Supporting Information

for

Steric and Electronic Parameters Characterizing Bulky and Electron-rich Dialkylbiarylphosphines

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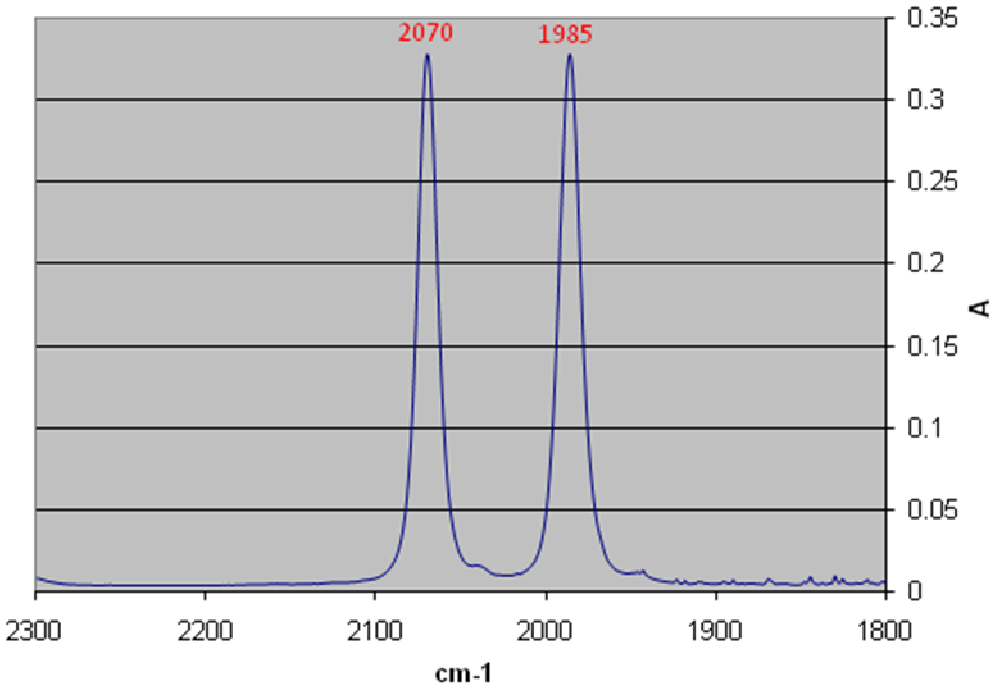
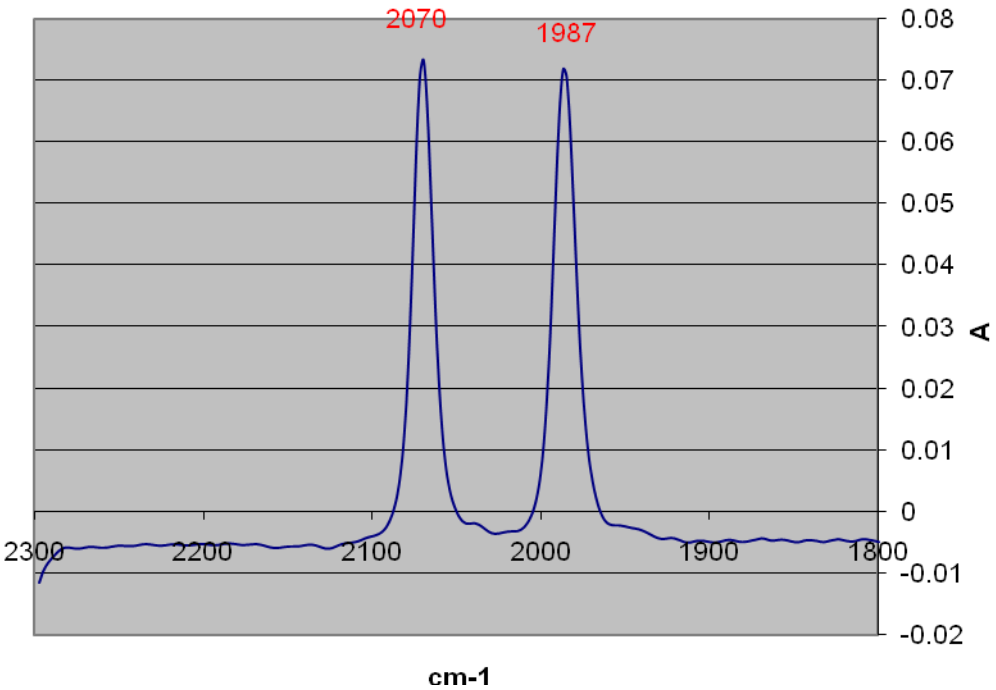
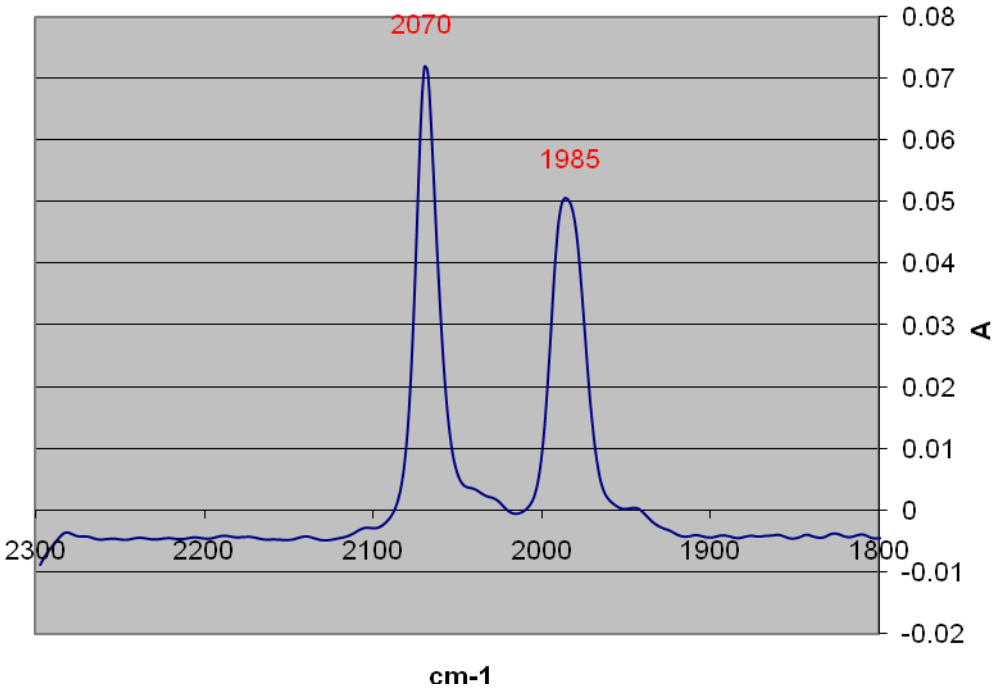
[IrCl(CO)2{PCy2(2-biphenyl)}] 4a



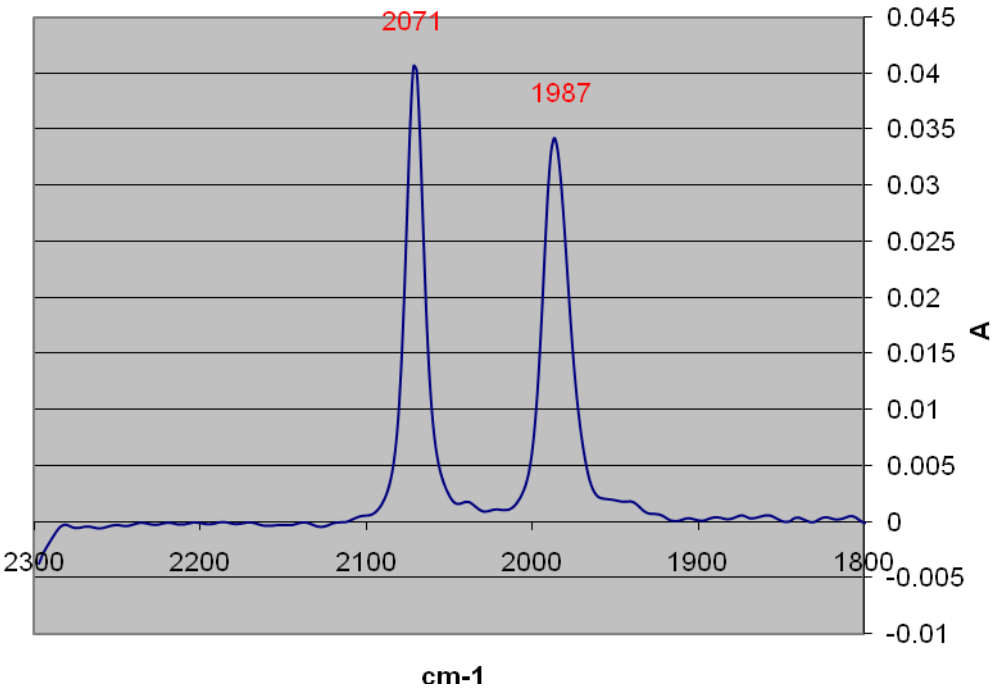
IrCl(CO)2{PCy2(2'-methyl-2-biphenyl)}] 4b

