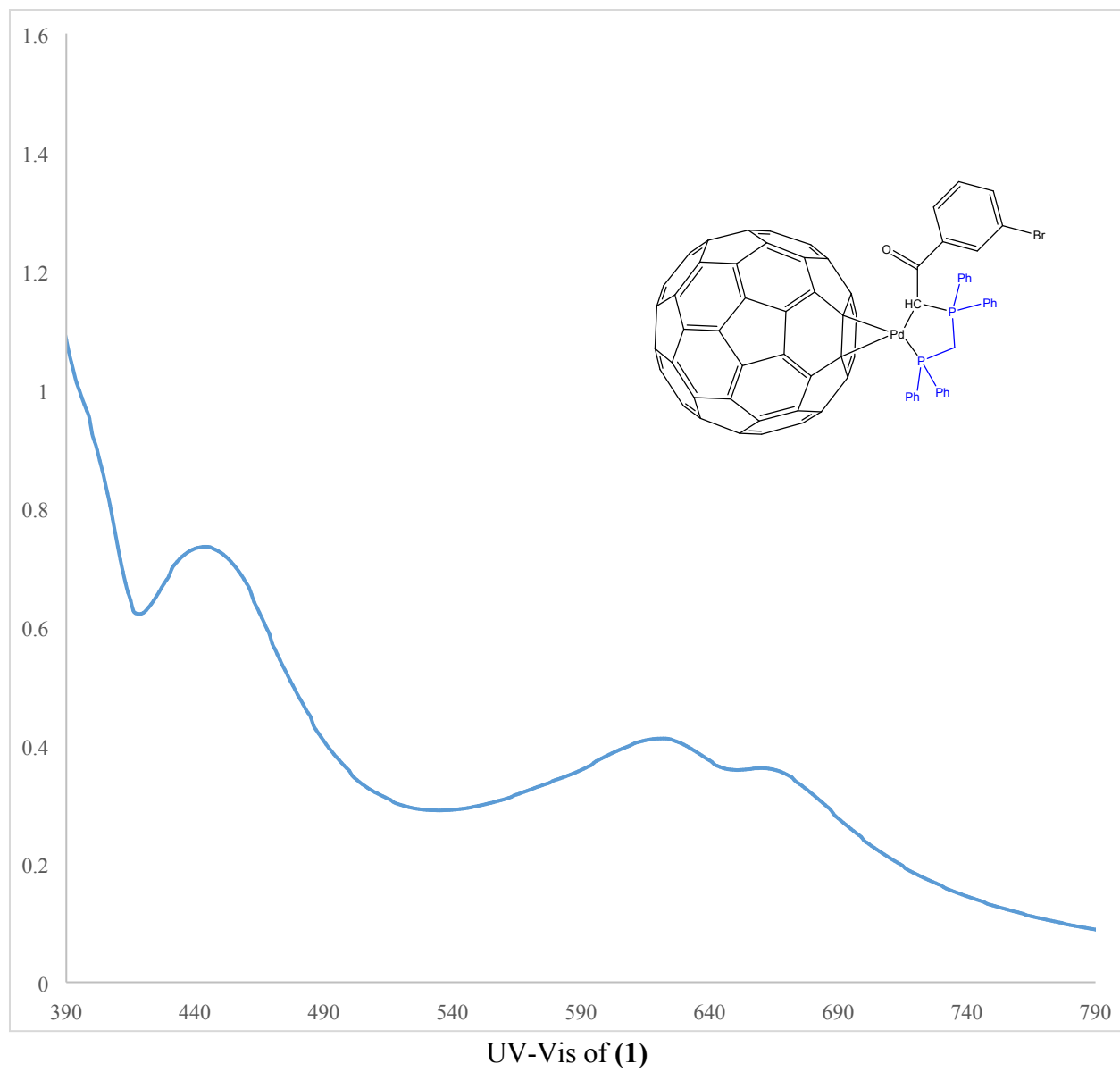


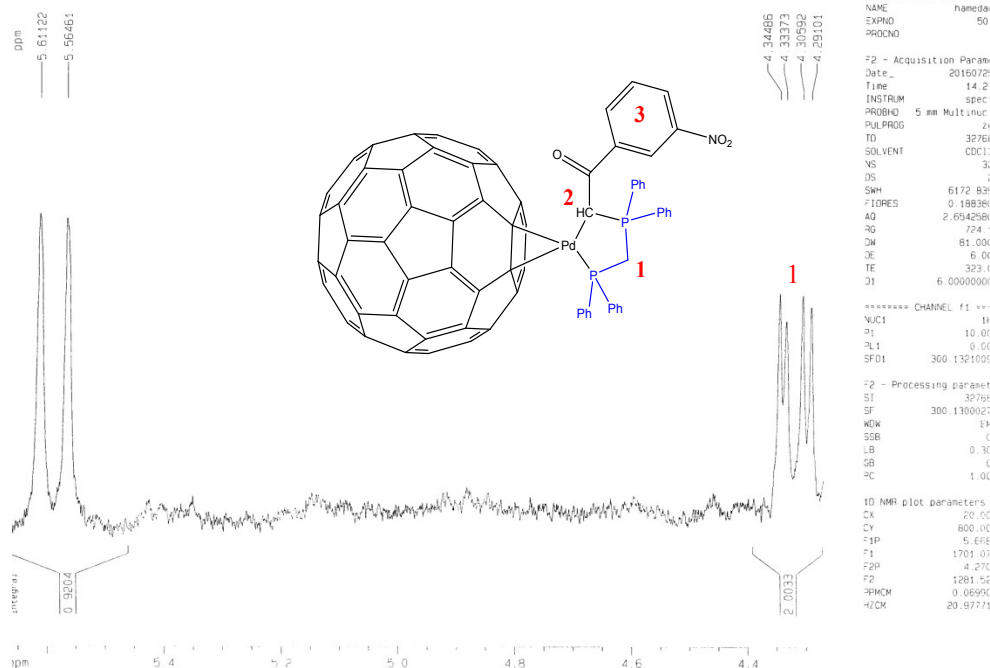
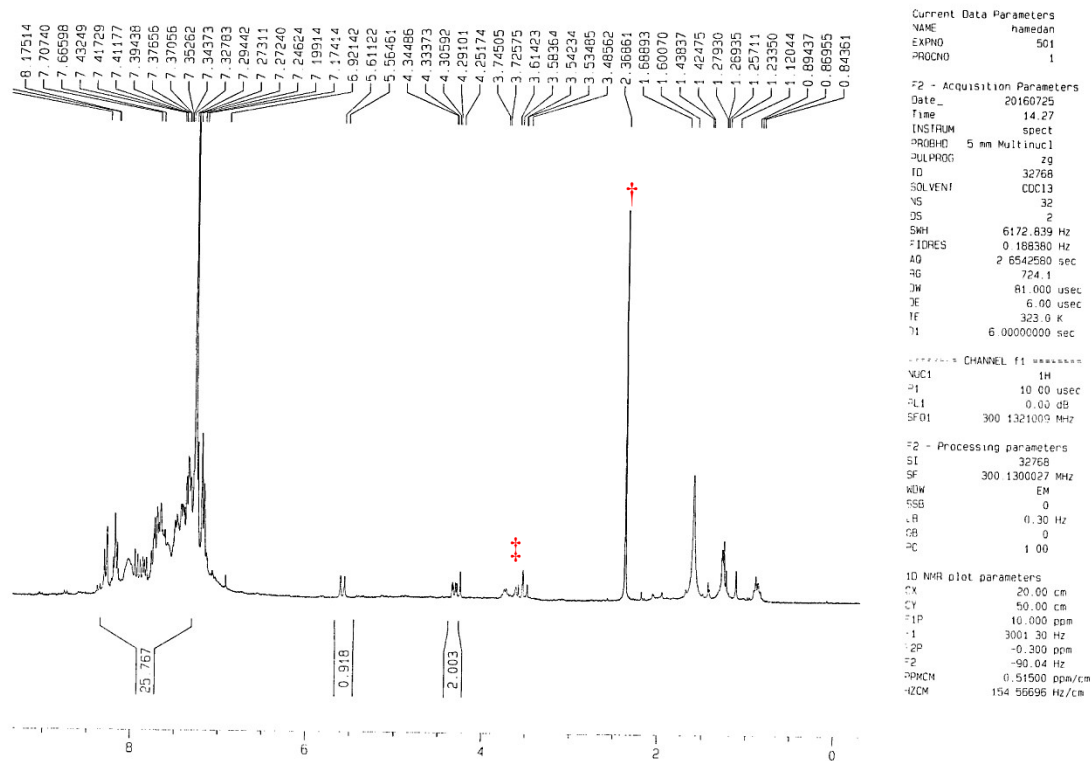
^{31}P NMR of (**1**)

† Ylide oxide
‡ Side product







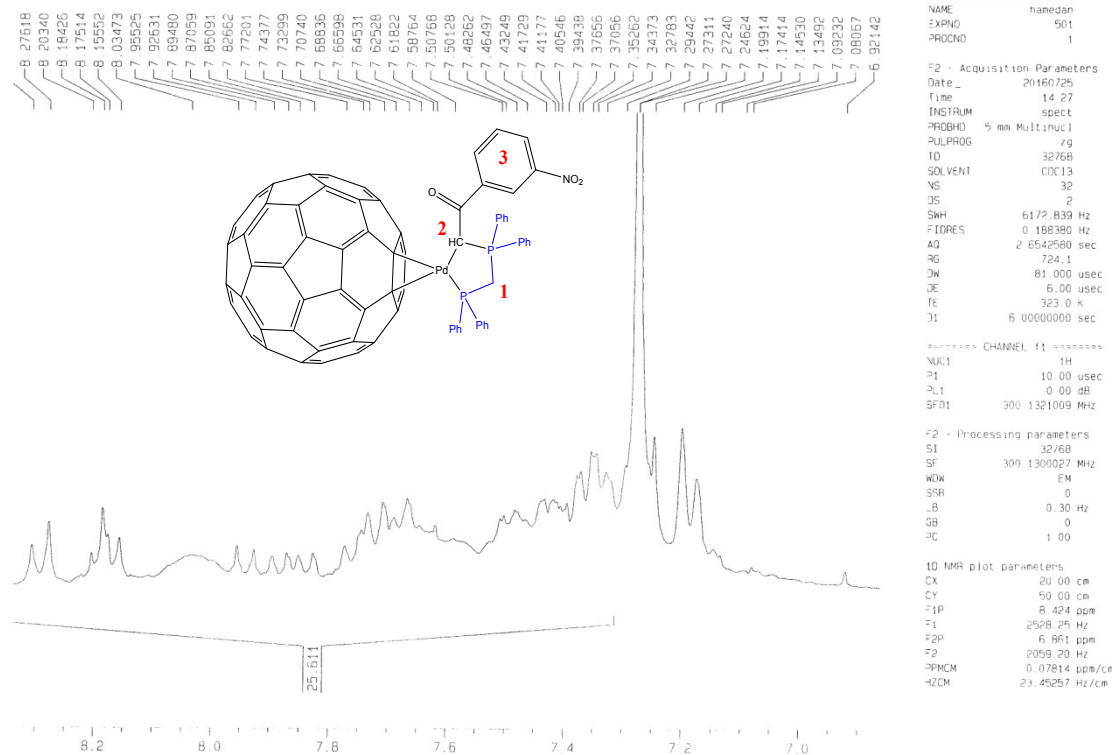


¹H NMR of (2)

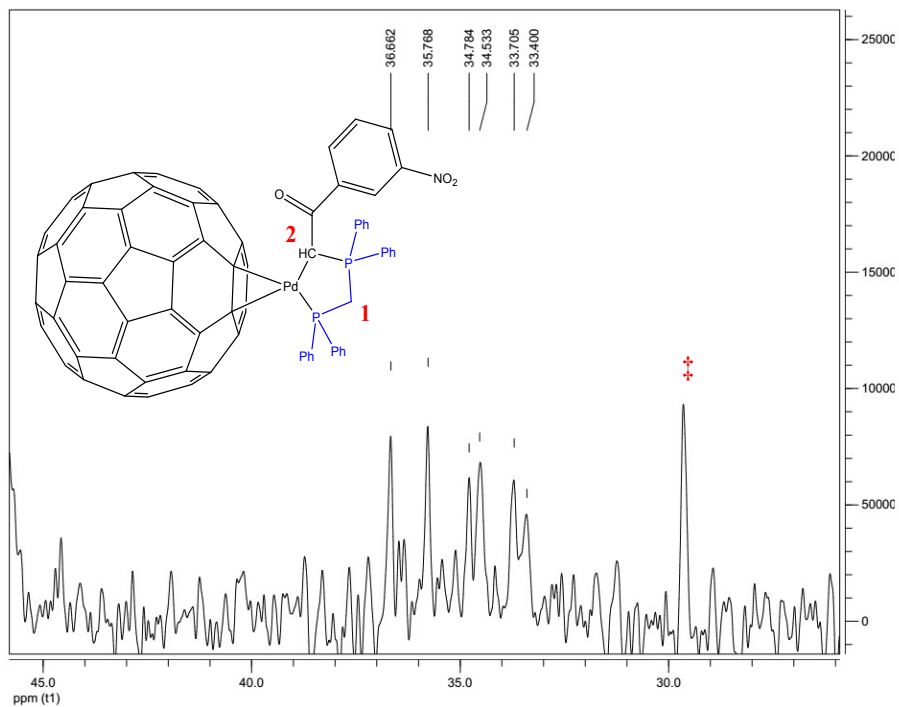
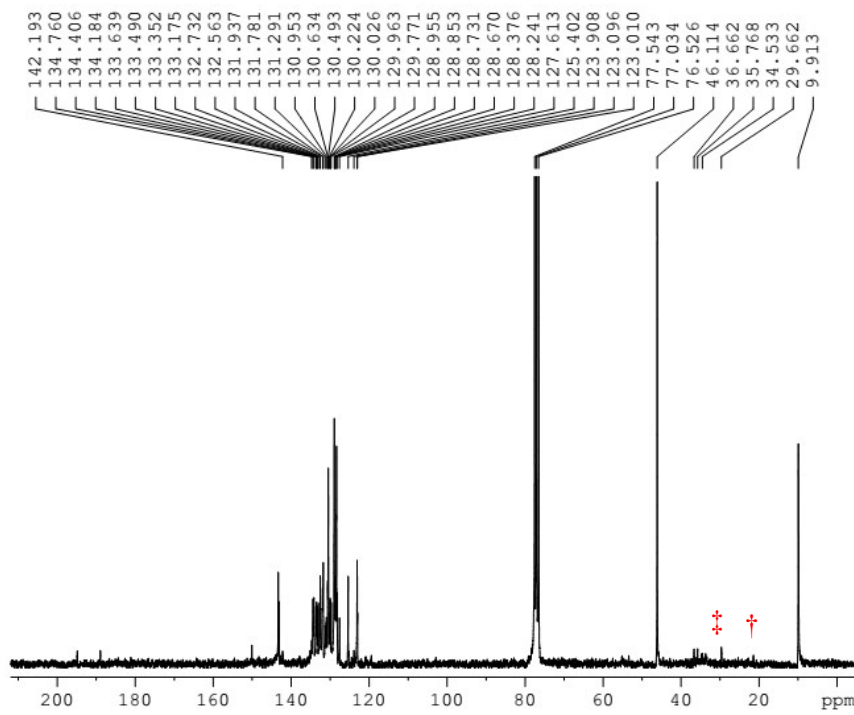
* n-Hexane