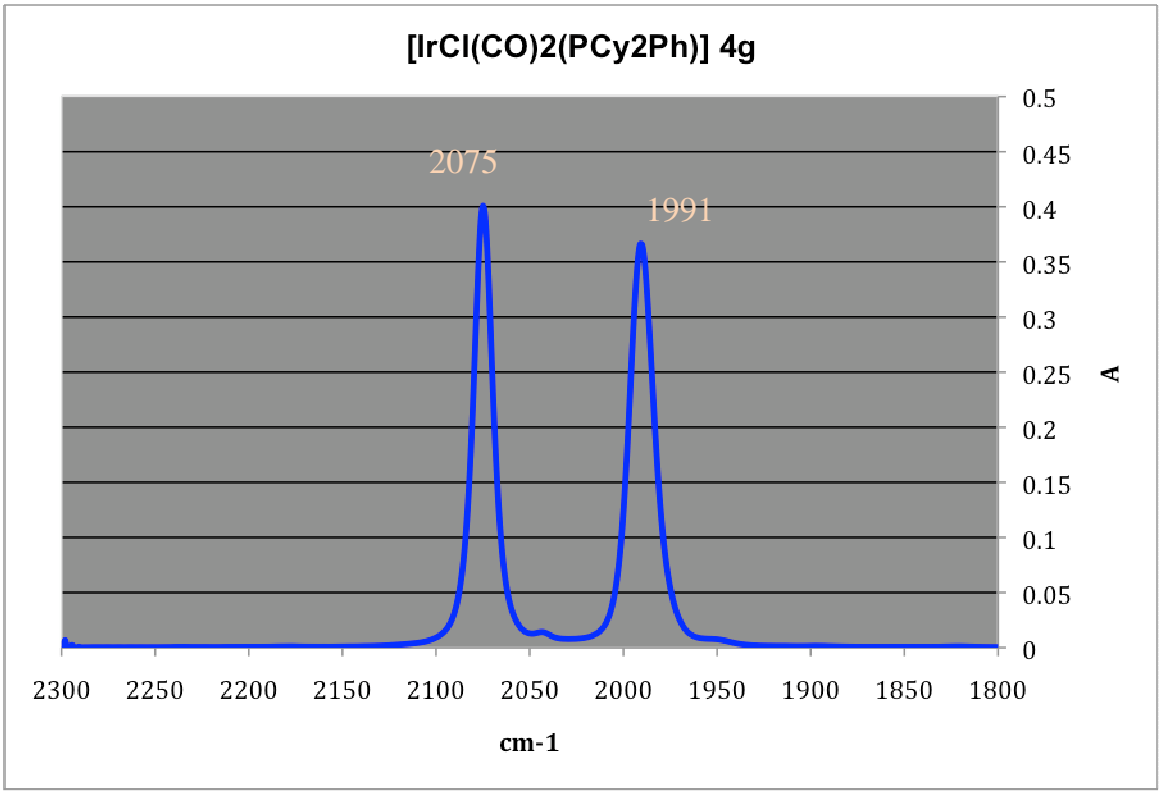


IrCl(CO)2(S-Phos)] 4c



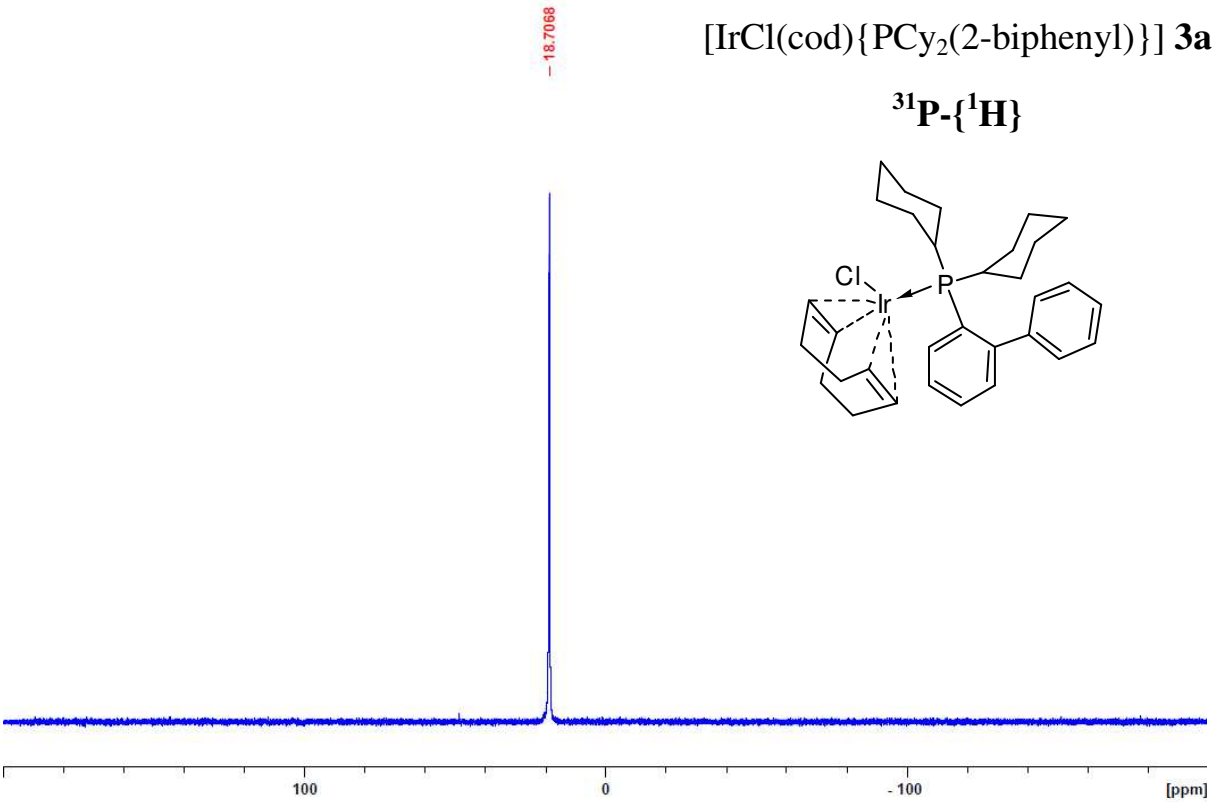
IrCl(CO)2(X-Phos) 4d




[IrCl(CO)2(PCy2Ph)] 4g
2075
1991
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
A
2300
2250
2200
2150
2100
2050
2000
1950
1900
1850
1800
cm-1