† Toluene

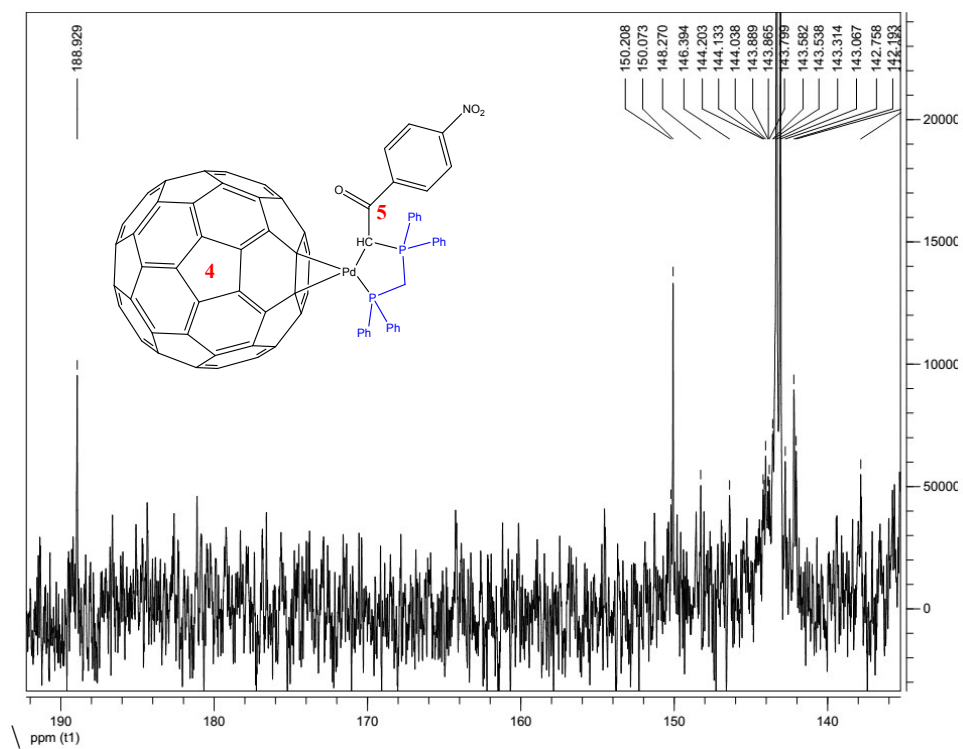
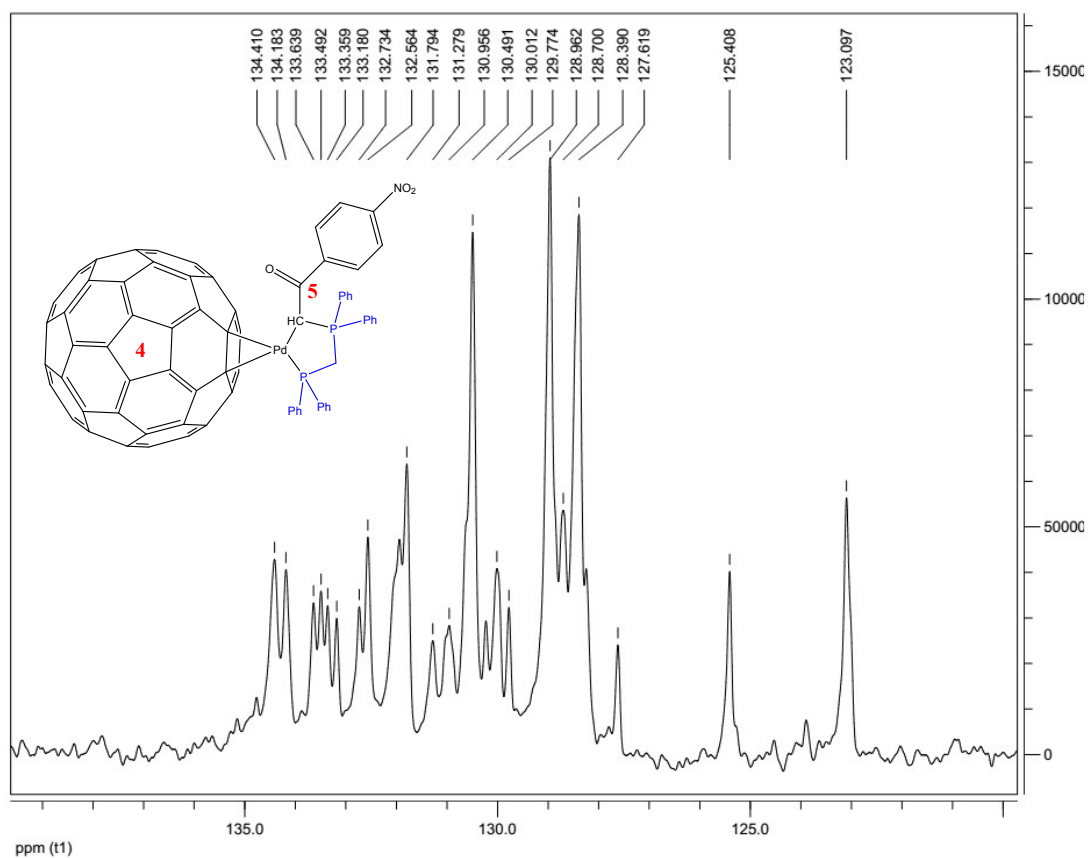
‡ dppm oxide



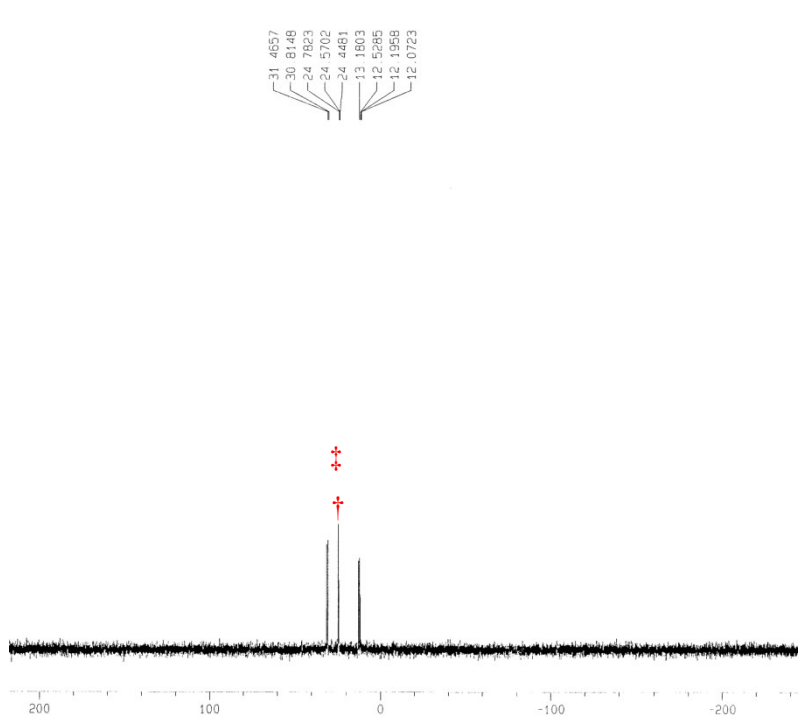
¹H NMR of (2)



* n-Hexane
† Toluene
‡ dppm oxide



^{13}C NMR of (2)



Current Data Parameters
NAME hamedan
EXPNO 502
PROCNO 1

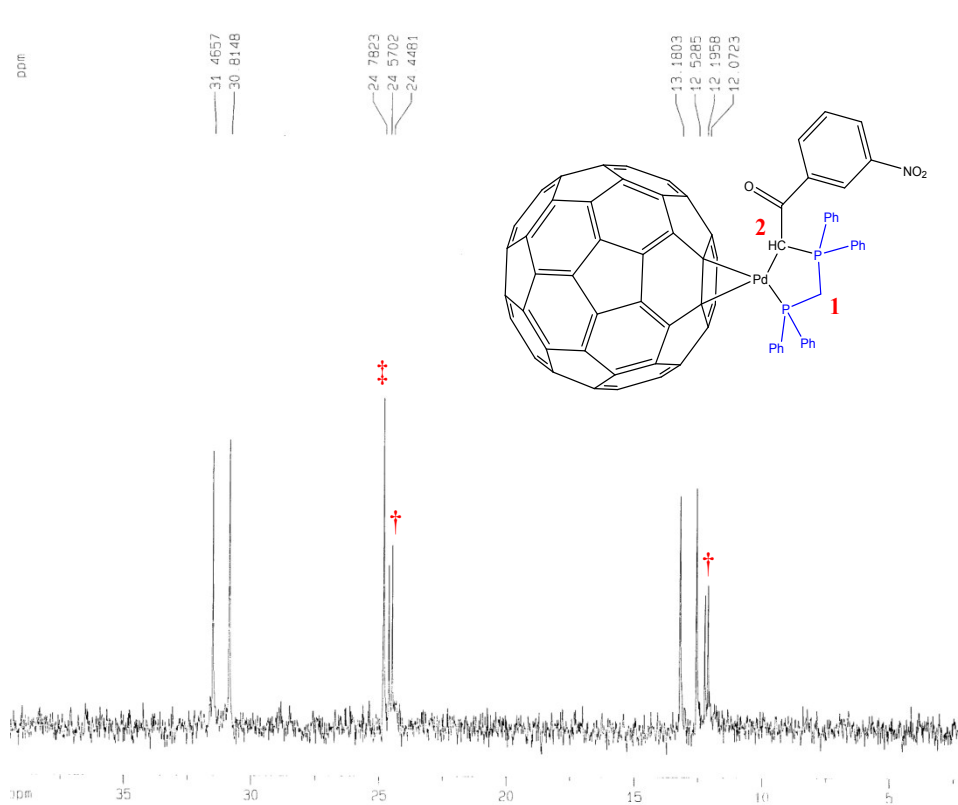
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Date_ 20160725
Time 14 19
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg
ID 65536
SOLVENT CDCl3
NS 128
DS 0
SWH 60606.062 Hz
FIDRES 0.924775 Hz
AQ 0.5407220 sec
RG 18390.4
JK 8.250 usec
JE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

***** CHANNEL f1 *****
NUC1 31P
P1 6.75 usec
PL1 0.00 dB
SFO1 121.4948360 MHz

***** CHANNEL f2 *****
CPDPRG2 wait116
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 21.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 121.4948360 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 3.00 cm
F1P -249.418 ppm
F1 30303.04 Hz
F2P -249.418 ppm
F2 -30303.03 Hz
PRMCM 24.94183 ppm/cm
HZCM 3030.30298 Hz/cm



Current Data Parameters
NAME hamed
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 201607
Time 14
INSTRUM spe
PROBHD 5 mm Multinucl
PULPROG zg
ID 655
SOLVENT CDCl3
NS 1
DS 0
SWH 60606.0
FIDRES 0.9247
AQ 0.54072
RG 18390
JK 8.2
JE 6.0
TE 300
D1 2.000000
d11 0.030000
d12 0.000020

***** CHANNEL f1 *****
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P1 6.75 usec
PL1 0.00 dB
SFO1 121.4948360 MHz

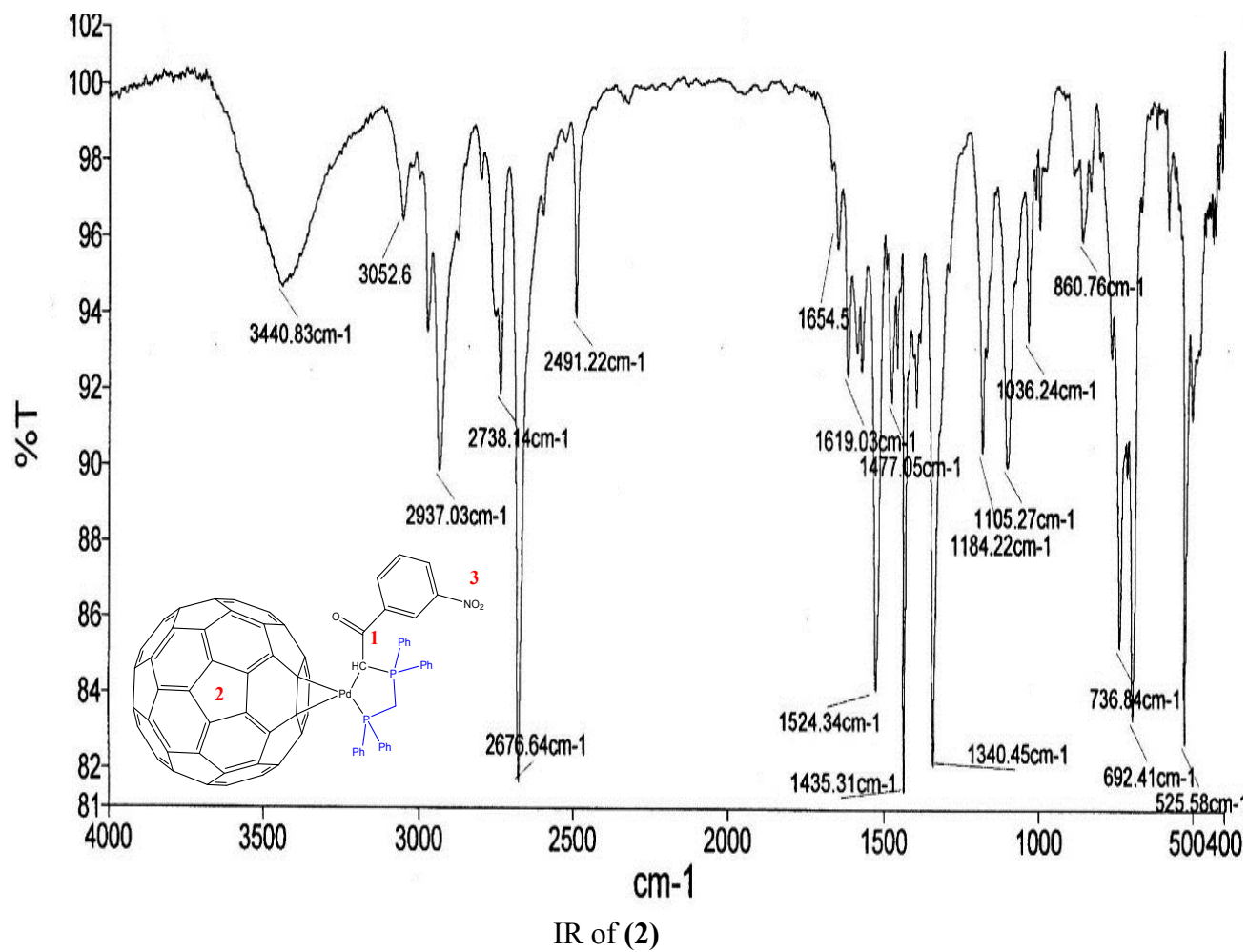
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PL12 21.00 dB
PL13 21.00 dB
SFO2 300.1312005 MHz

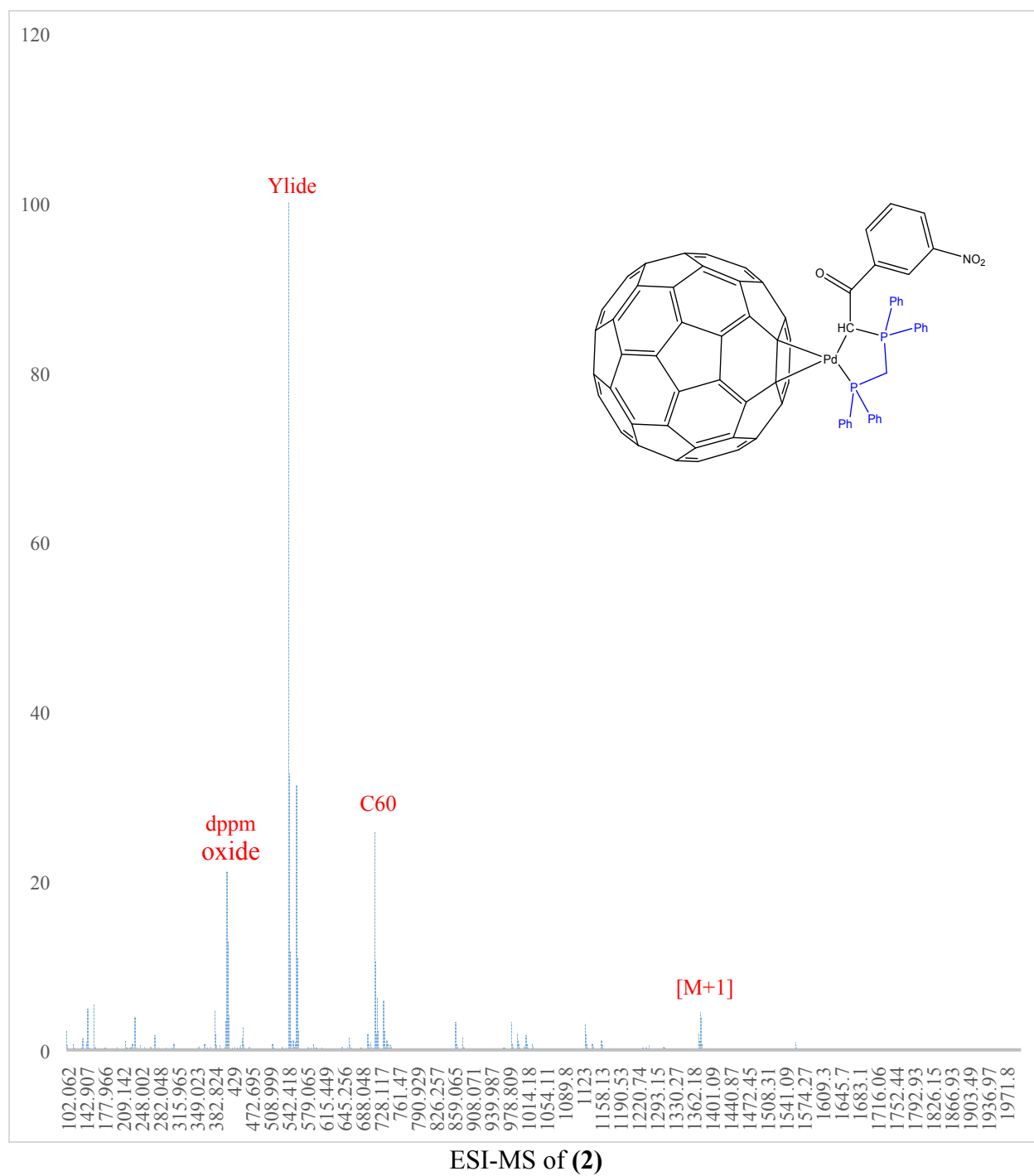
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GB 0
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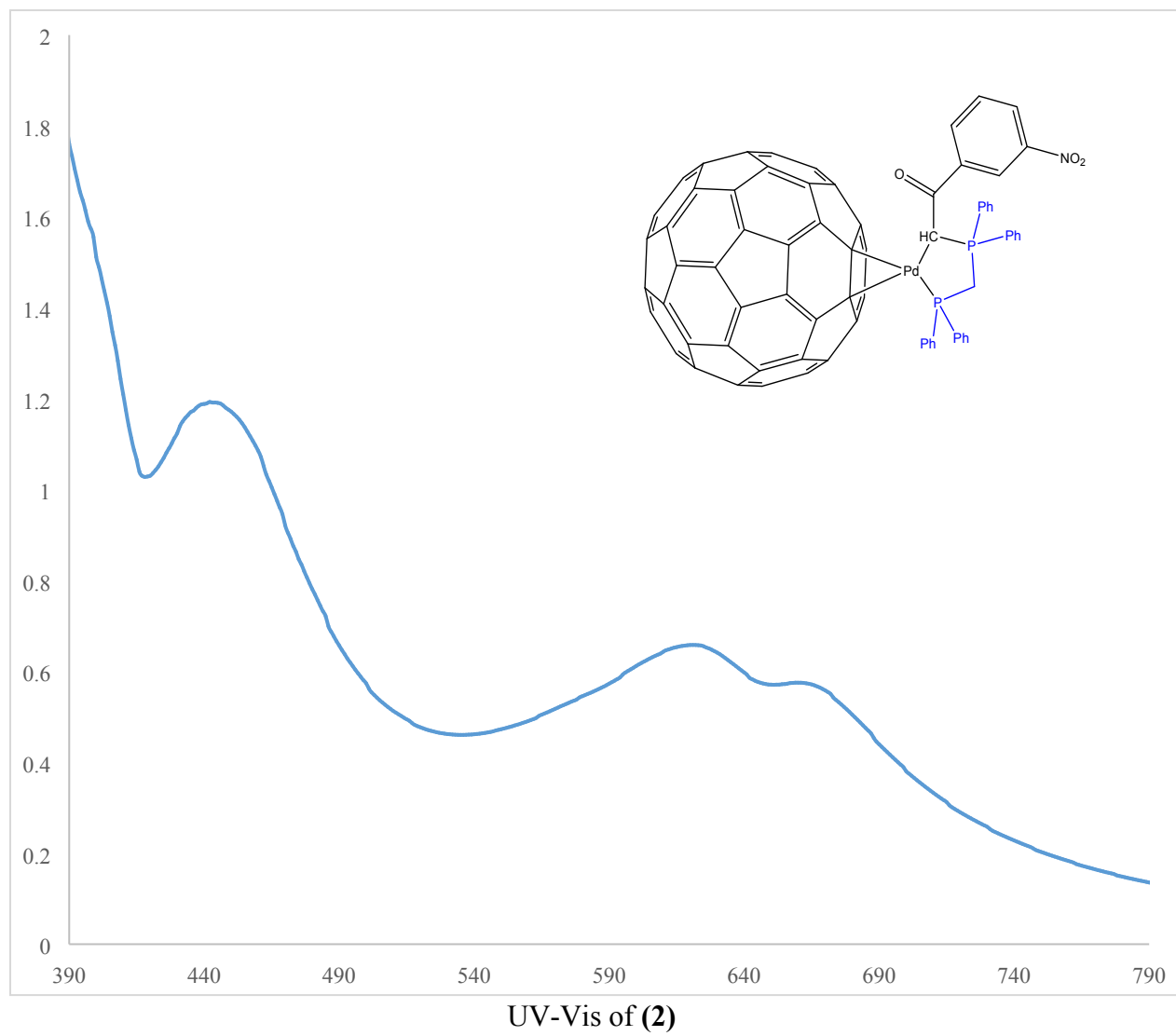
1D NMR plot parameters
CX 20.00 cm
CY 3.00 cm
F1P -249.418 ppm
F1 30303.04 Hz
F2P -249.418 ppm
F2 -30303.03 Hz
PRMCM 24.94183 ppm/cm
HZCM 3030.30298 Hz/cm

³¹P NMR of (2)

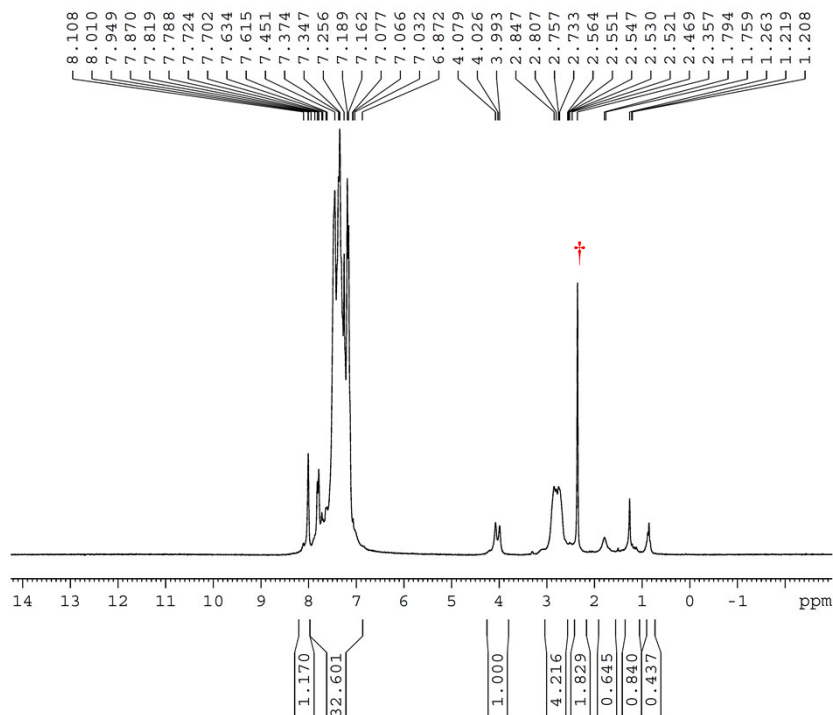
† Ylide oxide
‡ dppm oxide







Hashemi-dppe-m-Br

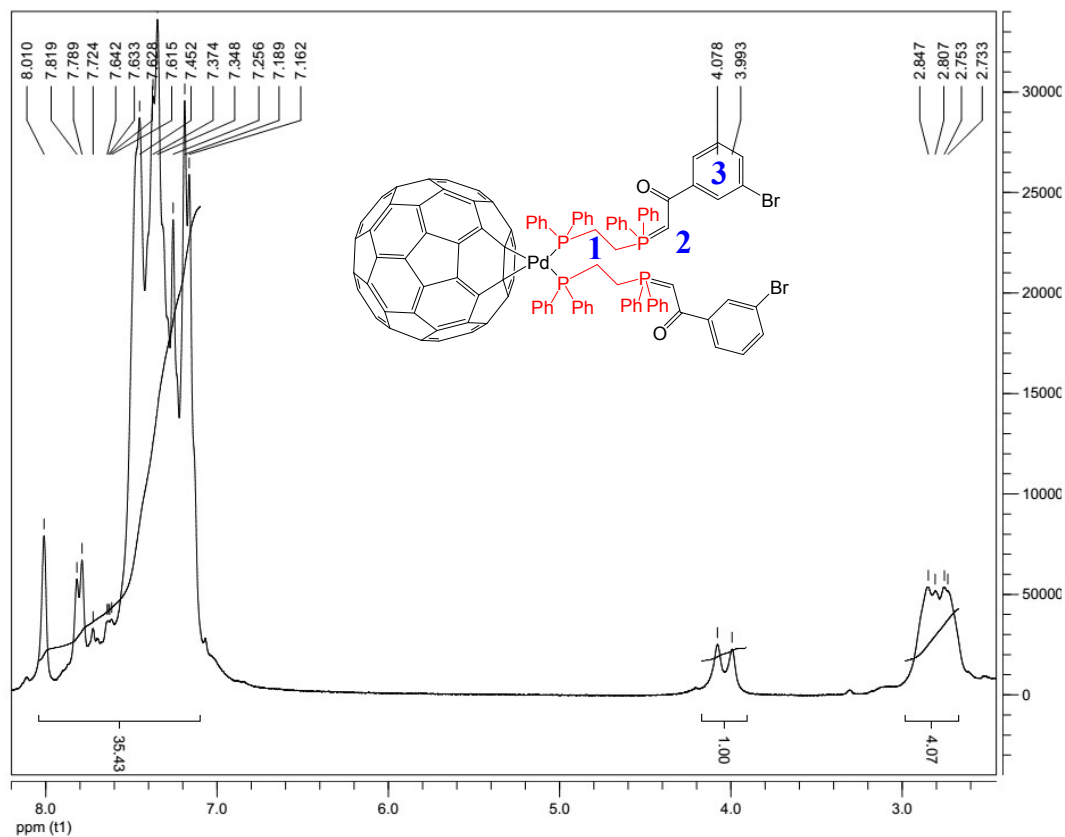


Current Data Parameters
NAME hamedan
EXPNO 235
PROCNO 1

F2 - Acquisition Parameters
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Time 12.25
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PULPROG zg
TD 16384
SOLVENT CDCl3
NS 10
DS 0
SWH 4496.403 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 256
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 3.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 3.00 dB
SFO1 250.1315008 MHz

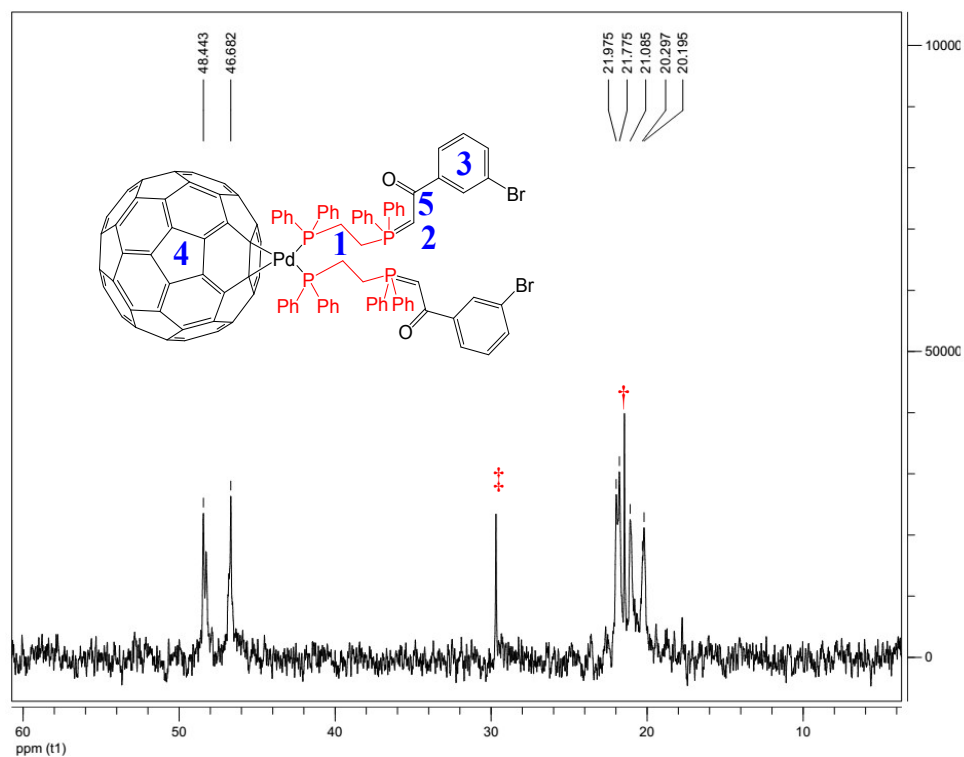
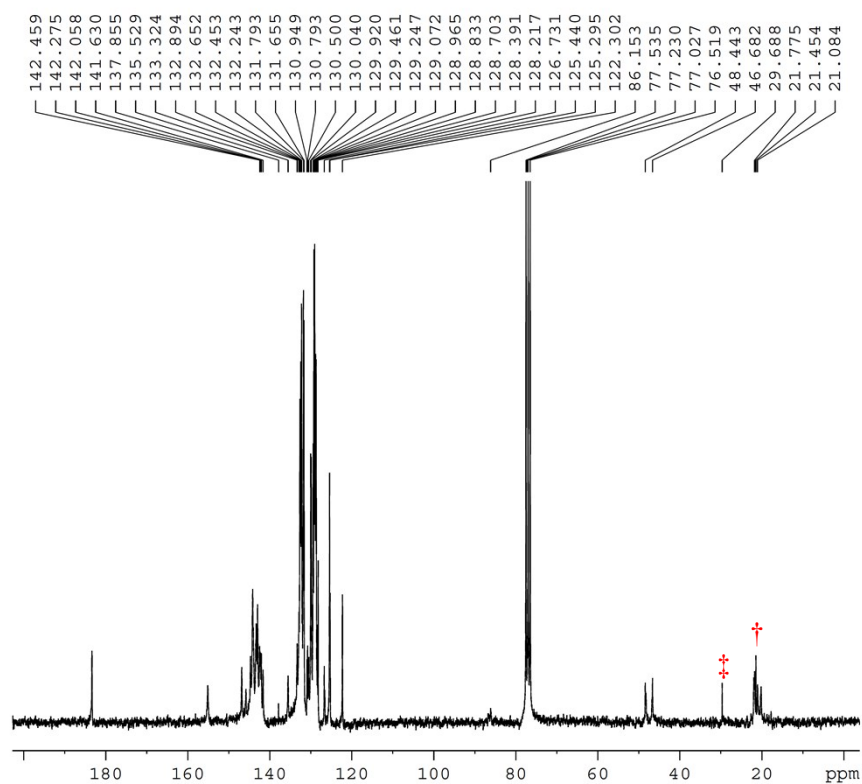
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^1H NMR of (3)

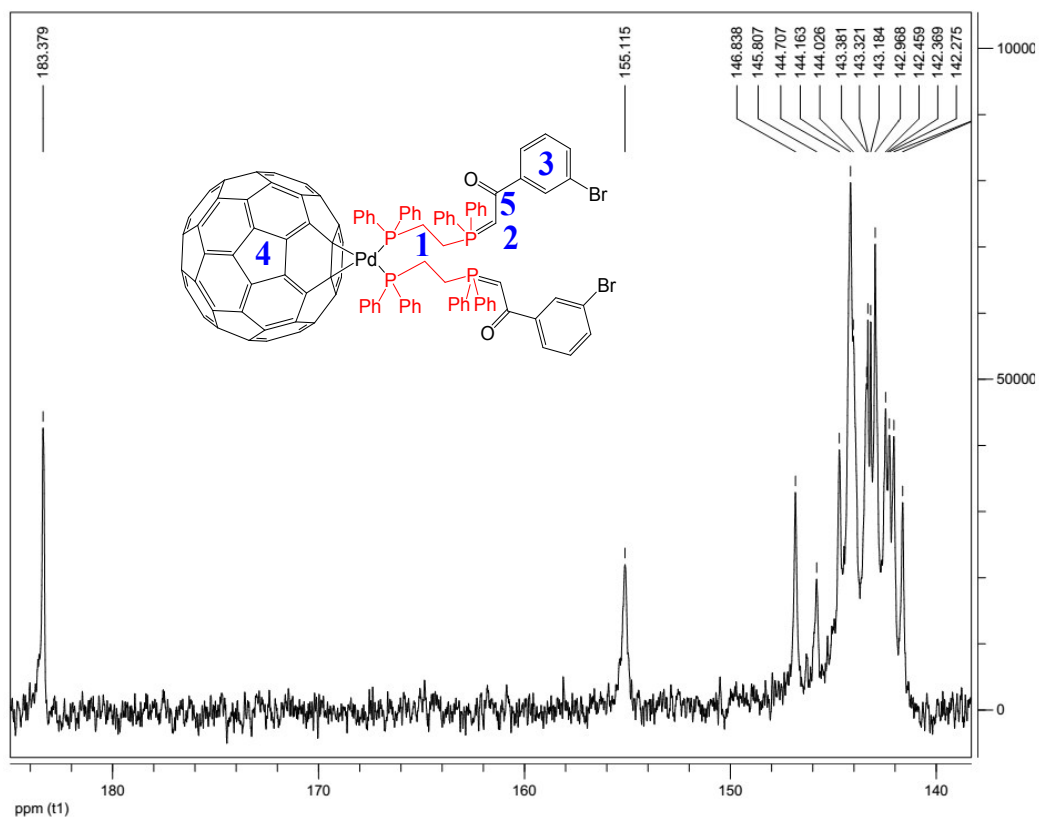
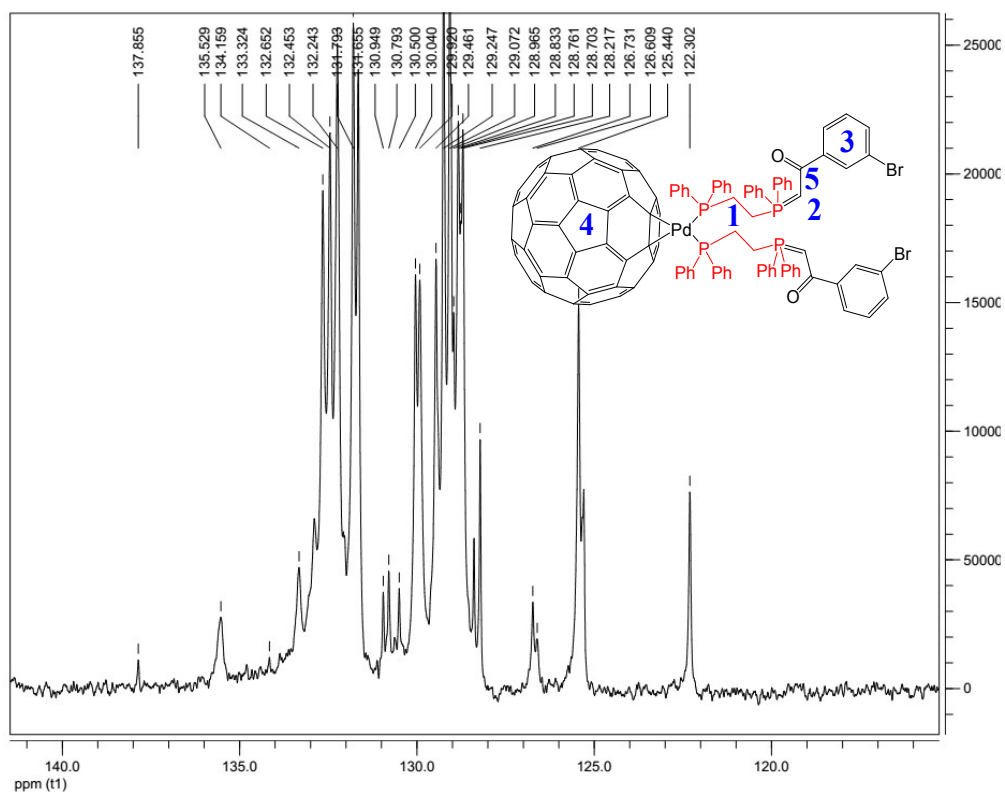
† Toluene