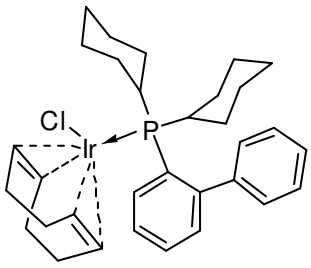
[IrCl(cod){PCy_2(2-biphenyl)}] **3a**

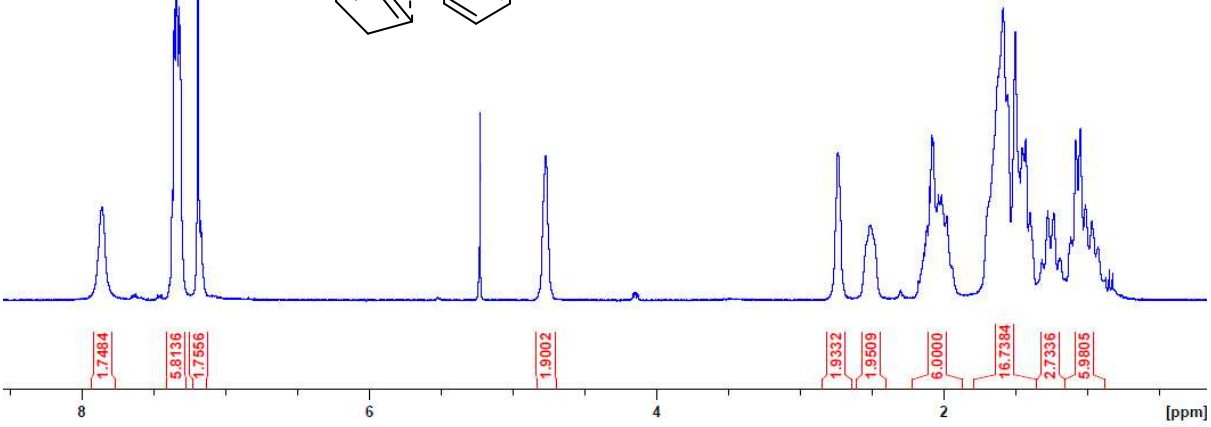
^{31}P-{^{1}H}



[IrCl(cod){PCy_2(2-biphenyl)}] **3a**

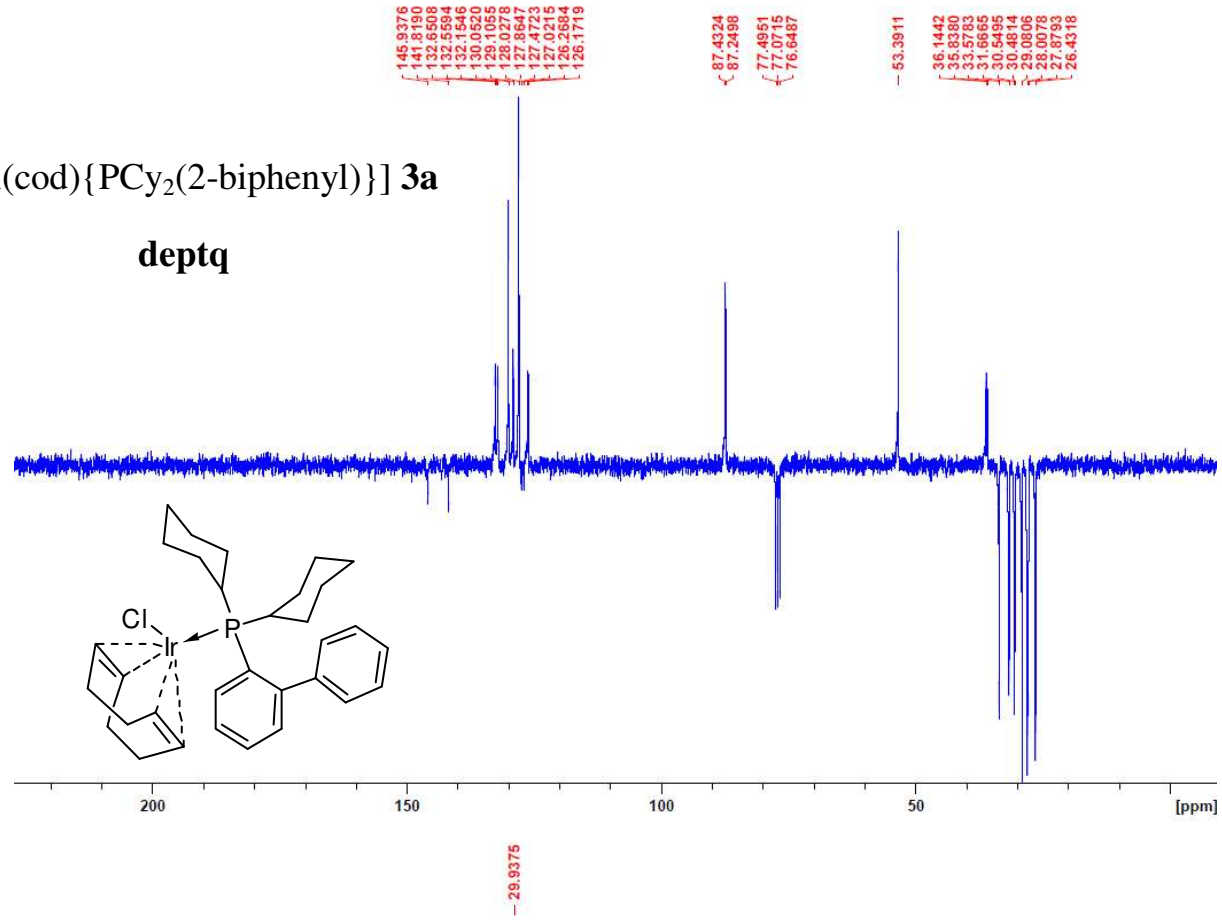
^{1}H





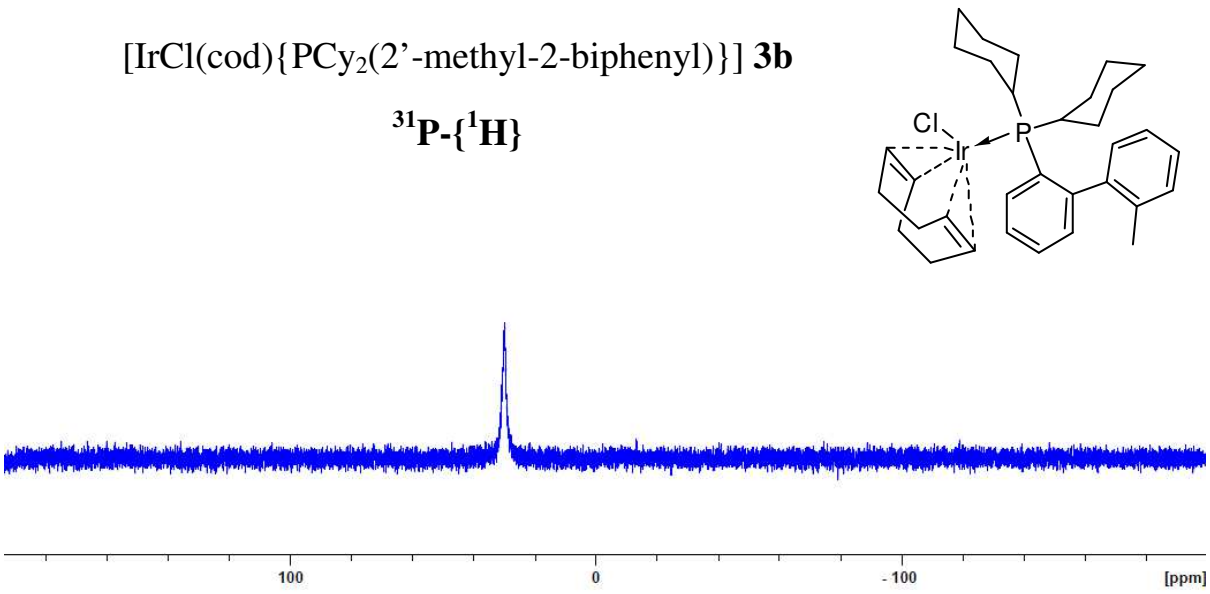
[IrCl(cod){PCy_2(2-biphenyl)}] **3a**

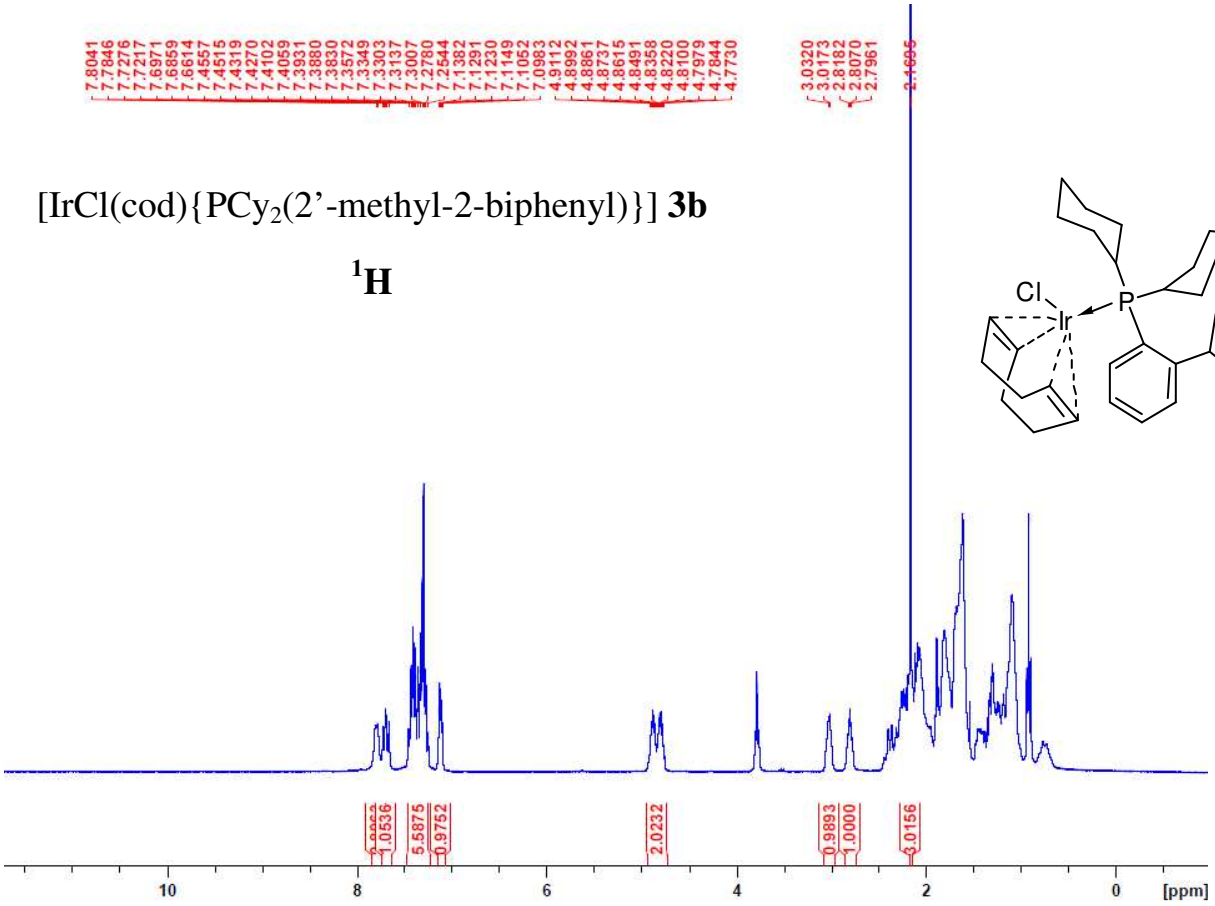
deptq



[IrCl(cod){PCy_2(2'-methyl-2-biphenyl)}] **3b**

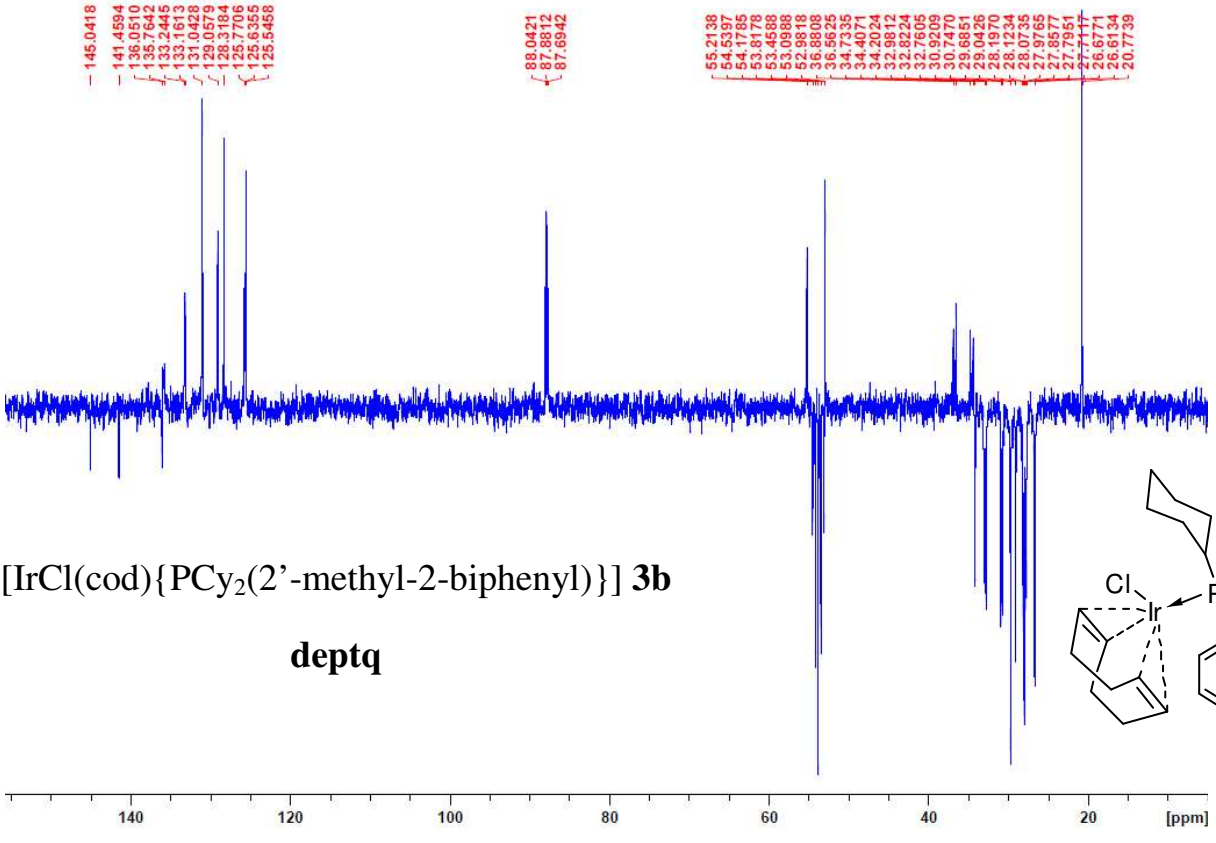
^{31}P-{^{1}H}





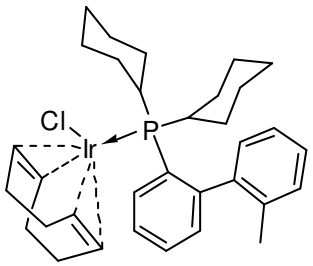
[IrCl(cod){PCy_2(2'-methyl-2-biphenyl)}] **3b**

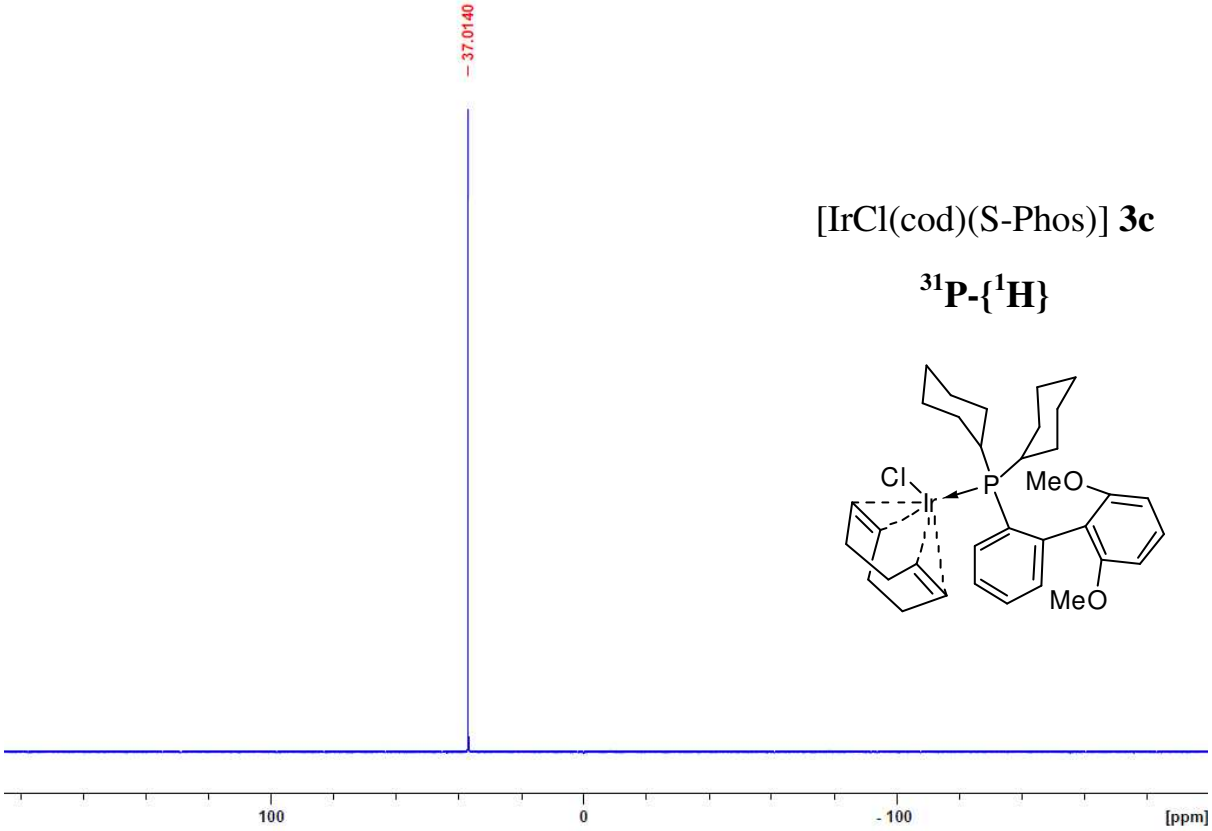
^{1}H



[IrCl(cod){PCy_2(2'-methyl-2-biphenyl)}] **3b**

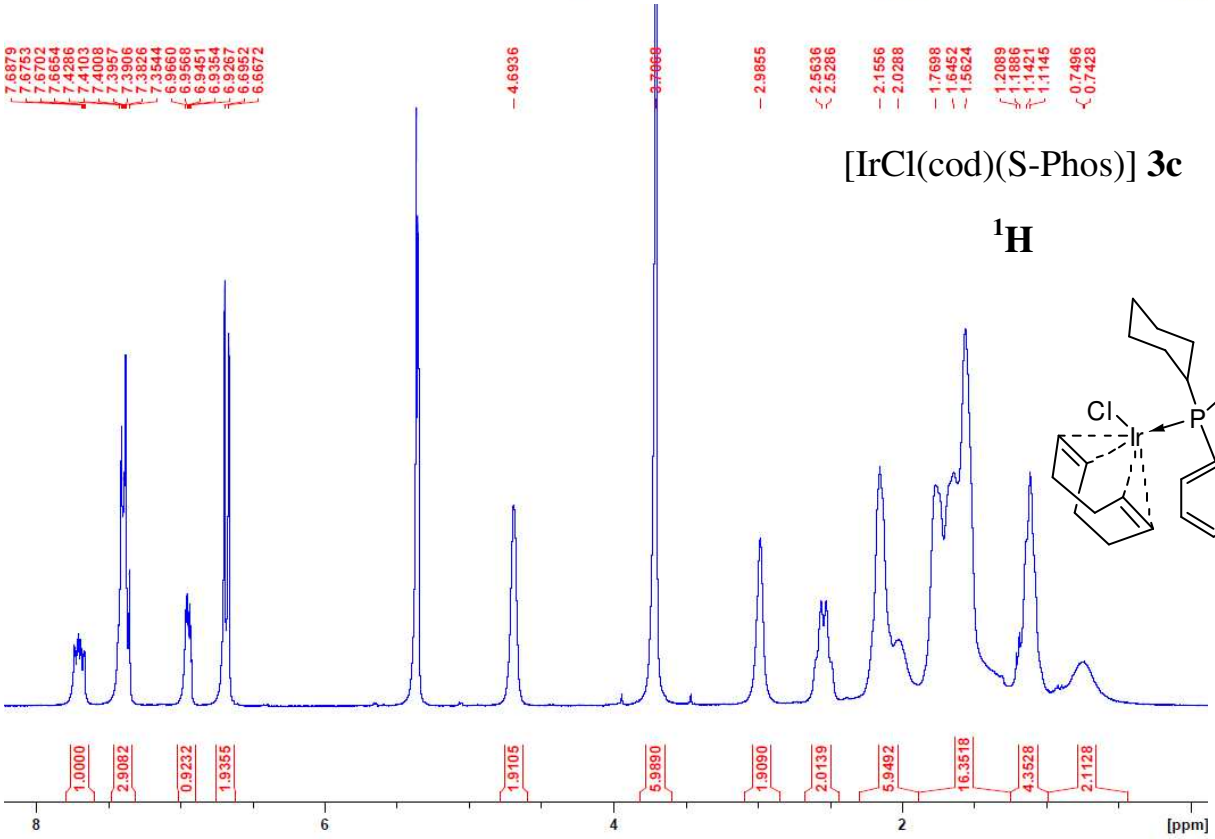
deptq





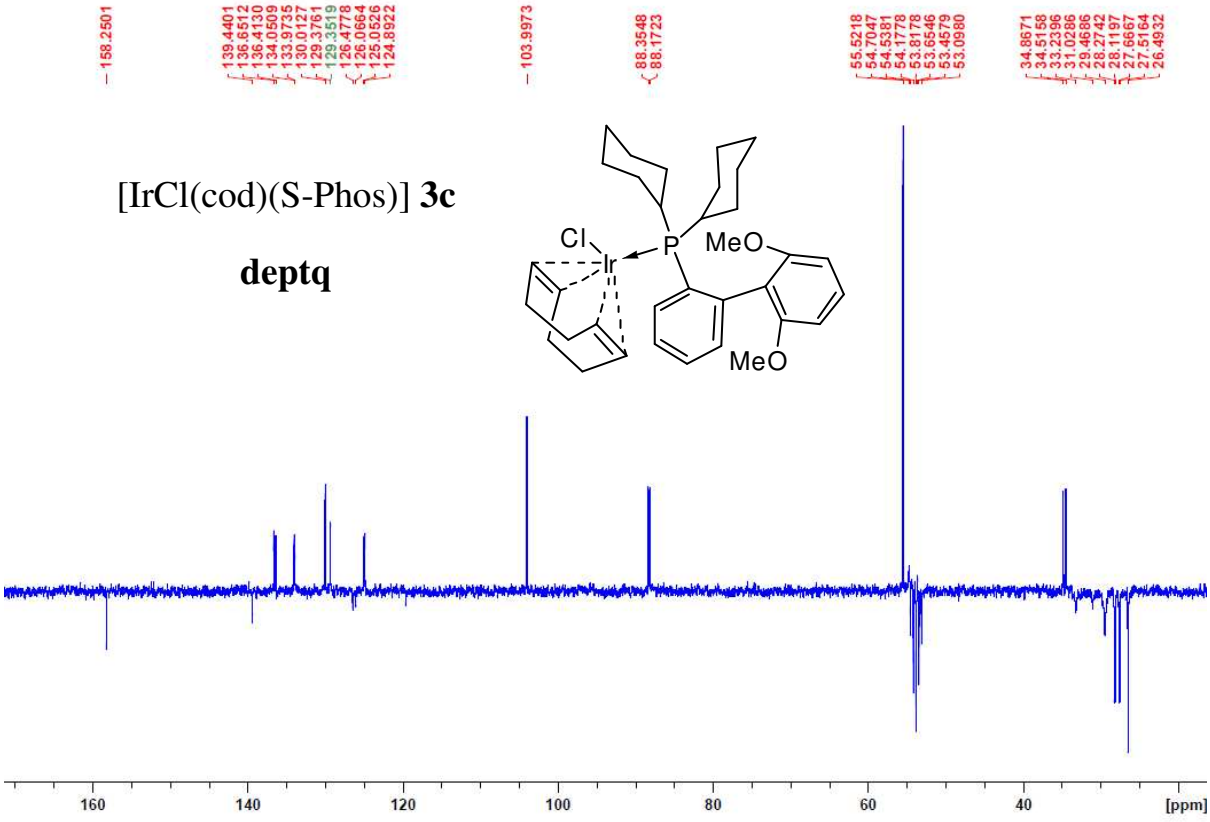
[IrCl(cod)(S-Phos)] **3c**

^{31}P-{^{1}H}



[IrCl(cod)(S-Phos)] **3c**

^{1}H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139.4401
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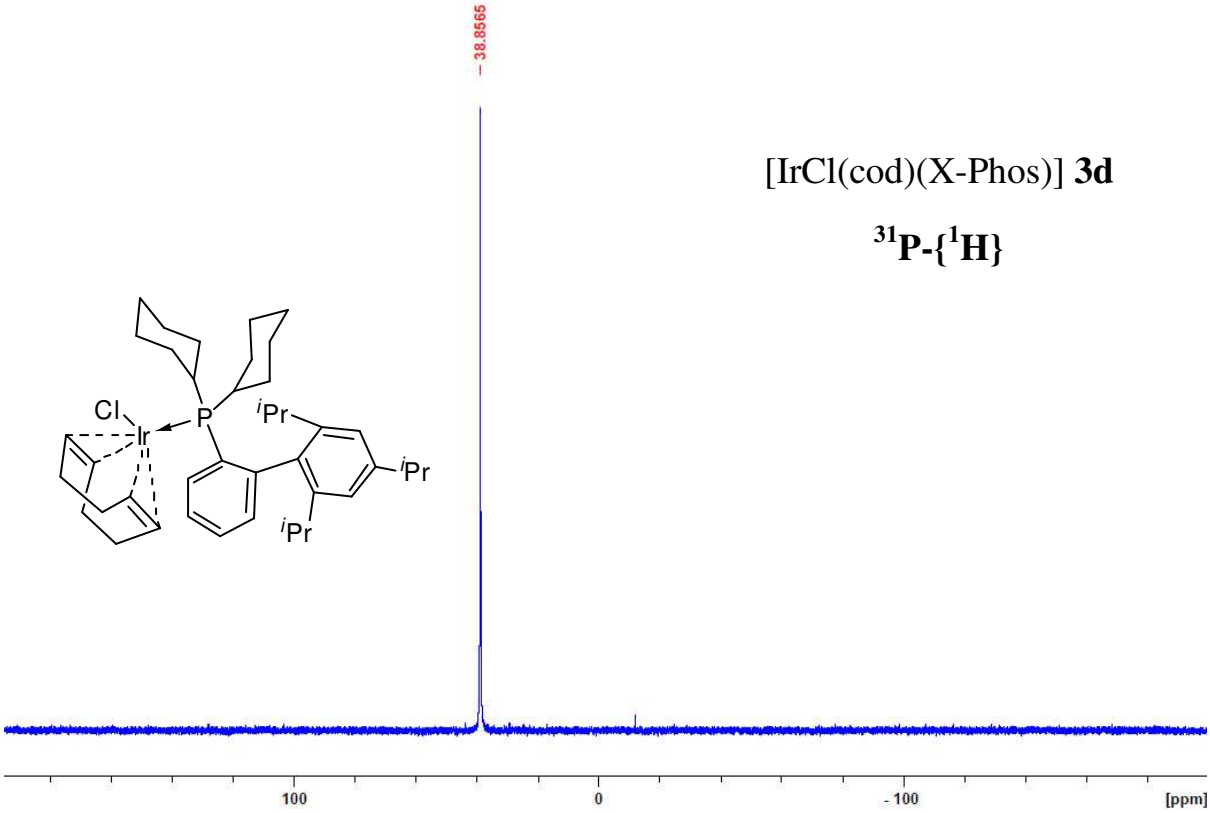