HAShemi-dppe m-Br



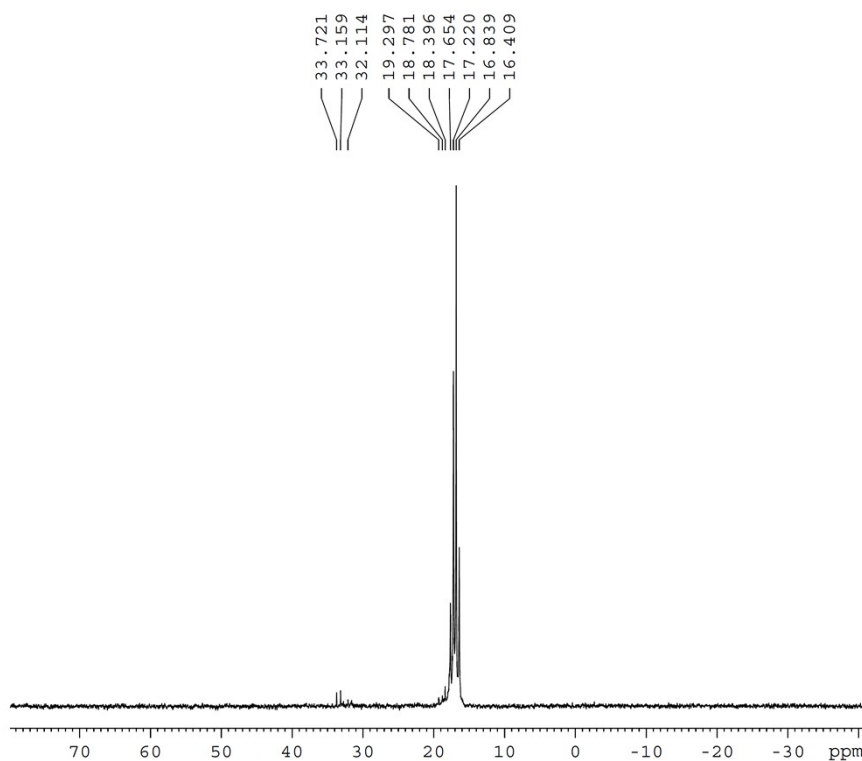
¹³C NMR of (3)

† Toluene
 ‡ dppe oxide



^{13}C NMR of (3)

hashemi-dppe-m-Br



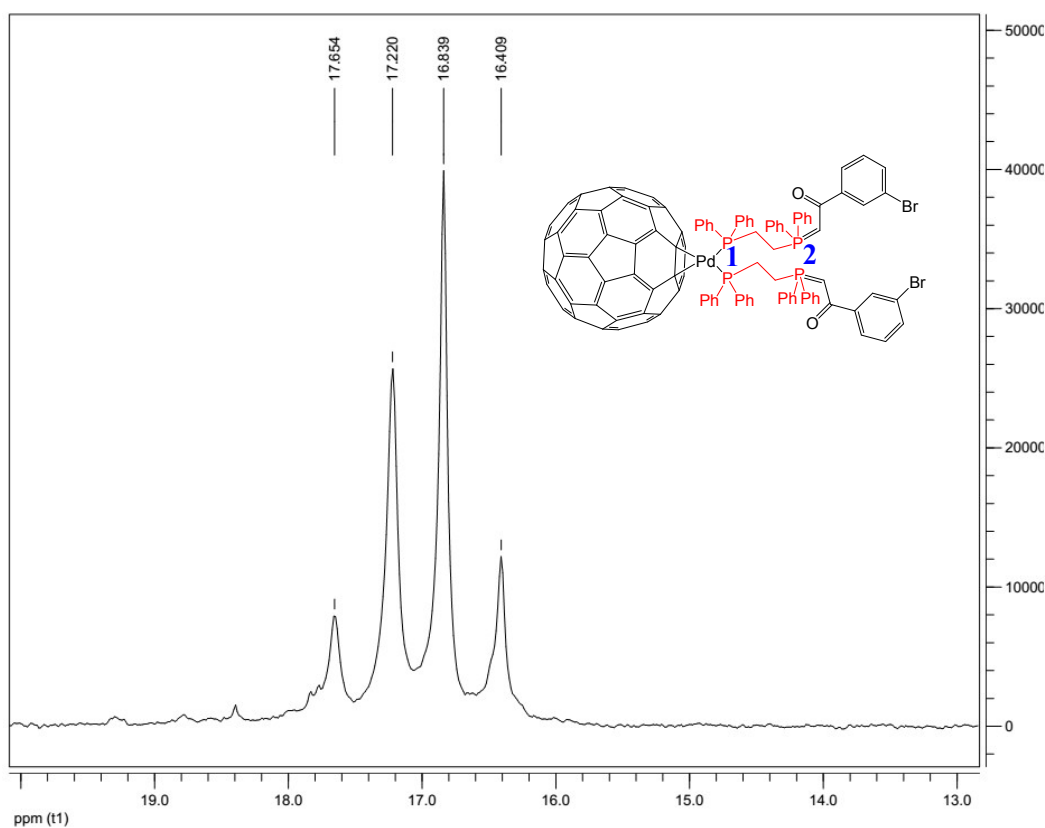
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EXPNO 234
PROCNO 1

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PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 20
DS
SWH 40650.406 Hz
FIDRES 0.620276 Hz
AQ 0.8061428 sec
RG 22800
DW 12.300 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

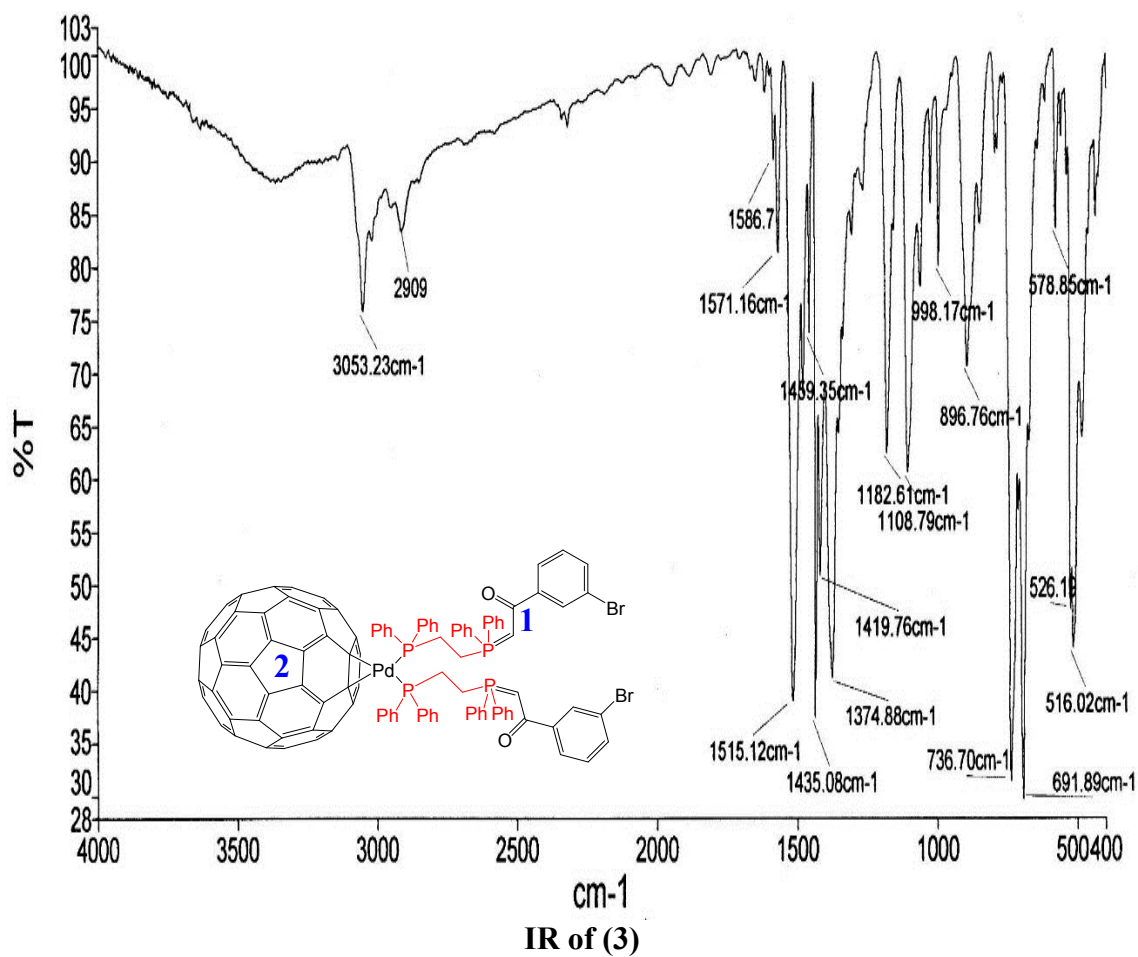
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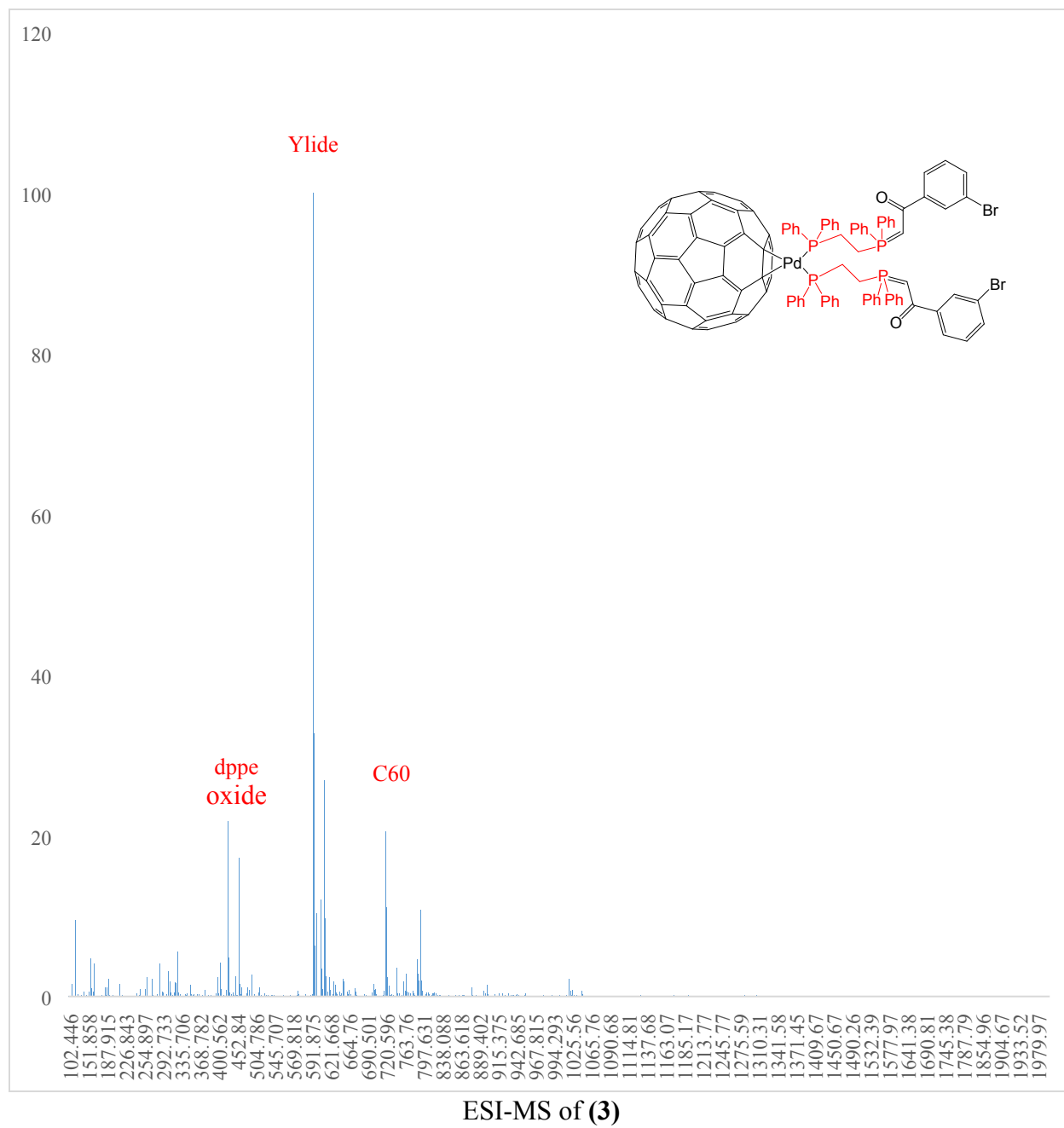
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PL13 23.00 dB
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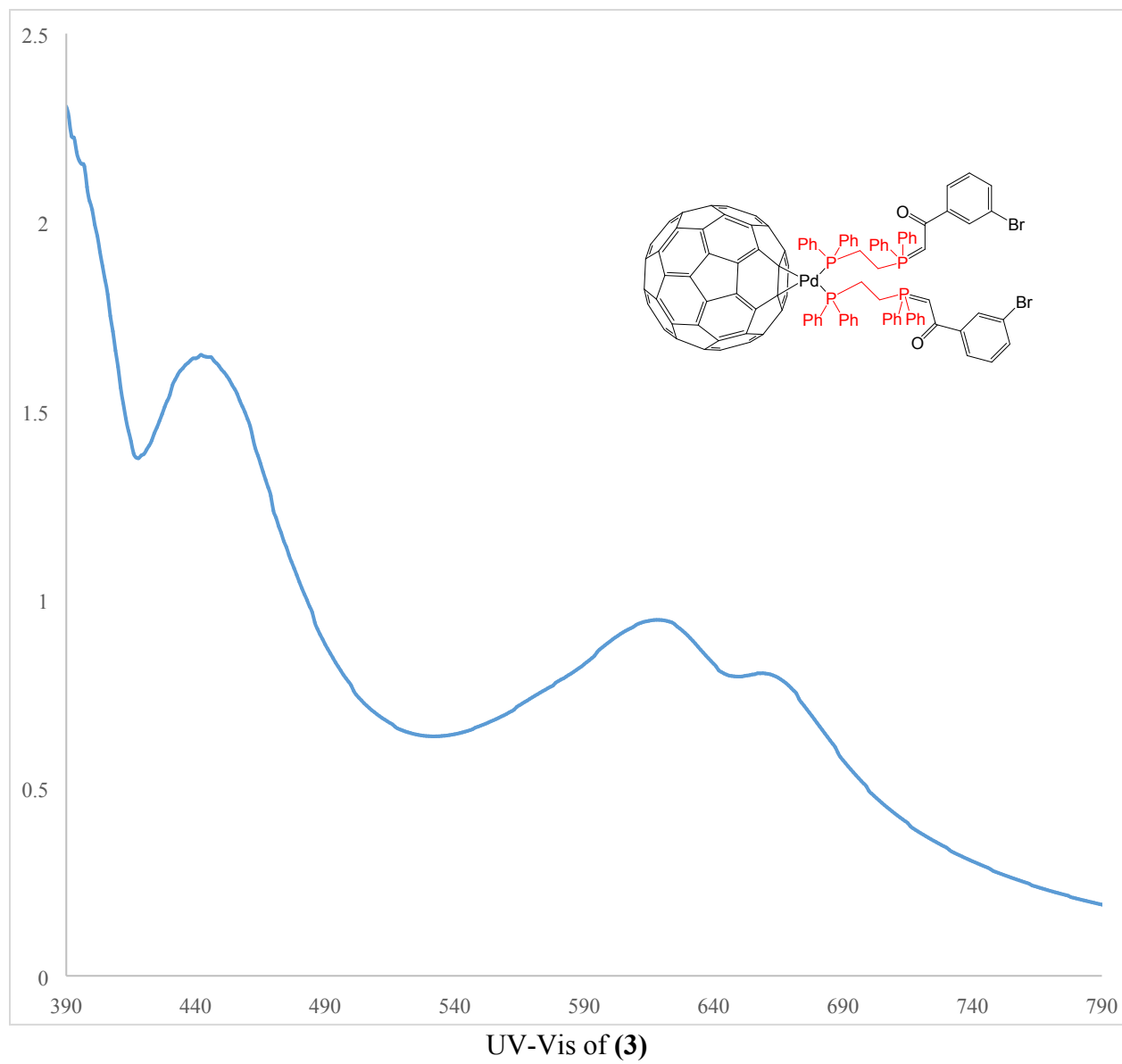
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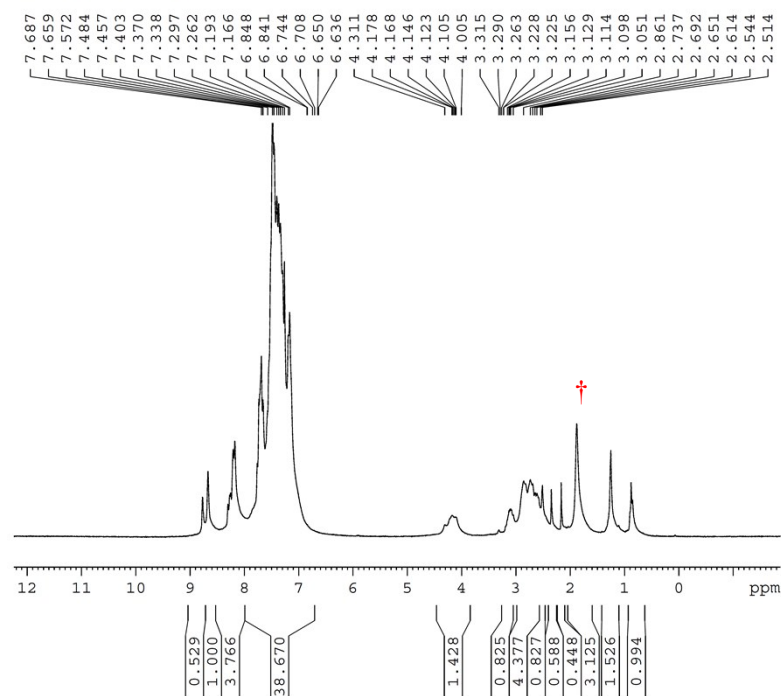
^{31}P NMR of (3)