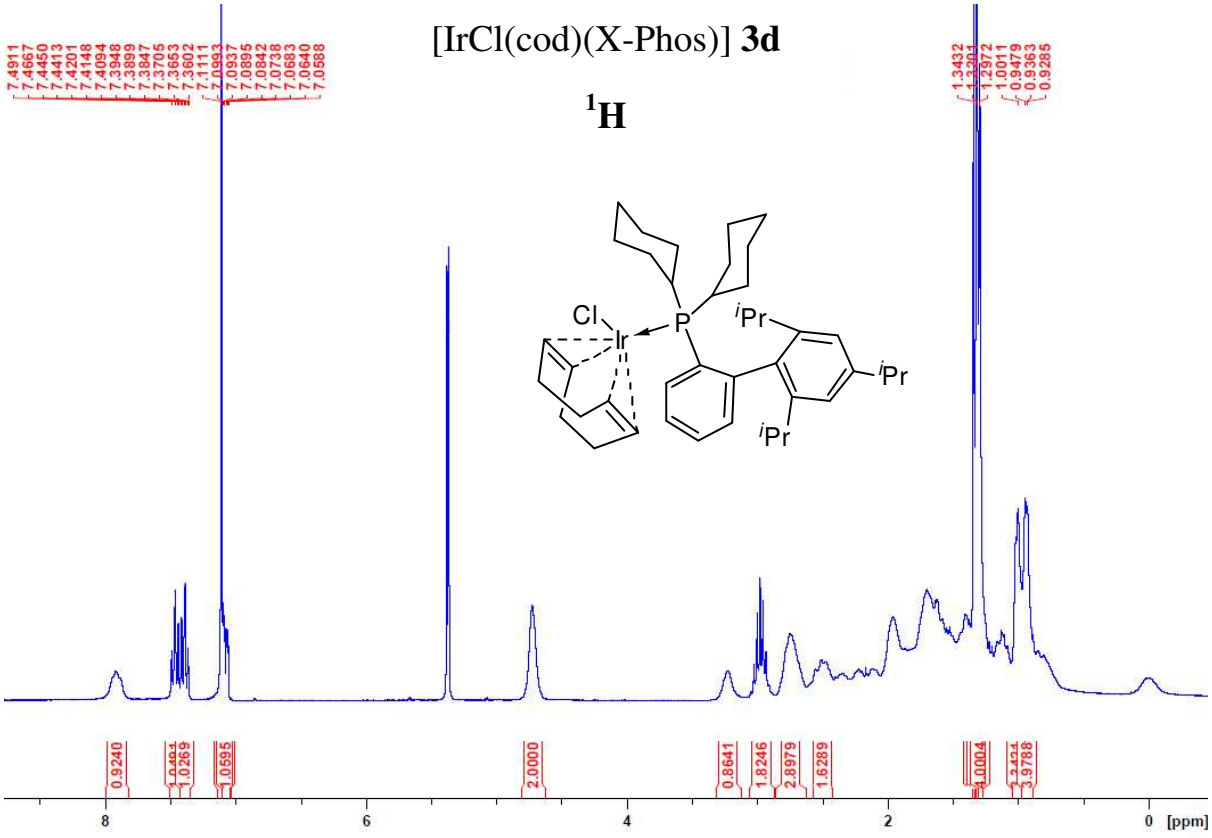
125.0526
124.8922
103.9973
88.3548
88.1723
55.5218
54.7047
54.5381
54.1778
53.8178
53.6546
53.4579
53.0980
34.8671
34.5158
33.2396
31.0286
29.4686
28.2742
28.1197
27.6667
27.5164
26.4932
[IrCl(cod)(S-Phos)] 3c
deptq
Cl
Ir
P
MeO
MeO
160
140
120
100
80
60
40
[ppm]


38.8565
[IrCl(cod)(X-Phos)] 3d
31P-{1H}
Cl
Ir
P
iPr
iPr
iPr
100
0
-100
[ppm]

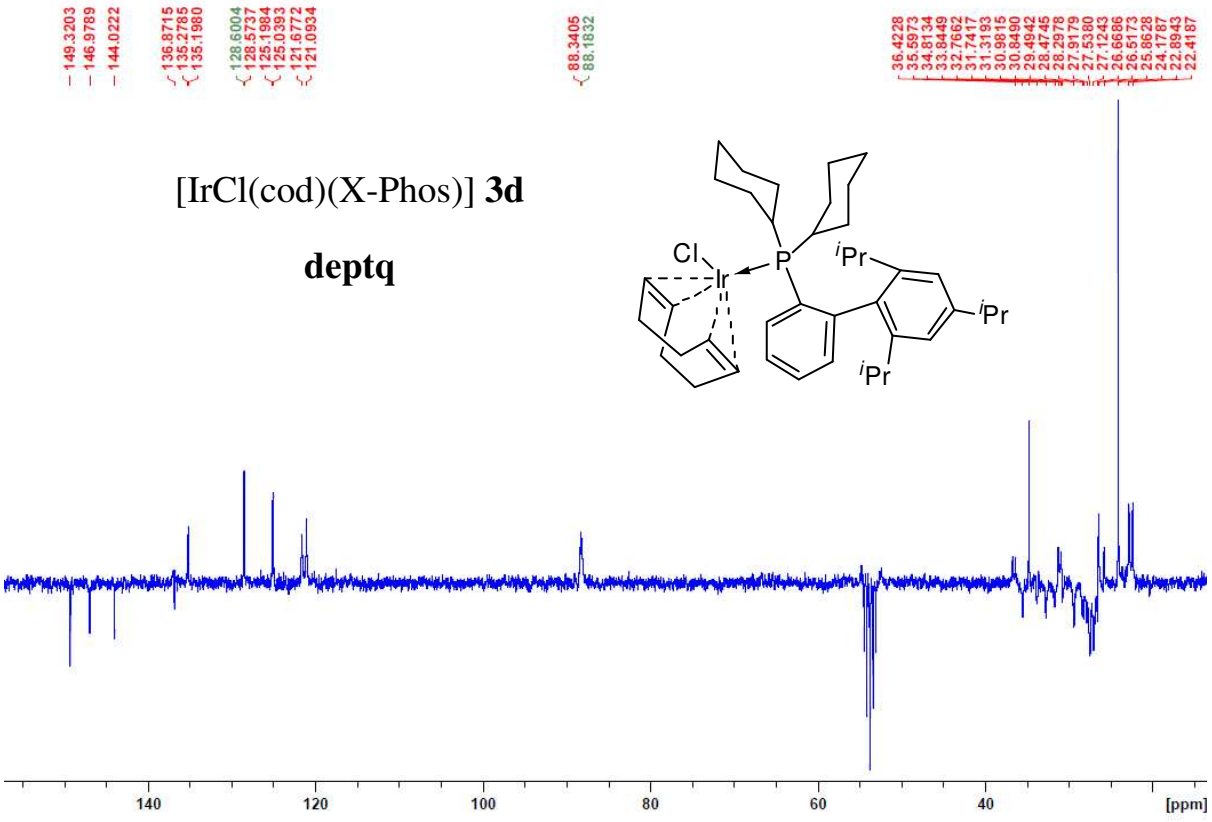
[IrCl(cod)(X-Phos)] **3d**

^{1}H



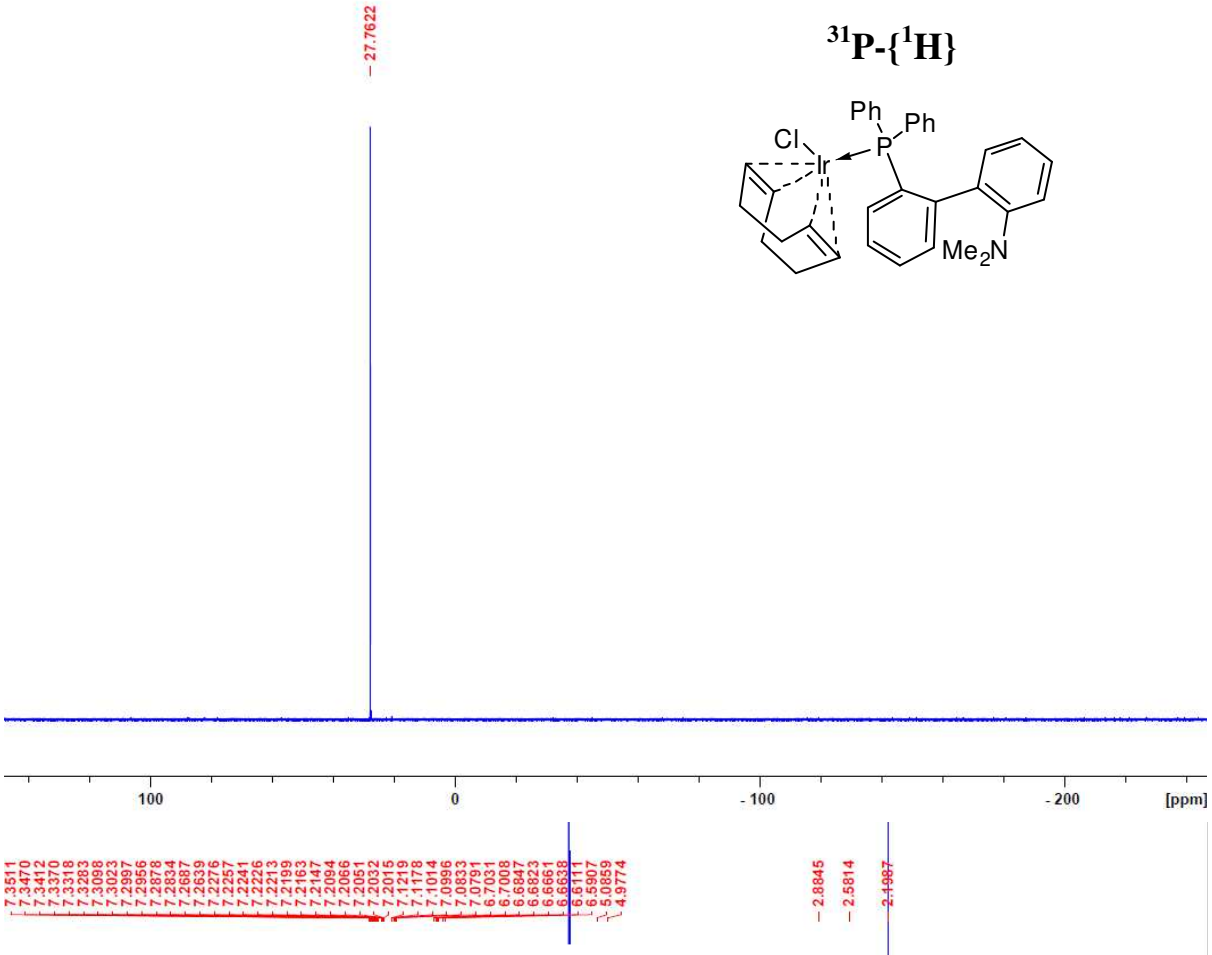
[IrCl(cod)(X-Phos)] **3d**

deptq



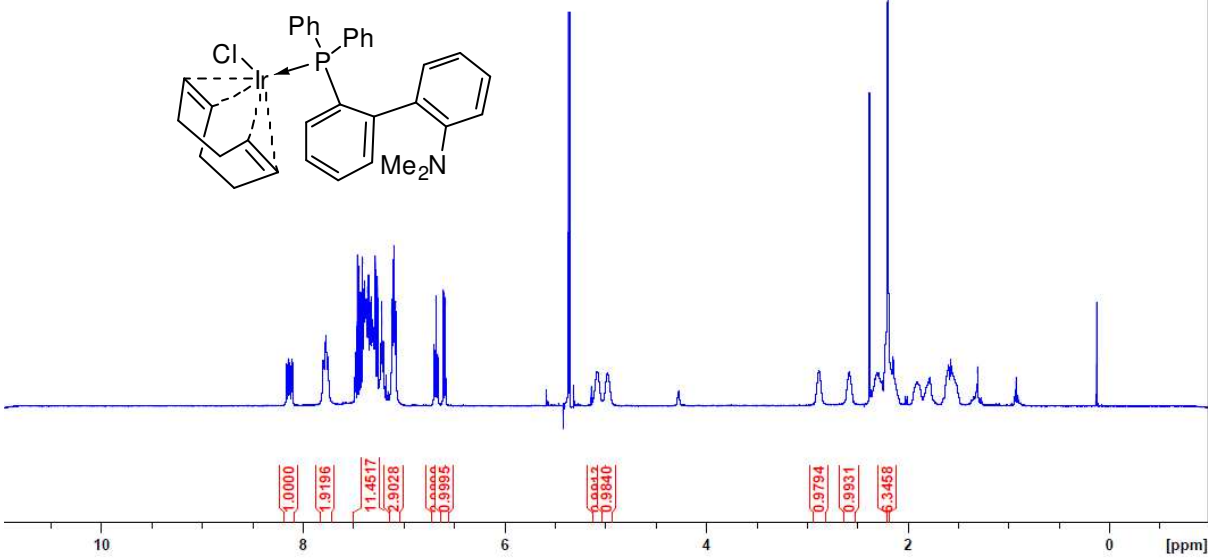
[IrCl(cod){PCy_2(2'-dimethylamino-2-biphenyl)}] **3e**