Hosseinzadeh-60-NE

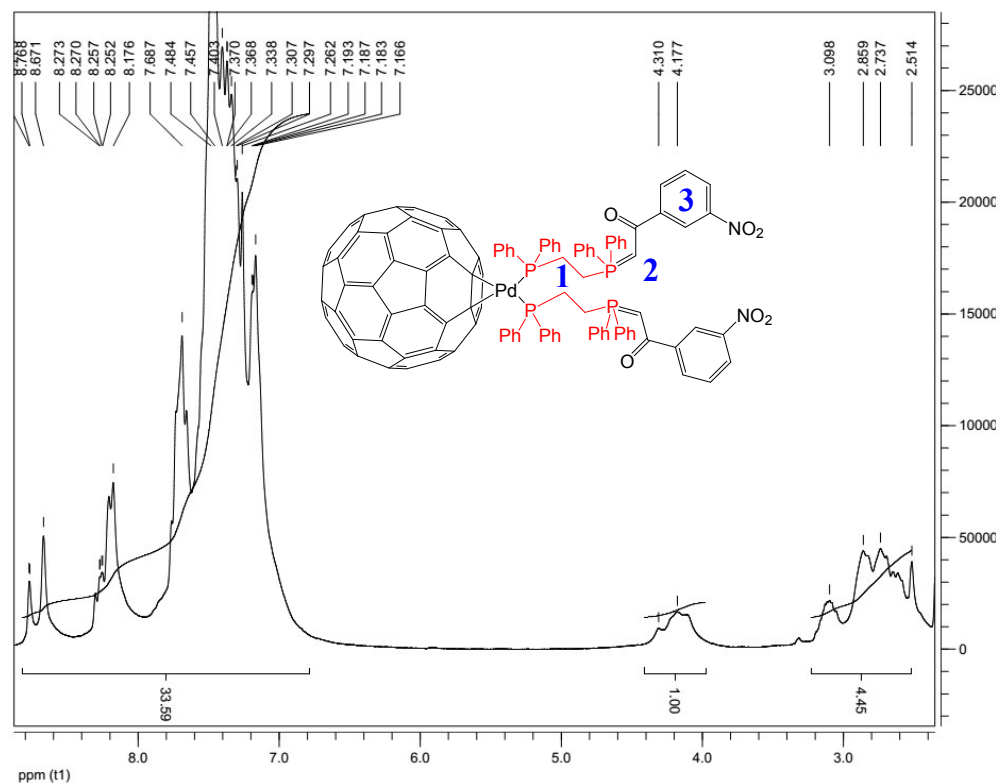


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PROCNO 1

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TD 16384
SOLVENT CDCl3
NS 30
DS 0
SWH 4496.403 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 256
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 3.0000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 9.00 usec
PL1 3.00 dB
SFO1 250.1315008 MHz

F2 - Processing parameters
SI 32768
SF 250.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

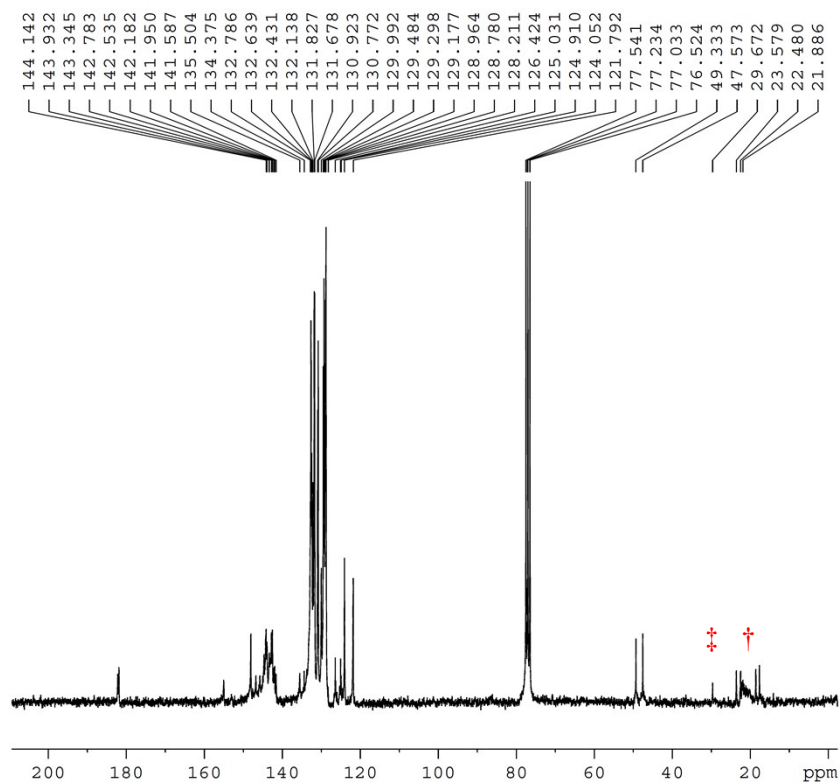


¹H NMR of (4)

* n-Hexane

† Toluene

Hosseinzadeh-60-NE



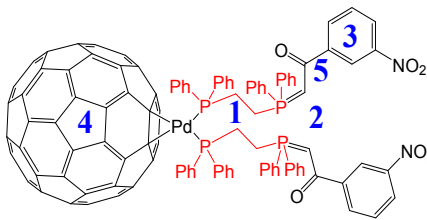
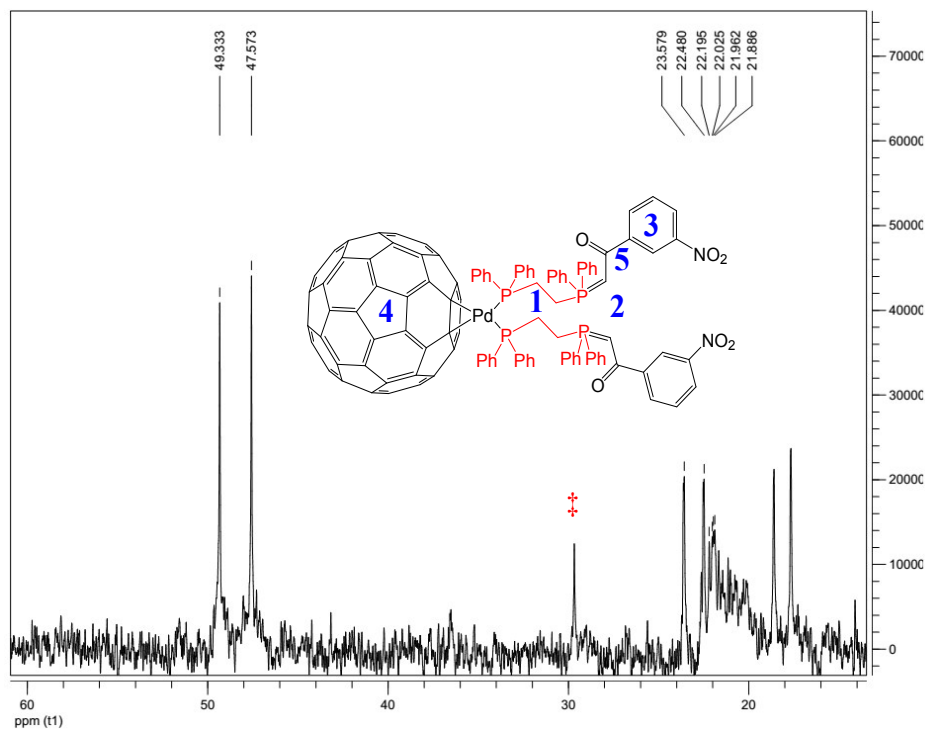
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SOLVENT CDCl3
NS 10000
DS 0
SWH 13812.154 Hz
FIDRES 0.210757 Hz
AQ 2.3724532 sec
RG 32768
DW 36.200 usec
DE 6.00 usec
TE 300.0 K
D1 3.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
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PL1 0.00 dB
SFO1 62.9018430 MHz

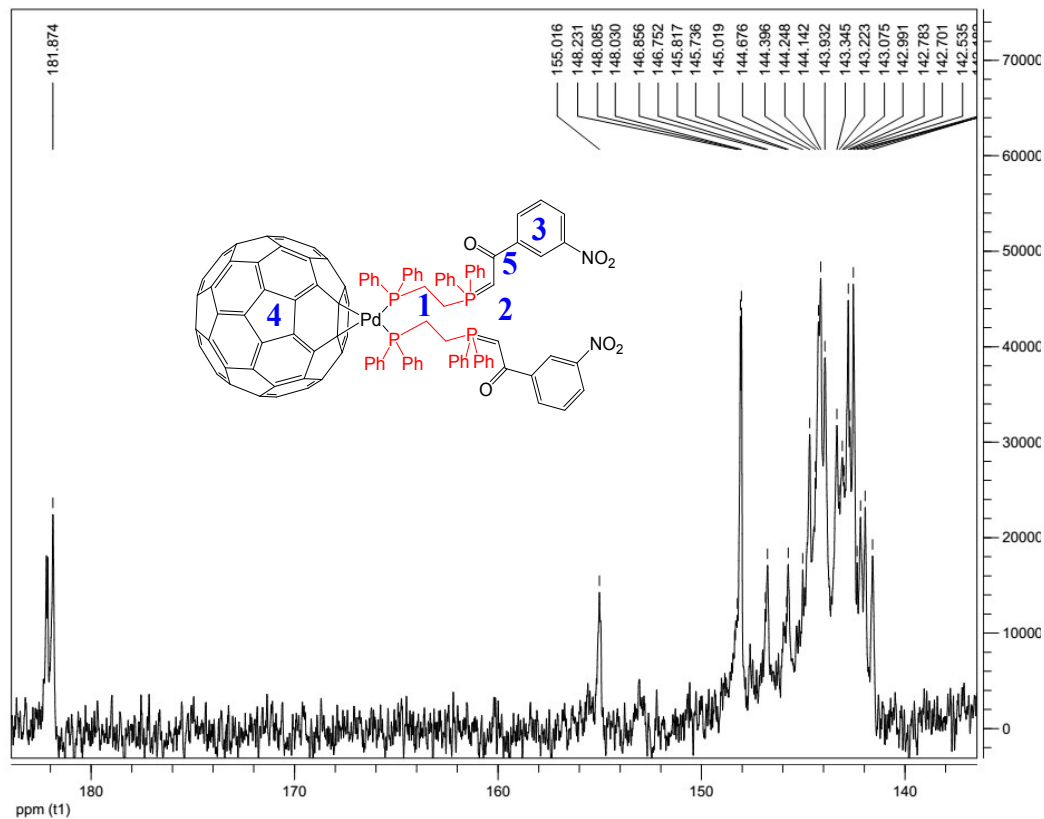
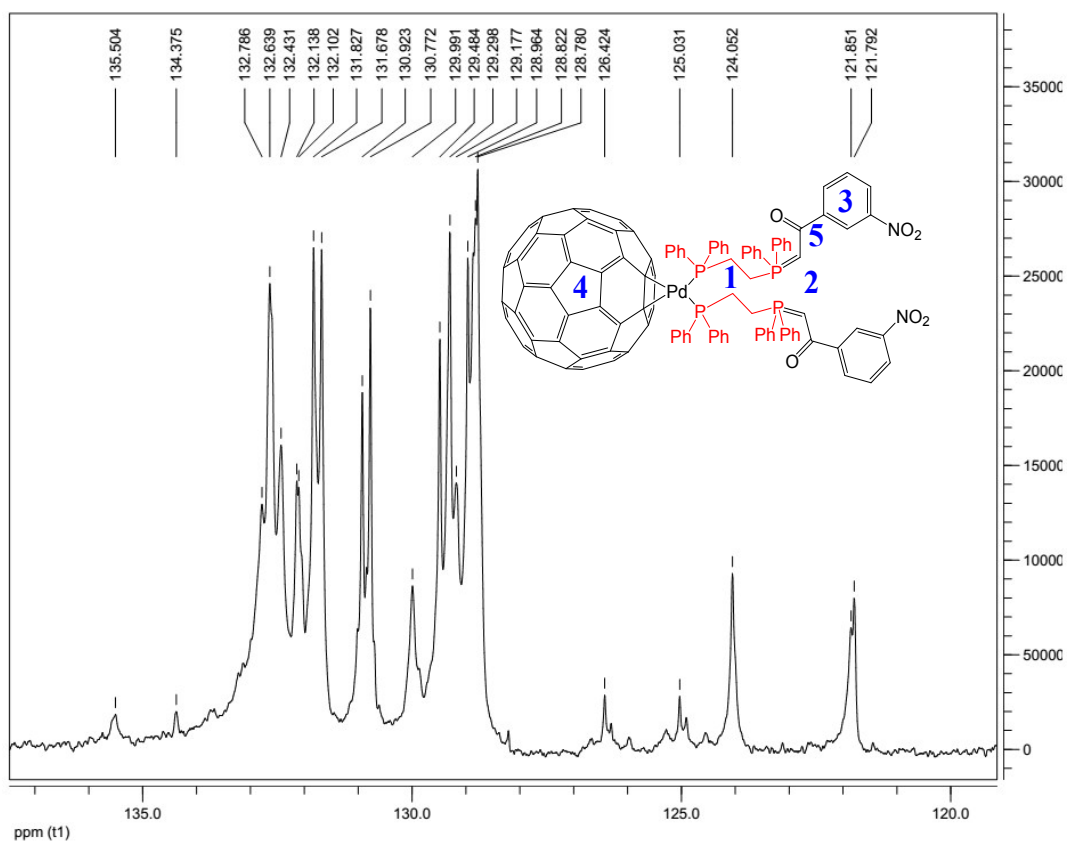
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NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 21.50 dB
PL13 23.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952390 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
FC 1.40

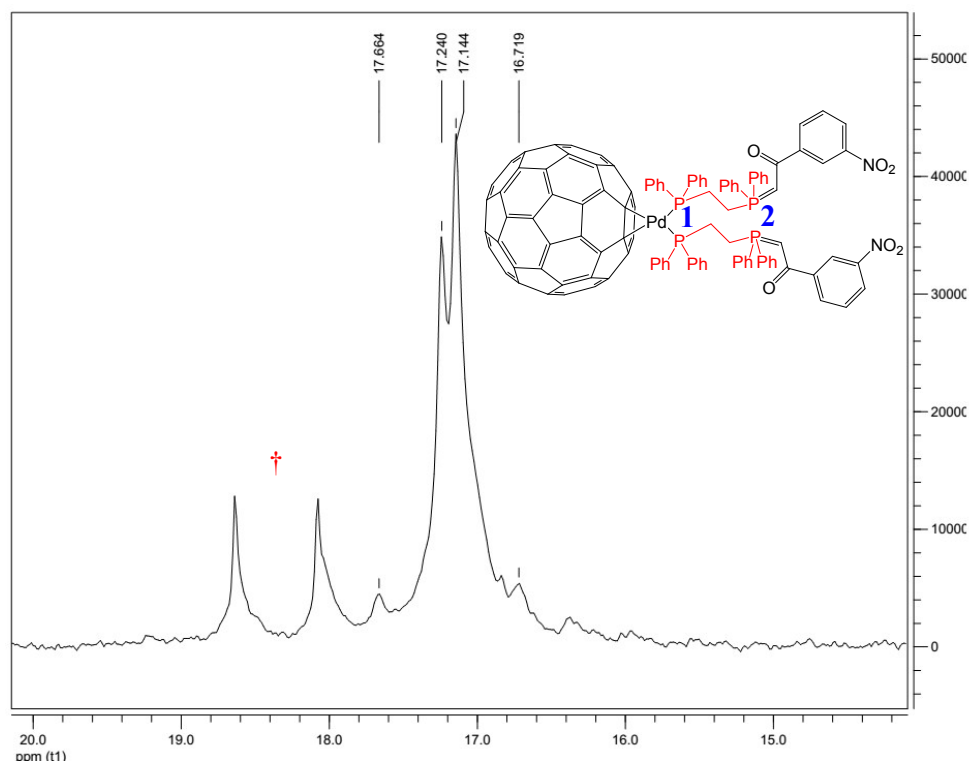
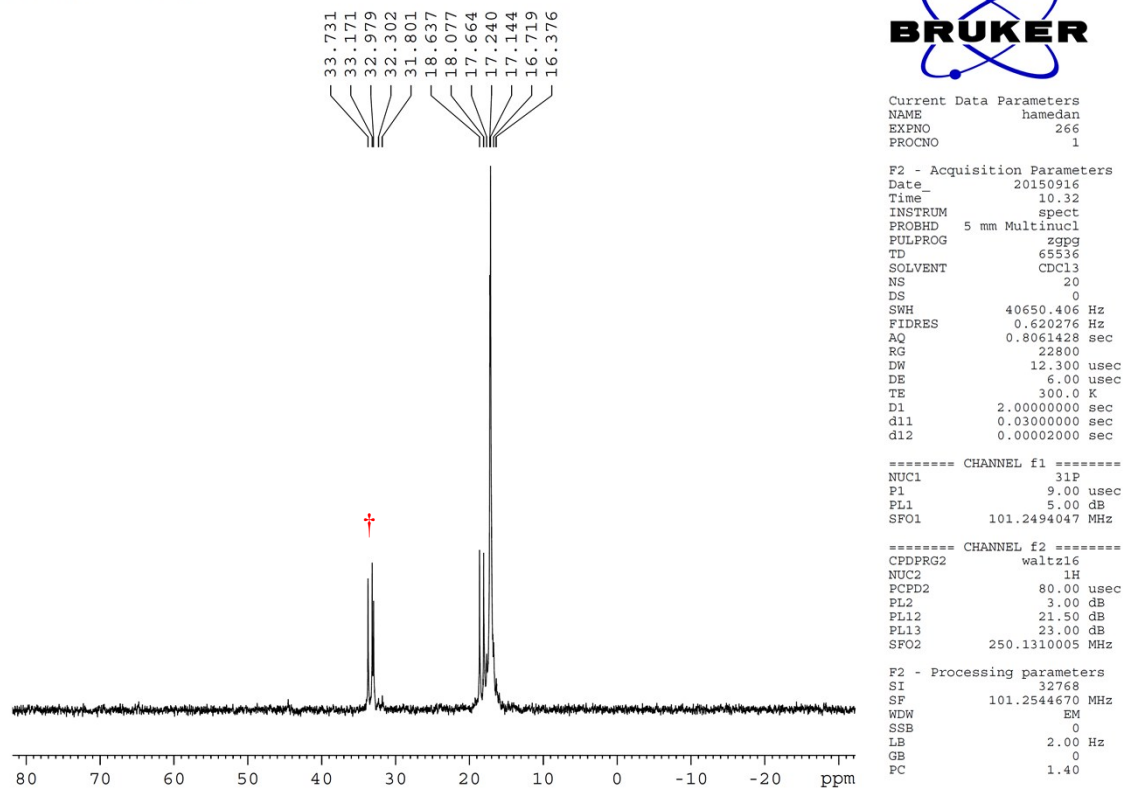