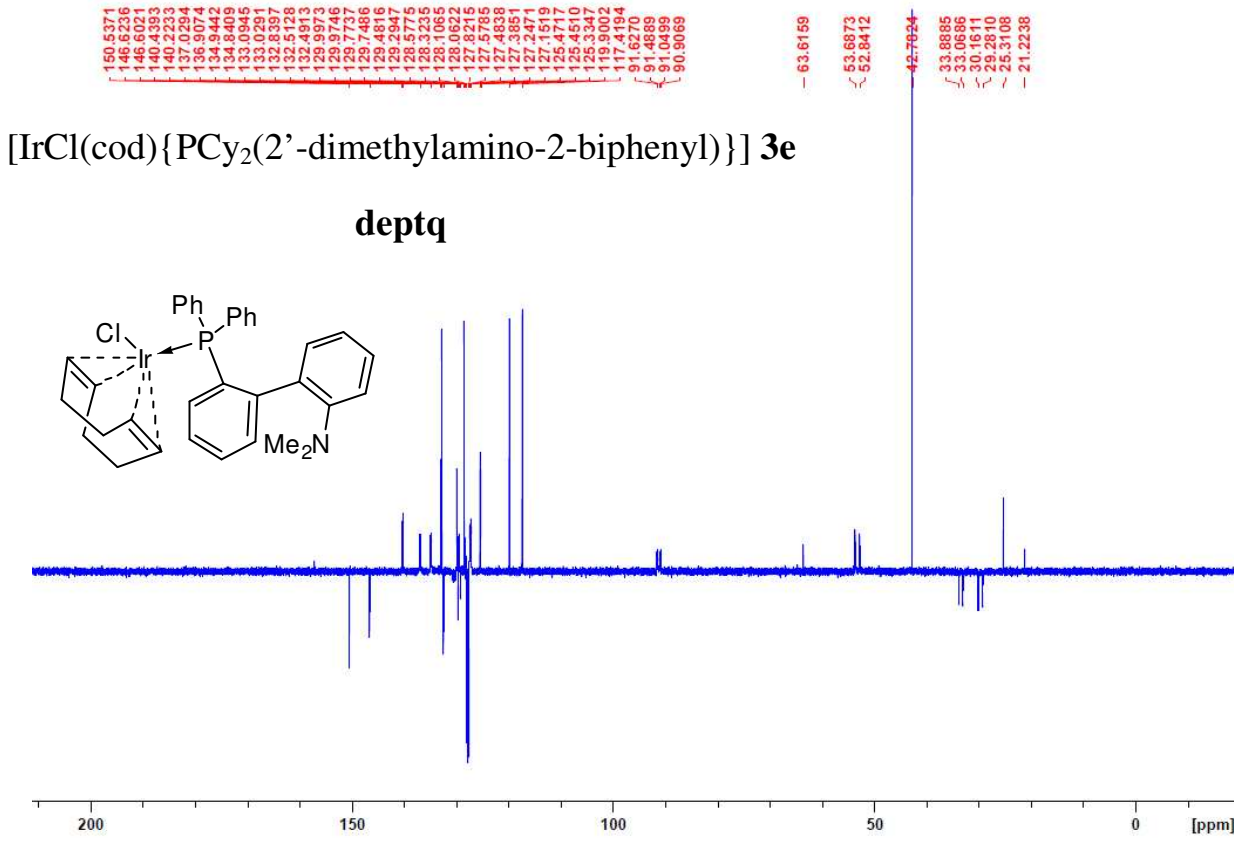
^{31}P-{^{1}H}



[IrCl(cod){PCy_2(2'-dimethylamino-2-biphenyl)}] **3e**

^{1}H

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132.8397
132.5128
132.4913
129.9973
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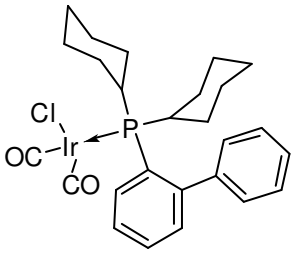
129.7737
129.7486
129.4816
129.2947
128.5775
128.3235
128.1065
128.0622
127.8215
127.5785
127.4838
127.3851
127.2471
127.1519
125.4717
125.4510
125.3347
119.9002
117.4194
91.6270
91.4889
91.0499
90.9069
63.6159
53.6873
52.8412
42.7024
33.8885
33.0886
30.1611
29.2810
25.3108
21.2238
[IrCl(cod){PCy2(2'-dimethylamino-2-biphenyl)}] 3e
deptq
Ph
Ph
Cl
Ir
P
Me2N
200
150
100
50
0
[ppm]

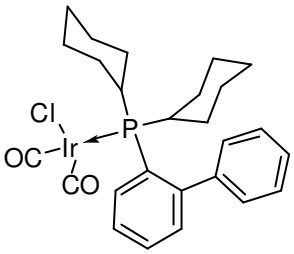
[IrCl(CO)$_2${PCy$_2$(2-biphenyl)}] **4a**

^{31}P-{^{1}H}



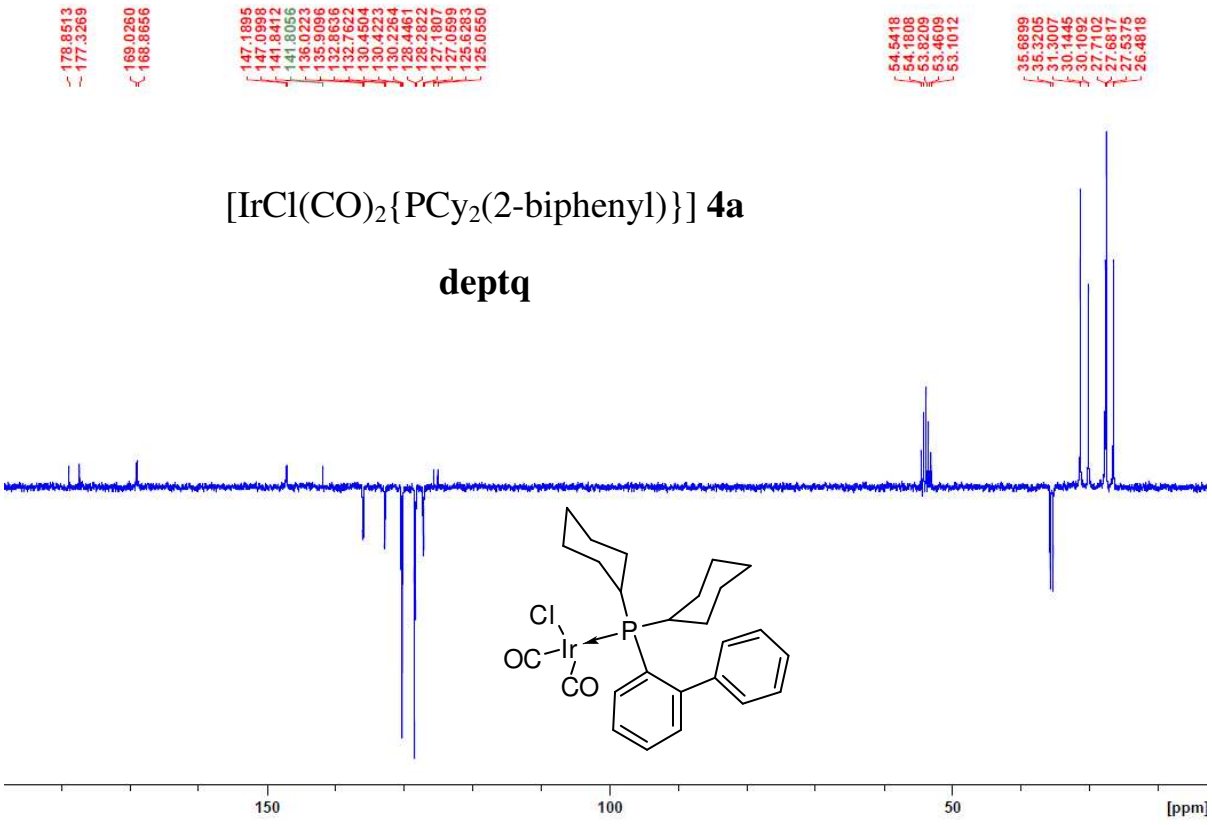
[IrCl(CO)$_2${PCy$_2$(2-biphenyl)}] **4a**

^{1}H



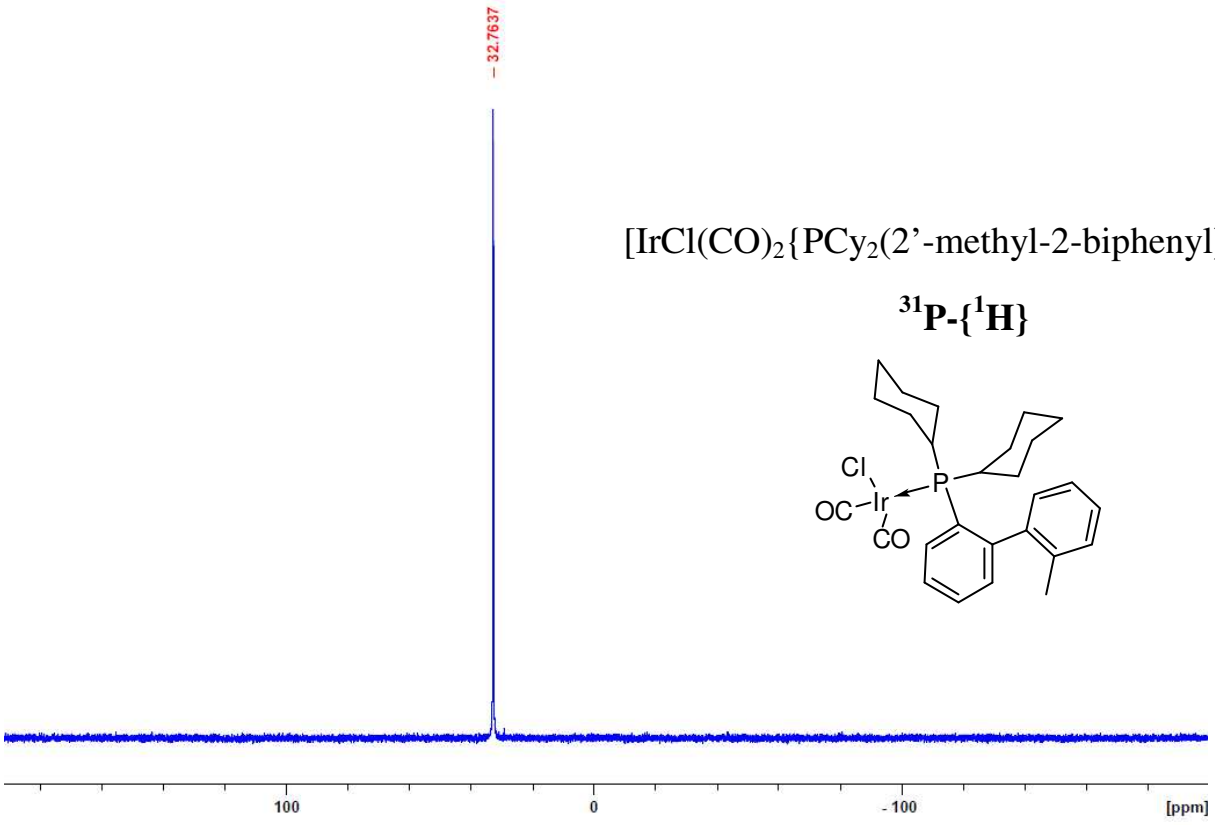
[IrCl(CO)$_2${PCy$_2$(2-biphenyl)}] **4a**