¹³C NMR of (4)

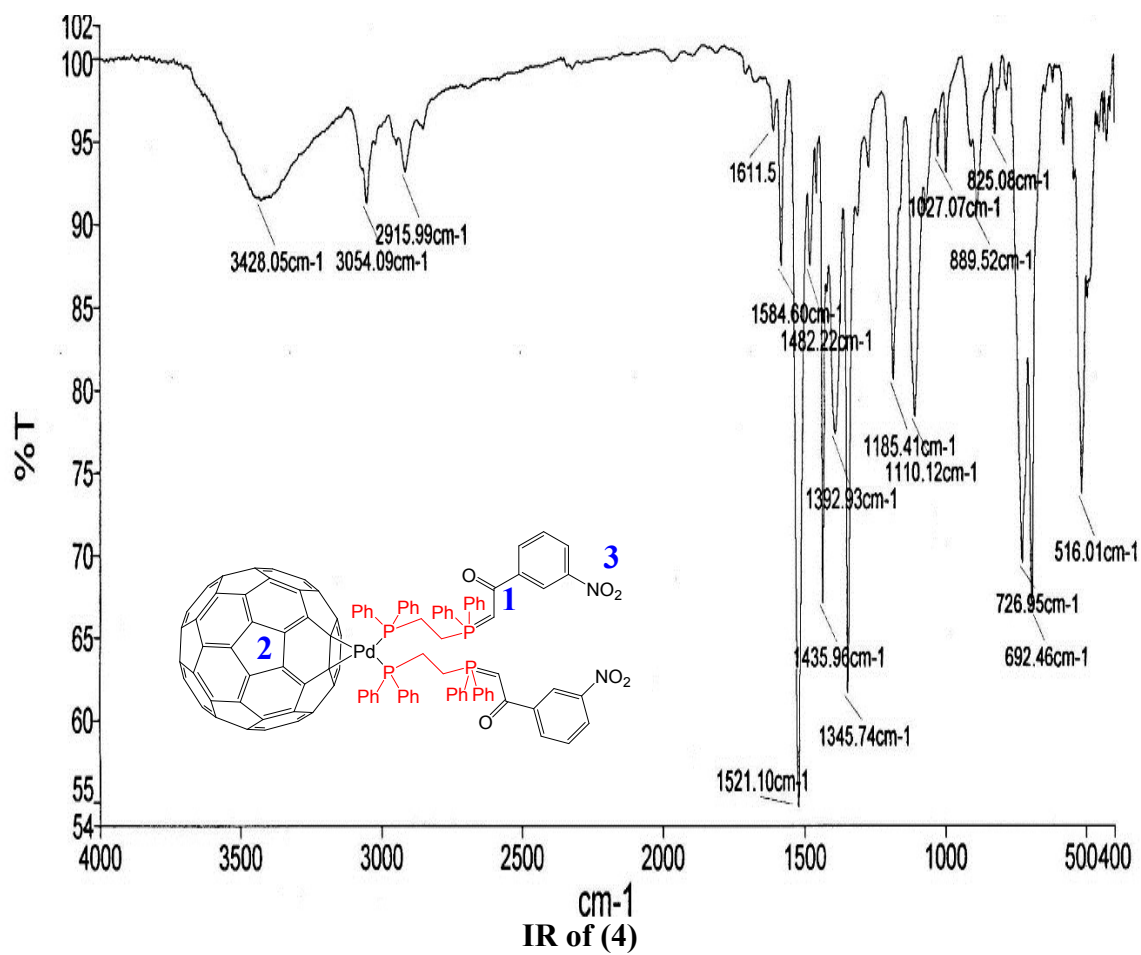
† Toluene
‡ dppe oxide

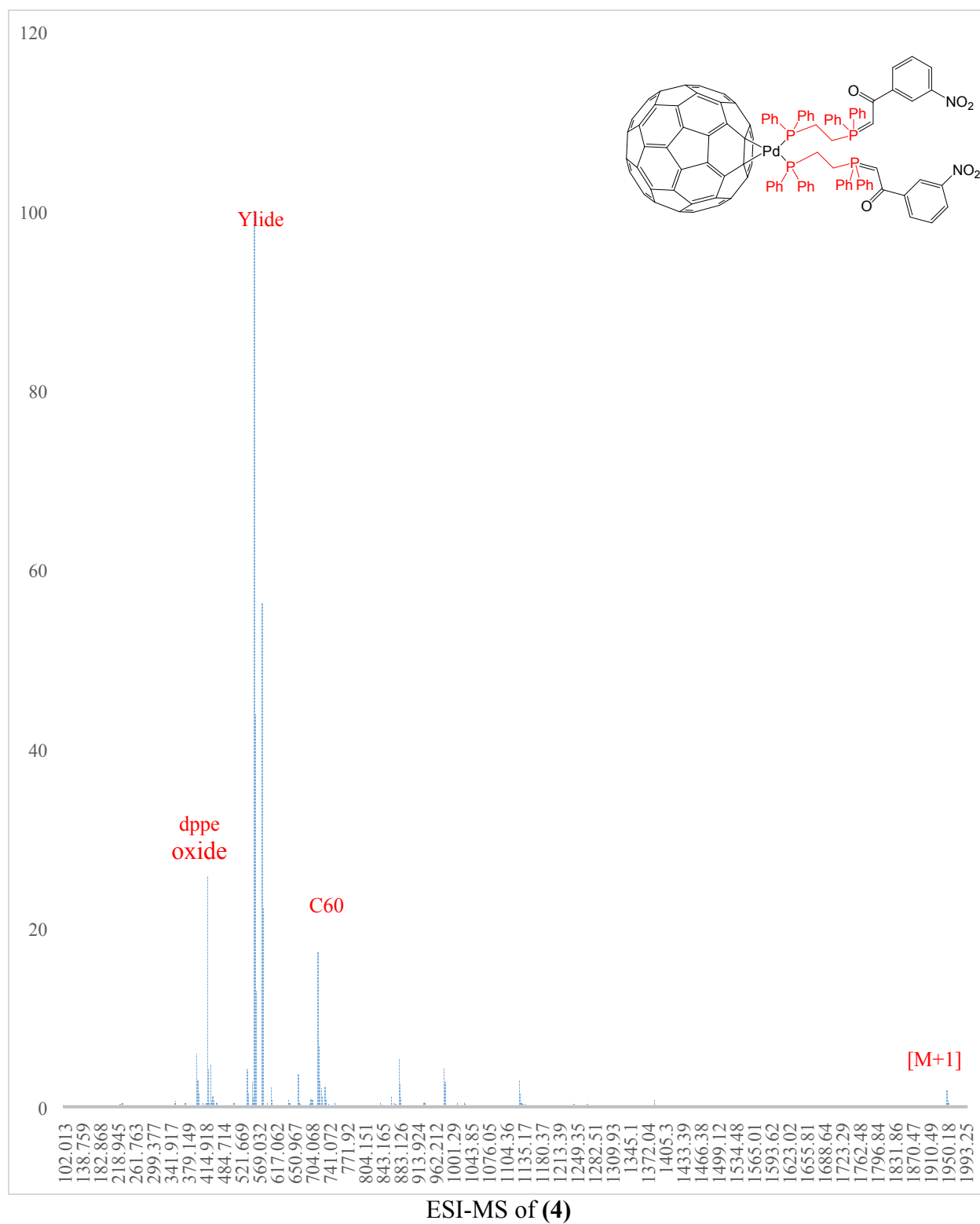


¹³C NMR of (4)

³¹P NMR of (4)

† Ylide oxide





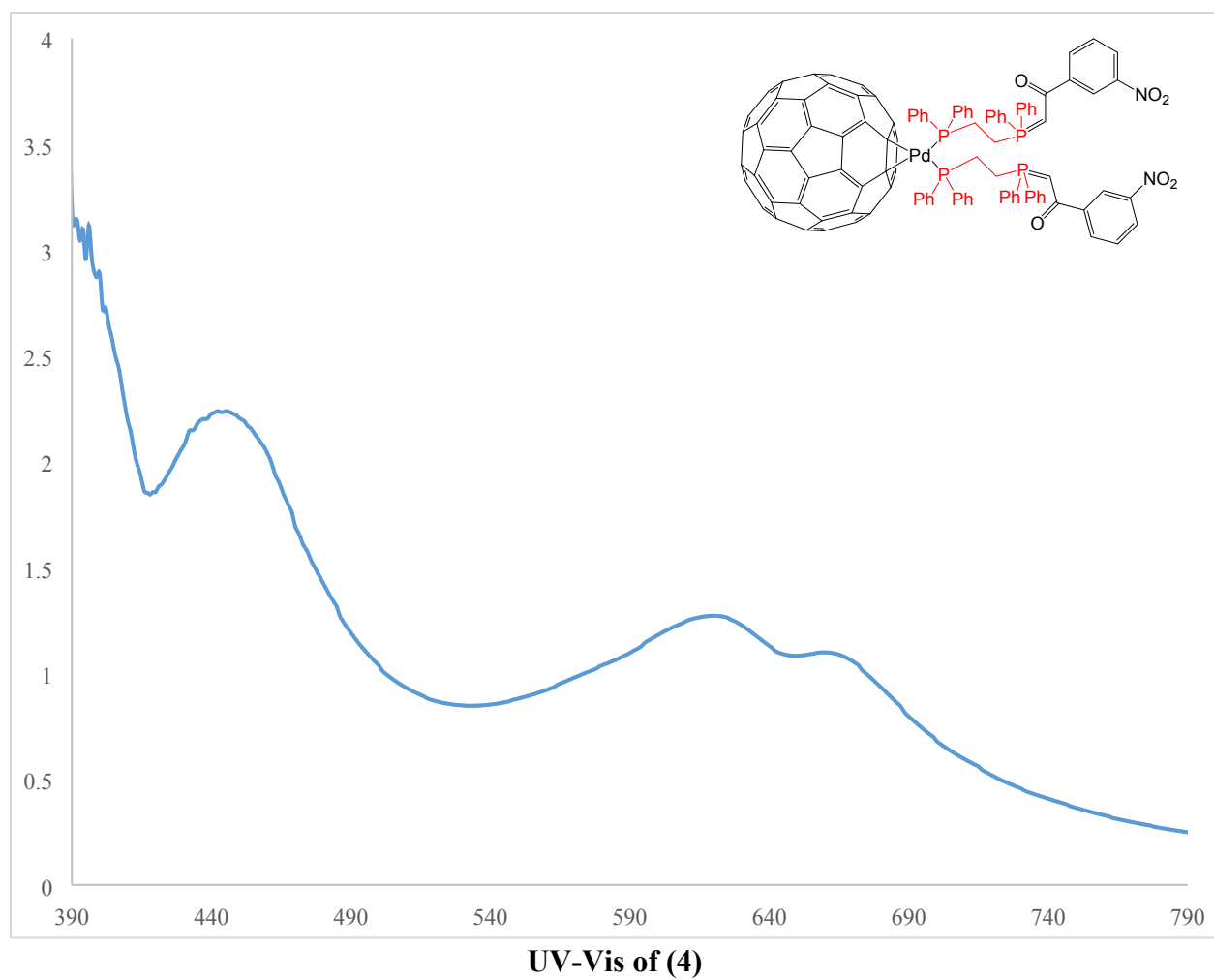


Table S1. The Cartesian atomic coordinates of all compounds involved

$(\eta^2\text{-C}_{60})\text{Pd}(\text{Y}^1)$							
Pd	1.740602000	0.677807000	-0.508459000	C	-4.124901000	-2.081558000	2.875893000
P	5.147349000	-0.032612000	-0.586122000	C	-4.837249000	-2.907278000	1.878558000
P	3.522316000	2.621142000	0.255405000	C	-4.119491000	-3.515228000	0.823959000
C	-0.277805000	1.060499000	0.106557000	C	-4.679020000	-3.517171000	-0.543801000
C	-0.177806000	-0.178902000	-0.747086000	C	-5.930374000	-2.910901000	-0.796836000
C	-0.883299000	-0.166510000	-2.086713000	C	-6.120348000	-2.088869000	-2.010093000
C	-1.515152000	0.988931000	-2.584432000	C	-6.986483000	-0.946411000	-1.656021000
C	-1.613468000	2.216114000	-1.739669000	C	-6.745656000	0.325297000	-2.224005000
C	-1.077690000	2.219596000	-0.436945000	C	-6.843774000	1.539469000	-1.386144000
C	-1.848121000	2.832657000	0.656802000	C	-7.178671000	1.427810000	-0.017483000
C	-1.658254000	2.013340000	1.865898000	C	-7.426897000	0.098144000	0.576075000
C	-0.769015000	0.891006000	1.523990000	C	-6.871193000	0.098732000	1.944783000
C	-1.013565000	-0.376907000	2.087410000	C	-6.242175000	-1.060776000	2.452307000
C	-0.916828000	-1.602230000	1.240596000	C	-6.144134000	-2.275022000	1.614475000
C	-0.576536000	-1.497910000	-0.120780000	C	-6.679212000	-2.275794000	0.306192000
C	-1.308502000	-2.301841000	-1.110879000	C	-7.332965000	-1.062282000	-0.224811000
C	-1.497936000	-1.482022000	-2.321470000	C	5.213368000	-0.840265000	1.183880000
C	-2.687676000	-1.602255000	-3.078743000	C	4.093198000	-0.719173000	2.032258000
C	-3.337173000	-0.395614000	-3.609736000	H	3.174604000	-0.219669000	1.678888000
C	-2.764190000	0.873545000	-3.354386000	C	4.163811000	-1.256653000	3.333924000
C	-3.633018000	2.012946000	-3.000313000	H	3.293970000	-1.171834000	4.000115000
C	-2.922232000	2.835182000	-2.000491000	C	5.336912000	-1.905722000	3.771731000
C	-3.648809000	3.454338000	-0.954432000	H	5.383338000	-2.327722000	4.785314000
C	-3.097175000	3.450443000	0.407664000	C	6.447615000	-2.022083000	2.910008000
C	-4.213619000	3.264220000	1.357459000	H	7.359762000	-2.531368000	3.249914000
C	-4.031693000	2.479011000	2.516507000	C	6.393725000	-1.486677000	1.608121000
C	-2.724815000	1.842337000	2.780688000	H	7.254980000	-1.570110000	0.933399000
C	-2.969787000	0.520903000	3.375688000	C	6.840818000	-0.545922000	-1.465218000
C	-2.134824000	-0.566545000	3.021140000	C	6.922475000	-1.832709000	-2.041420000
C	-2.728934000	-1.895014000	2.768972000	H	6.070568000	-2.523336000	-1.981283000
C	-1.977561000	-2.528465000	1.667759000	C	8.110688000	-2.221337000	-2.692883000
C	-2.658945000	-3.327763000	0.718563000	H	8.181141000	-3.222230000	-3.140831000
C	-2.315930000	-3.209764000	-0.705612000	C	9.200671000	-1.330368000	-2.772594000
C	-3.561944000	-3.328357000	-1.491447000	H	10.123971000	-1.636588000	-3.283704000
C	-3.743527000	-2.543337000	-2.650349000	C	9.106894000	-0.046176000	-2.198571000
C	-5.050762000	-1.909762000	-2.916295000	H	9.955259000	0.649444000	-2.259511000
C	-4.798547000	-0.579816000	-3.509294000	C	7.925238000	0.354367000	-1.541887000
C	-5.628544000	0.512465000	-3.169725000	H	7.860151000	1.353508000	-1.094669000
C	-5.032155000	1.840002000	-2.913430000	C	3.869403000	3.335738000	2.041619000
C	-5.787447000	2.476624000	-1.814643000	C	5.106915000	3.893842000	2.435656000
C	-5.109505000	3.264539000	-0.857020000	H	5.952635000	3.940350000	1.737809000
C	-5.460420000	3.148756000	0.574034000	C	5.258691000	4.394804000	3.744182000
C	-6.471358000	2.250482000	0.984263000	H	6.220403000	4.827490000	4.052166000
C	-6.280936000	1.428530000	2.197709000	C	4.181909000	4.344906000	4.652788000
C	-5.088110000	1.541024000	2.947078000	H	4.305315000	4.737845000	5.671383000
C	-4.430002000	0.328516000	3.477134000	C	2.948797000	3.789493000	4.255404000
C	-4.996086000	-0.943396000	3.234077000	H	2.107920000	3.747248000	4.961358000
				C	2.789845000	3.280650000	2.950146000
				H	1.833625000	2.839864000	2.632887000

C	3.417141000	4.208236000	-0.882328000
C	2.645098000	4.090901000	-2.057990000
H	2.135113000	3.140192000	-2.283812000
C	2.523481000	5.197381000	-2.923239000
H	1.922297000	5.107615000	-3.838473000
C	3.161992000	6.414104000	-2.607788000
H	3.061408000	7.277376000	-3.279953000
C	3.921711000	6.528182000	-1.425156000
H	4.411727000	7.479005000	-1.174647000
C	4.053398000	5.426004000	-0.557204000
H	4.635033000	5.520119000	0.368657000
C	5.293593000	1.909713000	-0.280905000
H	6.048627000	2.087994000	0.495727000
H	5.600503000	2.367060000	-1.232193000
C	3.412264000	-0.171903000	-1.641830000
H	3.687449000	0.556218000	-2.436049000
C	3.279680000	-1.511115000	-2.398024000
O	3.019613000	-1.492615000	-3.633725000
C	3.389935000	-2.882191000	-1.675984000
C	3.820850000	-3.988441000	-2.454011000
C	3.008239000	-3.087986000	-0.325951000
C	3.901585000	-5.280479000	-1.903541000
C	3.094512000	-4.394431000	0.185804000
C	3.536547000	-5.503665000	-0.557942000
H	4.072932000	-3.815132000	-3.510104000
H	2.628128000	-2.257451000	0.283004000
H	4.239199000	-6.126895000	-2.517608000
H	3.582517000	-6.503405000	-0.108439000
Br	2.528438000	-4.730983000	2.137402000

(η^2 -C₆₀)Pd(Y³)

Pd	1.730383000	0.873835000	-0.605060000
P	5.149634000	-0.023258000	-0.427569000
P	3.244979000	3.124162000	-0.140562000
C	-0.311216000	1.169406000	-0.013820000
C	-0.118119000	-0.145621000	-0.730083000
C	-0.843888000	-0.338226000	-2.045832000
C	-1.580103000	0.699217000	-2.649414000
C	-1.769962000	1.999328000	-1.940425000
C	-1.216939000	2.189572000	-0.659383000
C	-2.019382000	2.854001000	0.379635000
C	-1.742605000	2.191442000	1.665300000
C	-0.767046000	1.115583000	1.424800000
C	-0.894527000	-0.098154000	2.128907000
C	-0.707790000	-1.397469000	1.417695000
C	-0.398798000	-1.415303000	0.045096000
C	-1.075486000	-2.380505000	-0.833643000
C	-1.350569000	-1.717302000	-2.120892000
C	-2.537658000	-2.017894000	-2.831258000
C	-3.294591000	-0.934982000	-3.474087000
C	-2.826840000	0.397250000	-3.371236000

C	-3.783711000	1.493274000	-3.121793000
C	-3.129840000	2.476229000	-2.234809000
C	-3.890198000	3.145661000	-1.244830000
C	-3.319297000	3.336713000	0.095865000
C	-4.401427000	3.165057000	1.087313000
C	-4.136350000	2.529587000	2.319934000
C	-2.776420000	2.035426000	2.619552000
C	-2.899745000	0.771893000	3.359907000
C	-1.981328000	-0.275539000	3.104428000
C	-2.464735000	-1.667925000	3.012256000
C	-1.679593000	-2.355049000	1.968254000
C	-2.305631000	-3.307638000	1.128425000
C	-1.995853000	-3.318753000	-0.307987000
C	-3.239082000	-3.625849000	-1.045600000
C	-3.503578000	-2.990039000	-2.277779000
C	-4.863693000	-2.499507000	-2.579003000
C	-4.733618000	-1.226666000	-3.318550000
C	-5.647701000	-0.175783000	-3.078890000
C	-5.161784000	1.216373000	-2.982494000
C	-5.951321000	1.906075000	-1.941283000
C	-5.327740000	2.847779000	-1.091666000
C	-5.645694000	2.861393000	0.351780000
C	-6.570488000	1.933304000	0.881341000
C	-6.293247000	1.268449000	2.171554000
C	-5.102820000	1.560574000	2.874996000
C	-4.336698000	0.472035000	3.517120000
C	-4.796876000	-0.861149000	3.427303000
C	-3.838090000	-1.956210000	3.173279000
C	-4.493326000	-2.942642000	2.289331000
C	-3.743096000	-3.602085000	1.289465000
C	-4.321727000	-3.800297000	-0.056149000
C	-5.623239000	-3.330151000	-0.342536000
C	-5.900437000	-2.665157000	-1.632788000
C	-6.854564000	-1.565977000	-1.383455000
C	-6.730401000	-0.349002000	-2.091576000
C	-6.917760000	0.937761000	-1.388034000
C	-7.221491000	0.950337000	-0.007774000
C	-7.347572000	-0.321793000	0.732424000
C	-6.772858000	-0.125147000	2.078896000
C	-6.040437000	-1.166098000	2.693586000
C	-5.852795000	-2.452886000	1.990303000
C	-6.405968000	-2.641375000	0.703248000
C	-7.168065000	-1.551648000	0.060060000
C	4.944859000	-0.494266000	1.452515000
C	3.666245000	-0.480202000	2.041692000
H	2.775702000	-0.238514000	1.431908000
C	3.542100000	-0.763920000	3.418046000
H	2.544923000	-0.762133000	3.880114000
C	4.686768000	-1.051806000	4.188787000
H	4.585112000	-1.276921000	5.259609000
C	5.963996000	-1.049666000	3.589075000

H	6.857133000	-1.268643000	4.190161000
C	6.102202000	-0.767048000	2.216284000
H	7.095502000	-0.761339000	1.750395000
C	6.646319000	-1.129111000	-1.086403000
C	6.861550000	-2.413094000	-0.541469000
H	6.234100000	-2.781658000	0.280215000
C	7.896303000	-3.216803000	-1.062243000
H	8.072432000	-4.214559000	-0.636856000
C	8.696654000	-2.746050000	-2.123175000
H	9.501114000	-3.376826000	-2.526023000
C	8.460601000	-1.469532000	-2.673544000
H	9.076460000	-1.104394000	-3.506975000
C	7.429341000	-0.656219000	-2.162140000
H	7.242173000	0.331445000	-2.602768000
C	3.675495000	3.938798000	1.583354000
C	4.799747000	4.769146000	1.795289000
H	5.494879000	4.993554000	0.976517000
C	5.032857000	5.316943000	3.072896000
H	5.907271000	5.961597000	3.236469000
C	4.147310000	5.043502000	4.134847000
H	4.332379000	5.474027000	5.128536000
C	3.025151000	4.217743000	3.920847000
H	2.331829000	4.002546000	4.745523000
C	2.788829000	3.661504000	2.647311000
H	1.917612000	3.013239000	2.473745000
C	2.547883000	4.614542000	-1.199300000
C	1.788081000	4.286469000	-2.342837000
H	1.600962000	3.229293000	-2.591693000
C	1.264422000	5.317216000	-3.149361000
H	0.672608000	5.062852000	-4.039374000
C	1.491539000	6.666246000	-2.808239000
H	1.076615000	7.468198000	-3.434017000
C	2.243437000	6.987160000	-1.659720000
H	2.415067000	8.038020000	-1.389295000
C	2.776362000	5.963073000	-0.851397000
H	3.355222000	6.213476000	0.046964000
C	5.028434000	2.927576000	-0.995090000
H	5.569742000	3.886209000	-0.942342000
H	4.830509000	2.701185000	-2.053033000
C	5.902216000	1.834132000	-0.335735000
H	6.044714000	2.028038000	0.738428000
H	6.889397000	1.779758000	-0.822782000
C	3.483506000	0.002932000	-1.595488000
H	3.846411000	0.755737000	-2.324998000
C	3.319652000	-1.277097000	-2.441147000
O	3.045317000	-1.144396000	-3.667545000
C	3.405538000	-2.707590000	-1.847098000
C	3.586545000	-3.766269000	-2.774656000
C	3.280052000	-3.007750000	-0.467489000
C	3.662997000	-5.104845000	-2.351123000
C	3.368217000	-4.356665000	-0.082014000

C	3.559050000	-5.422933000	-0.978628000
H	3.652076000	-3.506140000	-3.841284000
H	3.099116000	-2.219094000	0.271436000
H	3.802650000	-5.913293000	-3.082239000
H	3.617355000	-6.458841000	-0.621920000
Br	3.228255000	-4.812334000	1.923854000

(η^2 -C₆₀)Pd(Y¹)₂

P	-3.617111000	4.225947000	0.249473000
P	-0.867215000	2.102980000	0.678248000
C	-5.236864000	3.798835000	-0.773766000
C	-5.765458000	4.810821000	-1.600823000
H	-5.248835000	5.777806000	-1.669390000
C	-6.948830000	4.563412000	-2.325644000
H	-7.363867000	5.347245000	-2.974307000
C	-7.599852000	3.317720000	-2.213405000
H	-8.524168000	3.128289000	-2.776610000
C	-7.068933000	2.315321000	-1.376048000
H	-7.577695000	1.345520000	-1.286753000
C	-5.883706000	2.551482000	-0.650044000
H	-5.473831000	1.768468000	-0.000730000
C	-4.209495000	4.747365000	2.044241000
C	-5.311669000	4.081636000	2.621114000
H	-5.828231000	3.272733000	2.089169000
C	-5.749723000	4.492793000	3.894727000
H	-6.606784000	3.990263000	4.362963000
C	-5.093938000	5.549570000	4.561985000
H	-5.442766000	5.865389000	5.555092000
C	-3.997362000	6.200096000	3.960226000
H	-3.493312000	7.022331000	4.487410000
C	-3.537292000	5.804722000	2.685438000
H	-2.654486000	6.257199000	2.143533000
C	-0.083690000	3.157494000	-0.760984000
C	-0.512884000	2.914633000	-2.085947000
H	-1.328192000	2.205884000	-2.283923000
C	0.112502000	3.586846000	-3.153974000
H	-0.223429000	3.402218000	-4.183462000
C	1.171449000	4.483994000	-2.904387000
H	1.661550000	5.002028000	-3.739824000
C	1.606938000	4.708190000	-1.583352000
H	2.436063000	5.401513000	-1.385423000
C	0.984544000	4.043498000	-0.506564000
H	1.327705000	4.214672000	0.521919000
C	-0.346076000	2.971403000	2.343207000
C	0.154336000	2.100686000	3.338272000
H	0.208817000	1.019145000	3.134048000
C	0.589128000	2.618292000	4.573556000
H	0.979972000	1.938555000	5.342623000
C	0.526026000	4.005977000	4.812096000
H	0.868788000	4.414989000	5.772617000
C	0.026849000	4.867580000	3.815386000

H	-0.021619000	5.949784000	3.999384000	C	6.258950000	-3.293155000	-3.516332000
C	-0.412671000	4.364760000	2.571334000	C	5.420185000	-4.218368000	-2.855026000
H	-0.806289000	5.096051000	1.827751000	C	5.920682000	-4.956317000	-1.676687000
Pd	0.205505000	-0.334518000	0.502615000	C	7.236692000	-4.736205000	-1.210968000
P	-1.776378000	-2.074650000	0.823449000	C	7.499218000	-4.632990000	0.239618000
P	-5.121904000	-2.575022000	1.716578000	C	8.537174000	-3.602340000	0.443052000
C	2.274348000	-0.039923000	0.107566000	C	8.464724000	-2.737594000	1.558613000
C	1.962412000	-1.501747000	0.265139000	C	8.772112000	-1.300333000	1.400819000
C	2.601406000	-2.235028000	1.422509000	C	9.138349000	-0.791494000	0.134265000
C	3.377707000	-1.565086000	2.388137000	C	9.210842000	-1.695219000	-1.032101000
C	3.688744000	-0.115323000	2.229191000	C	8.713517000	-0.958198000	-2.211967000
C	3.208828000	0.593410000	1.111430000	C	7.941414000	-1.626999000	-3.188703000
C	4.100469000	1.533372000	0.414349000	C	7.634031000	-3.064406000	-3.030873000
C	3.837695000	1.430577000	-1.032525000	C	8.112443000	-3.769311000	-1.903132000
C	2.780909000	0.426906000	-1.238084000	C	8.917268000	-3.069059000	-0.881215000
C	2.859808000	-0.441145000	-2.344556000	C	-2.329860000	-2.871243000	-0.861292000
C	2.550964000	-1.891221000	-2.185791000	C	-1.900083000	-2.214794000	-2.035109000
C	2.178503000	-2.402435000	-0.928202000	H	-1.296273000	-1.296849000	-1.953256000
C	2.745511000	-3.680844000	-0.471025000	C	-2.238140000	-2.744437000	-3.296861000
C	3.007071000	-3.577575000	0.976019000	H	-1.901169000	-2.234080000	-4.209367000
C	4.137308000	-4.217581000	1.537698000	C	-3.002102000	-3.925906000	-3.383825000
C	4.936646000	-3.522249000	2.557434000	H	-3.266216000	-4.338628000	-4.367331000
C	4.566679000	-2.217888000	2.962795000	C	-3.426909000	-4.580876000	-2.209472000
C	5.606844000	-1.189937000	3.165612000	H	-4.028186000	-5.498314000	-2.273340000
C	5.063806000	0.104253000	2.707928000	C	-3.091336000	-4.059430000	-0.943601000
C	5.910957000	1.032402000	2.057048000	H	-3.426383000	-4.576453000	-0.035879000
C	5.416549000	1.763045000	0.880750000	C	-1.111784000	-3.551387000	1.911912000
C	6.529345000	1.892504000	-0.082635000	C	-0.796088000	-4.804310000	1.345143000
C	6.278042000	1.793548000	-1.468287000	H	-0.992220000	-4.997104000	0.282827000
C	4.902542000	1.561108000	-1.955301000	C	-0.220232000	-5.807433000	2.152072000
C	4.973505000	0.663880000	-3.118086000	H	0.023504000	-6.783501000	1.710480000
C	3.975854000	-0.323206000	-3.298402000	C	0.047270000	-5.559734000	3.512775000
C	4.357598000	-1.680776000	-3.735388000	H	0.499906000	-6.342969000	4.135889000
C	3.479997000	-2.645521000	-3.043718000	C	-0.252705000	-4.299765000	4.070494000
C	4.000080000	-3.890840000	-2.617867000	H	-0.031837000	-4.096844000	5.127346000
C	3.624120000	-4.419622000	-1.298418000	C	-0.824469000	-3.290900000	3.271429000
C	4.808282000	-5.081661000	-0.713178000	H	-1.035355000	-2.302500000	3.702018000
C	5.058974000	-4.982638000	0.672612000	C	-6.141261000	-1.577488000	3.103588000
C	6.434046000	-4.754170000	1.160581000	C	-5.590112000	-1.211574000	4.348813000
C	6.358028000	-3.849358000	2.326361000	H	-4.547020000	-1.443244000	4.598462000
C	7.351681000	-2.863516000	2.519609000	C	-6.398458000	-0.536388000	5.286466000
C	6.967432000	-1.504109000	2.952746000	H	-5.976738000	-0.247402000	6.259041000
C	7.849020000	-0.538425000	2.264461000	C	-7.741276000	-0.233864000	4.979467000
C	7.331268000	0.701165000	1.826270000	H	-8.366326000	0.290567000	5.715284000
C	7.714911000	1.234126000	0.502468000	C	-8.283012000	-0.606364000	3.732267000
C	8.597762000	0.504010000	-0.324871000	H	-9.330174000	-0.374327000	3.493315000
C	8.334808000	0.400779000	-1.775283000	C	-7.481755000	-1.283490000	2.790777000
C	7.200782000	1.032217000	-2.334387000	H	-7.879452000	-1.588775000	1.811937000
C	6.392950000	0.332441000	-3.354960000	C	-4.832037000	-4.386345000	2.398734000
C	6.756312000	-0.967963000	-3.771782000	C	-5.327605000	-5.459261000	1.637896000
C	5.714226000	-1.996642000	-3.969900000	H	-5.854783000	-5.223001000	0.640979000

C	-5.143493000	-6.759451000	2.162428000
H	-5.516529000	-7.626198000	1.598367000
C	-4.493256000	-6.958919000	3.396322000
H	-4.358877000	-7.976220000	3.790041000
C	-4.012030000	-5.855837000	4.135762000
H	-3.505936000	-6.011676000	5.097898000
C	-4.179941000	-4.549428000	3.641132000
H	-3.811337000	-3.688744000	4.211867000
C	-6.040900000	-2.376596000	0.122915000
H	-6.136137000	-1.325311000	-0.134709000
C	-2.770729000	5.558302000	-0.723110000
H	-2.823973000	5.363280000	-1.791912000
C	-1.812536000	6.459257000	-0.154842000
O	-1.470359000	6.590844000	1.085698000
C	-6.508839000	-3.405709000	-0.756441000
O	-6.496547000	-4.688542000	-0.634318000
C	-7.194099000	-2.859239000	-2.054794000
C	-6.861052000	-1.640042000	-2.693969000
C	-8.174639000	-3.699286000	-2.646097000
C	-7.498573000	-1.249355000	-3.889030000
C	-8.793744000	-3.274545000	-3.829187000
C	-8.489053000	-2.063646000	-4.477891000
H	-6.081172000	-0.996220000	-2.267804000
H	-8.408976000	-4.661643000	-2.170607000
H	-7.222747000	-0.304427000	-4.377483000
H	-8.995940000	-1.773661000	-5.406404000
C	-1.123017000	7.431853000	-1.164891000
C	-0.070129000	8.215026000	-0.622812000
C	-1.475070000	7.604740000	-2.526112000
C	0.592752000	9.121056000	-1.458634000
C	-0.787216000	8.529714000	-3.337875000
C	0.268613000	9.306963000	-2.815443000
H	0.173909000	8.081367000	0.441021000
H	-2.296645000	7.023269000	-2.962460000
H	-1.072166000	8.654913000	-4.391793000
H	0.812898000	10.029391000	-3.436166000
Br	-10.231696000	-4.485744000	-4.674137000
Br	2.127270000	10.248091000	-0.667783000
C	-2.808360000	2.362077000	0.475991000
H	-3.098080000	1.796036000	-0.419990000
H	-3.287541000	1.923366000	1.363173000
C	-3.407325000	-1.509379000	1.783067000
H	-3.127291000	-1.398441000	2.840173000
H	-3.674458000	-0.523423000	1.380507000

(η^2 -C₆₀)Pd(Y³)₂

P	-1.096878000	4.739649000	0.316882000
P	-0.867068000	0.796013000	-2.377317000
C	-0.975830000	4.533590000	2.266727000
C	-2.193574000	4.422393000	2.963224000
H	-3.149552000	4.495918000	2.348649000
C	-2.127554000	4.256466000	4.363957000

H	-3.056323000	4.170700000	4.945593000
C	-0.882287000	4.204174000	5.024269000
H	-0.844653000	4.076582000	6.115173000
C	0.320656000	4.319512000	4.294582000
H	1.288326000	4.281828000	4.813014000
C	0.284838000	4.486561000	2.895923000
H	1.213432000	4.586039000	2.318946000
C	0.488017000	5.656000000	-0.346195000
C	1.703061000	4.958702000	-0.514676000
H	1.775150000	3.883535000	-0.302429000
C	2.839418000	5.662418000	-0.963828000
H	3.789067000	5.124734000	-1.095097000
C	2.757683000	7.043216000	-1.237134000
H	3.646867000	7.586144000	-1.586699000
C	1.538787000	7.729986000	-1.058682000
H	1.475662000	8.807125000	-1.266019000
C	0.396222000	7.039659000	-0.606956000
H	-0.554833000	7.566666000	-0.454953000
C	-2.751338000	0.329943000	-2.644520000
C	-3.817566000	1.166750000	-2.252741000
H	-3.629478000	2.132834000	-1.768391000
C	-5.147840000	0.759380000	-2.487688000
H	-5.975406000	1.414437000	-2.182402000
C	-5.413870000	-0.477308000	-3.106884000
H	-6.450936000	-0.789738000	-3.289423000
C	-4.346072000	-1.316377000	-3.487789000
H	-4.548156000	-2.284729000	-3.965951000
C	-3.015785000	-0.917940000	-3.253794000
H	-2.182557000	-1.571128000	-3.547539000
C	-0.294441000	0.939090000	-4.243145000
C	0.894095000	0.295211000	-4.641162000
H	1.480056000	-0.275169000	-3.906577000
C	1.322836000	0.388748000	-5.982047000
H	2.249364000	-0.113446000	-6.292490000
C	0.565305000	1.120635000	-6.917525000
H	0.900434000	1.191638000	-7.961422000
C	-0.626403000	1.759721000	-6.515795000
H	-1.220425000	2.327271000	-7.245129000
C	-1.061510000	1.670150000	-5.179410000
H	-1.994572000	2.159772000	-4.871247000
Pd	0.710653000	-0.401372000	-0.588859000
P	-1.053183000	-1.711357000	1.002208000
P	-5.899137000	-1.572898000	1.310128000
C	2.769002000	-0.078637000	-1.021191000
C	2.599936000	-0.834779000	0.267736000
C	3.097240000	-0.178746000	1.535958000
C	3.599851000	1.136585000	1.545803000
C	3.768592000	1.884690000	0.267068000
C	3.425622000	1.280945000	-0.958152000
C	4.320013000	1.440370000	-2.115589000
C	4.344549000	0.167120000	-2.856887000

C	3.464615000	-0.786083000	-2.162898000
C	3.845070000	-2.138926000	-2.078064000
C	3.676240000	-2.888968000	-0.799940000
C	3.137906000	-2.246448000	0.331076000
C	3.751815000	-2.470696000	1.649035000
C	3.728164000	-1.197245000	2.390625000
C	4.799561000	-0.859440000	3.250928000
C	5.312219000	0.518540000	3.269726000
C	4.727810000	1.490861000	2.423861000
C	5.589200000	2.451969000	1.707479000
C	4.997987000	2.688340000	0.375839000
C	5.840180000	2.869953000	-0.747077000
C	5.492585000	2.227443000	-2.023073000
C	6.742780000	1.770090000	-2.663982000
C	6.765556000	0.550413000	-3.374524000
C	5.539571000	-0.267785000	-3.477338000
C	5.925958000	-1.684332000	-3.401321000
C	5.097253000	-2.595467000	-2.704434000
C	5.703837000	-3.620735000	-1.832429000
C	4.827905000	-3.795370000	-0.656889000
C	5.398028000	-4.036079000	0.615674000
C	4.846561000	-3.355294000	1.796478000
C	5.969042000	-2.998989000	2.688798000
C	5.946052000	-1.779631000	3.399807000
C	7.172115000	-0.963281000	3.506929000
C	6.779275000	0.459181000	3.425329000
C	7.602110000	1.379637000	2.737953000
C	6.992452000	2.401073000	1.861597000
C	7.871096000	2.579694000	0.686914000
C	7.307010000	2.808843000	-0.588155000
C	7.866105000	2.128990000	-1.774964000
C	8.963636000	1.249728000	-1.634353000
C	8.987786000	-0.026694000	-2.378548000
C	7.913147000	-0.368202000	-3.230466000
C	7.392773000	-1.751223000	-3.246022000
C	7.971249000	-2.731600000	-2.408952000
C	7.107279000	-3.690437000	-1.689137000
C	7.701886000	-3.932367000	-0.358288000
C	6.865364000	-4.100682000	0.767973000
C	7.219316000	-3.459747000	2.051568000
C	8.392961000	-2.678939000	2.152292000
C	8.368415000	-1.402176000	2.896070000
C	9.227192000	-0.439079000	2.177686000
C	8.852471000	0.921508000	2.101334000
C	9.018822000	1.663323000	0.833608000
C	9.553059000	1.011950000	-0.301243000
C	9.942697000	-0.410807000	-0.221270000
C	9.592399000	-1.052665000	-1.504964000
C	9.094624000	-2.375288000	-1.520457000
C	8.928272000	-3.117667000	-0.252950000
C	9.266483000	-2.503944000	0.974436000

C	9.783095000	-1.120050000	0.990327000
C	-1.220867000	-3.540069000	0.349114000
C	-0.532821000	-3.873683000	-0.837121000
H	0.073521000	-3.105583000	-1.346050000
C	-0.627262000	-5.178846000	-1.361378000
H	-0.088579000	-5.435318000	-2.283790000
C	-1.414363000	-6.147269000	-0.705913000
H	-1.492280000	-7.163178000	-1.117111000
C	-2.105747000	-5.811899000	0.476359000
H	-2.723814000	-6.563346000	0.986744000
C	-2.010975000	-4.510434000	1.008585000
H	-2.553742000	-4.259511000	1.928859000
C	-0.178113000	-1.914494000	2.743161000
C	0.229857000	-3.169656000	3.241513000
H	0.062627000	-4.079820000	2.651225000
C	0.853364000	-3.247922000	4.504042000
H	1.172497000	-4.225274000	4.891382000
C	1.064753000	-2.081949000	5.266031000
H	1.549197000	-2.148231000	6.249612000
C	0.659022000	-0.829066000	4.762286000
H	0.825237000	0.083143000	5.351307000
C	0.042383000	-0.740964000	3.498694000
H	-0.268295000	0.235633000	3.101843000
C	-6.551852000	0.262694000	1.184256000
C	-5.671474000	1.363574000	1.236600000
H	-4.589725000	1.202559000	1.324991000
C	-6.186389000	2.676143000	1.168652000
H	-5.484361000	3.554524000	1.203910000
C	-7.580981000	2.862980000	1.053370000
H	-7.993345000	3.880695000	1.000863000
C	-8.456566000	1.758124000	1.007022000
H	-9.540725000	1.914768000	0.920850000
C	-7.945729000	0.446872000	1.075747000
H	-8.611595000	-0.425368000	1.045654000
C	-5.675194000	-2.060751000	3.196706000
C	-5.790184000	-3.425790000	3.520931000
H	-6.048002000	-4.144219000	2.669439000
C	-5.628133000	-3.787237000	4.876659000
H	-5.715669000	-4.842661000	5.171196000
C	-5.361161000	-2.809750000	5.857381000
H	-5.237902000	-3.105504000	6.908563000
C	-5.259308000	-1.448036000	5.499851000
H	-5.059975000	-0.688097000	6.267328000
C	-5.417251000	-1.058846000	4.155528000
H	-5.351541000	-0.001899000	3.866385000
C	-7.091890000	-2.643668000	0.380816000
H	-7.495744000	-2.126375000	-0.485635000
C	-2.599449000	5.628241000	-0.323487000
H	-2.392761000	6.214876000	-1.213645000
C	-3.910926000	5.406515000	0.184788000
O	-4.271237000	4.757641000	1.249431000

C	-7.143616000	-4.073890000	0.505107000
O	-6.577155000	-4.846357000	1.367107000
C	-8.037070000	-4.789641000	-0.565544000
C	-9.012687000	-4.165914000	-1.381446000
C	-7.845431000	-6.192238000	-0.677511000
C	-9.774908000	-4.915246000	-2.300838000
C	-8.614310000	-6.902569000	-1.606686000
C	-9.583104000	-6.306872000	-2.435088000
H	-9.194435000	-3.087428000	-1.294009000
H	-7.106901000	-6.667934000	-0.016601000
H	-10.531772000	-4.417766000	-2.923180000
H	-10.165767000	-6.902545000	-3.148171000
C	-5.051227000	6.083522000	-0.640705000
C	-6.246841000	6.388392000	0.062278000
C	-4.979885000	6.369879000	-2.026444000
C	-7.307631000	6.972228000	-0.643224000
C	-6.067066000	6.958477000	-2.703181000
C	-7.258742000	7.274640000	-2.016276000
H	-6.312643000	6.153833000	1.133386000
H	-4.071050000	6.120802000	-2.589001000
H	-5.996729000	7.172051000	-3.778901000
H	-8.114521000	7.731526000	-2.528302000
Br	-8.315058000	-8.938087000	-1.782415000
Br	-9.043238000	7.405494000	0.381042000
C	-0.944500000	2.818808000	-0.312592000
H	-1.825610000	2.325913000	0.125484000
H	-0.029880000	2.399092000	0.140396000
C	-0.926120000	2.714681000	-1.848287000
H	-0.012776000	3.164734000	-2.265183000
H	-1.805304000	3.196593000	-2.301335000
C	-2.920964000	-1.360453000	1.679401000
H	-3.094436000	-2.066688000	2.504991000
H	-2.901764000	-0.339484000	2.086911000
C	-3.973028000	-1.520692000	0.573664000
H	-3.874680000	-2.485898000	0.055846000
H	-3.944277000	-0.705278000	-0.164410000

Y¹

P	0.009706000	-0.075822000	0.120646000
P	-3.148679000	-0.309768000	-0.940536000
C	0.621409000	-1.947905000	-0.289562000
C	-0.224522000	-2.777311000	-1.056674000
H	-1.210208000	-2.419802000	-1.382375000
C	0.209319000	-4.069692000	-1.415388000
H	-0.450100000	-4.718976000	-2.007618000
C	1.485589000	-4.523923000	-1.024868000
H	1.822189000	-5.530040000	-1.309698000
C	2.335013000	-3.681088000	-0.280670000
H	3.337649000	-4.022084000	0.011877000
C	1.908540000	-2.386735000	0.082984000
H	2.579882000	-1.732291000	0.652611000

C	0.893781000	0.302093000	1.837956000
C	1.152413000	1.650298000	2.153583000
H	0.920400000	2.428591000	1.413772000
C	1.700502000	1.974503000	3.410860000
H	1.912915000	3.023339000	3.659596000
C	1.967946000	0.955921000	4.348508000
H	2.393233000	1.210277000	5.329089000
C	1.681223000	-0.388430000	4.033815000
H	1.880371000	-1.181184000	4.767881000
C	1.136880000	-0.721969000	2.777079000
H	0.908291000	-1.767107000	2.532560000
C	-4.676657000	-1.283896000	-0.157322000
C	-4.884865000	-1.431473000	1.232348000
H	-4.181109000	-0.999208000	1.954165000
C	-6.005602000	-2.146540000	1.701641000
H	-6.162911000	-2.260832000	2.782926000
C	-6.921119000	-2.710032000	0.790924000
H	-7.793539000	-3.265543000	1.161038000
C	-6.713354000	-2.562351000	-0.595239000
H	-7.422625000	-3.002636000	-1.309419000
C	-5.591312000	-1.854828000	-1.071245000
H	-5.421891000	-1.746111000	-2.150529000
C	-3.773329000	1.554509000	-0.765022000
C	-3.554008000	2.420334000	-1.858881000
H	-3.053750000	2.046865000	-2.762033000
C	-3.978412000	3.763191000	-1.783694000
H	-3.802881000	4.437262000	-2.633240000
C	-4.623432000	4.237451000	-0.624174000
H	-4.953718000	5.283706000	-0.567729000
C	-4.848245000	3.368233000	0.462967000
H	-5.355801000	3.734649000	1.365741000
C	-4.424917000	2.026068000	0.395799000
H	-4.612297000	1.350327000	1.239931000
C	-1.885988000	-0.410737000	0.598973000
H	-1.931169000	-1.424497000	1.019201000
H	-2.150335000	0.327175000	1.367583000
C	0.033011000	1.397209000	-0.961956000
H	-0.887030000	1.462580000	-1.545060000
C	1.173101000	2.182188000	-1.425111000
O	1.034007000	3.154063000	-2.236177000
C	2.619207000	1.924812000	-0.865026000
C	3.342253000	3.029863000	-0.345082000
C	3.280867000	0.678000000	-1.005983000
C	4.681707000	2.904673000	0.066177000
C	4.623898000	0.596553000	-0.597713000
C	5.353137000	1.667935000	-0.056754000
H	2.837220000	4.003411000	-0.274729000
H	2.771210000	-0.191762000	-1.438158000
H	5.220634000	3.769442000	0.477752000
H	6.400462000	1.547670000	0.245001000
Br	5.618664000	-1.206669000	-0.819768000

Y ³							
P	0.348795000	0.205283000	0.686798000	C	-4.245350000	-2.535048000	-0.513063000
P	-3.239165000	0.184663000	-0.398483000	H	-3.547872000	-2.607013000	-1.357821000
C	0.383055000	-1.504467000	-0.355074000	C	-4.569828000	1.619296000	-0.664284000
C	0.403291000	-1.410022000	-1.759771000	C	-4.099460000	2.946589000	-0.791092000
H	0.408588000	-0.420592000	-2.238669000	H	-3.027288000	3.165510000	-0.701227000
C	0.396861000	-2.587184000	-2.536591000	C	-5.009472000	3.992441000	-1.040486000
H	0.414328000	-2.518532000	-3.633074000	H	-4.639845000	5.022858000	-1.132948000
C	0.366394000	-3.847910000	-1.906321000	C	-6.385168000	3.718030000	-1.179858000
H	0.364153000	-4.764432000	-2.511974000	H	-7.092083000	4.534827000	-1.378254000
C	0.335499000	-3.934943000	-0.499228000	C	-6.848914000	2.392580000	-1.071719000
H	0.308291000	-4.917686000	-0.008648000	H	-7.918918000	2.171803000	-1.186718000
C	0.341100000	-2.761890000	0.283315000	C	-5.944814000	1.341198000	-0.816456000
H	0.315794000	-2.834984000	1.378682000	H	-6.310932000	0.310392000	-0.733303000
C	1.865391000	0.029851000	1.920772000	C	-2.501606000	0.775881000	1.371605000
C	2.787672000	-1.030255000	1.818887000	H	-3.296080000	0.698641000	2.130725000
H	2.694713000	-1.772708000	1.015925000	H	-2.216798000	1.832918000	1.265292000
C	3.839990000	-1.119690000	2.753473000	C	-1.292835000	-0.079360000	1.812778000
H	4.565932000	-1.940626000	2.674381000	H	-1.512333000	-1.156522000	1.774630000
C	3.964053000	-0.158677000	3.777118000	H	-0.986677000	0.192445000	2.836333000
H	4.785964000	-0.232751000	4.502409000	C	0.279205000	1.826791000	-0.125922000
C	3.038386000	0.901198000	3.867945000	H	-0.733329000	2.110787000	-0.404274000
H	3.137177000	1.654546000	4.661420000	C	1.381026000	2.677264000	-0.554928000
C	1.983966000	1.000195000	2.938514000	O	1.195839000	3.850428000	-1.013611000
H	1.266122000	1.829093000	2.995536000	C	2.867768000	2.180841000	-0.446131000
C	-4.366801000	-1.315883000	0.190452000	C	3.844838000	3.086214000	0.042018000
C	-5.263924000	-1.218502000	1.279042000	C	3.292482000	0.926574000	-0.954769000
H	-5.370511000	-0.272896000	1.826239000	C	5.211716000	2.752334000	0.062865000
C	-6.031807000	-2.336783000	1.660133000	C	4.665770000	0.632865000	-0.925880000
H	-6.728489000	-2.256616000	2.505756000	C	5.650259000	1.502159000	-0.428205000
C	-5.908888000	-3.553229000	0.958165000	H	3.513633000	4.071310000	0.399593000
H	-6.509337000	-4.423118000	1.257589000	H	2.575224000	0.209702000	-1.371370000
C	-5.016769000	-3.650970000	-0.127945000	H	5.951935000	3.463551000	0.455283000
H	-4.919166000	-4.596919000	-0.677888000	H	6.710613000	1.222541000	-0.430552000
				Br	5.288786000	-1.199231000	-1.667573