deptq



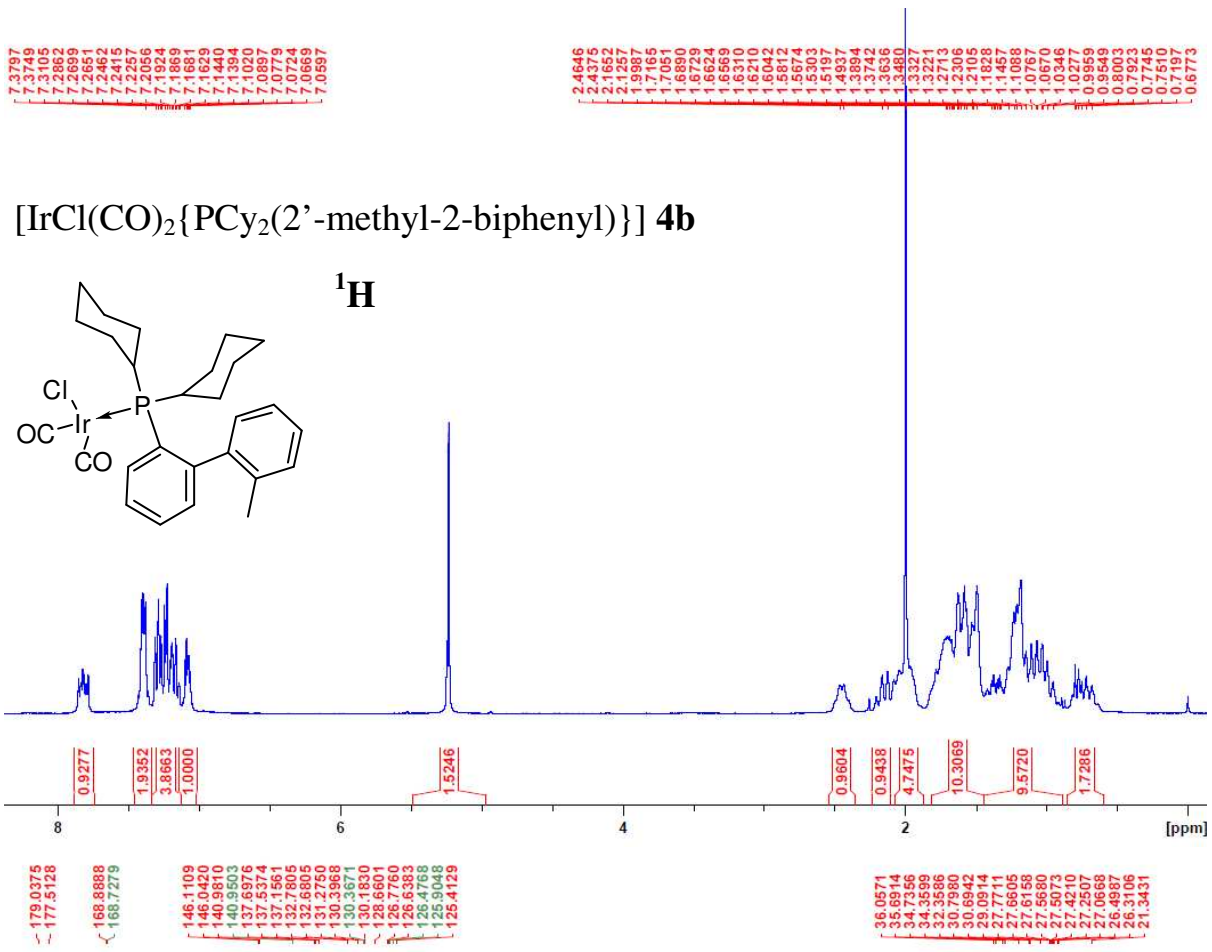
[IrCl(CO)$_2${PCy$_2$(2'-methyl-2-biphenyl)}] **4b**

^{31}P-{^{1}H}



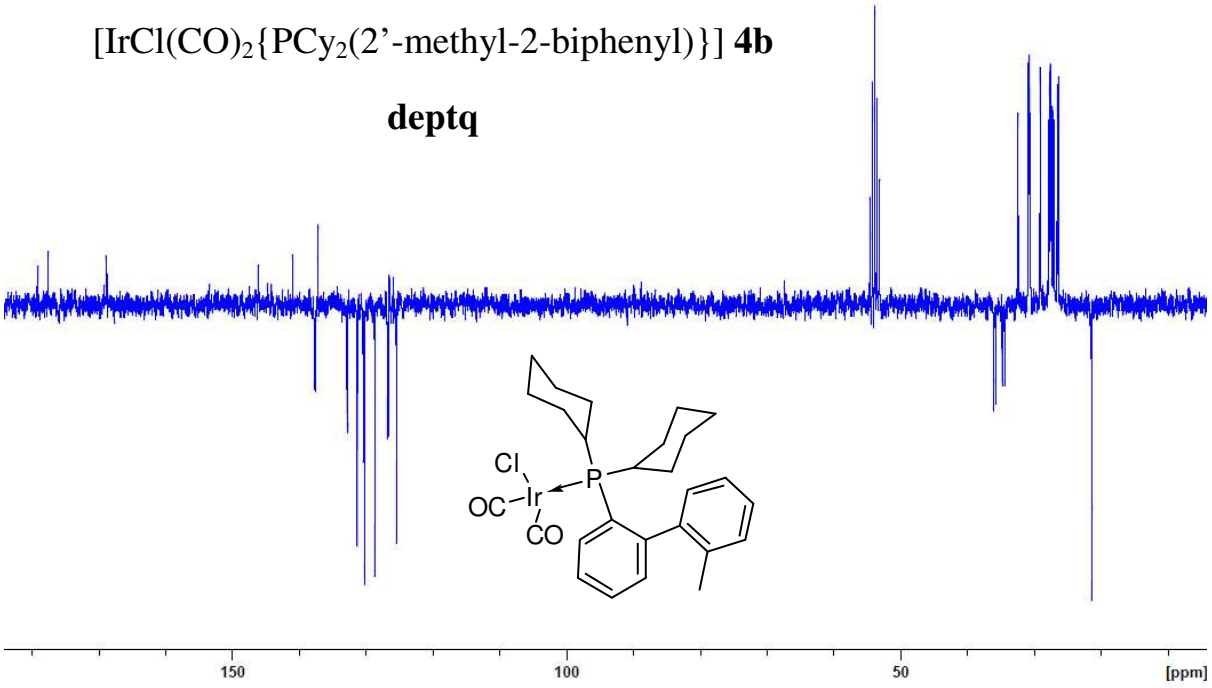
[IrCl(CO)$_2${PCy$_2$(2'-methyl-2-biphenyl)}] **4b**

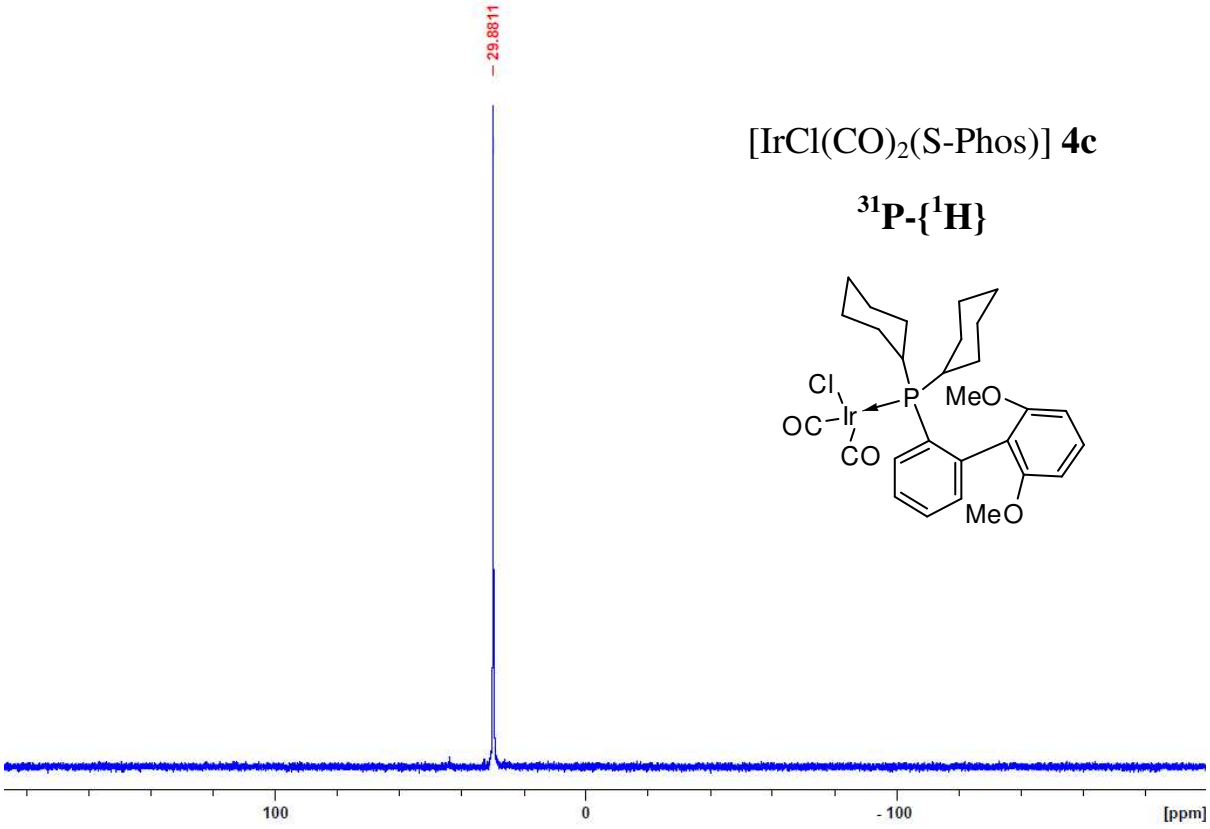
^{1}H



[IrCl(CO)$_2${PCy$_2$(2'-methyl-2-biphenyl)}] **4b**

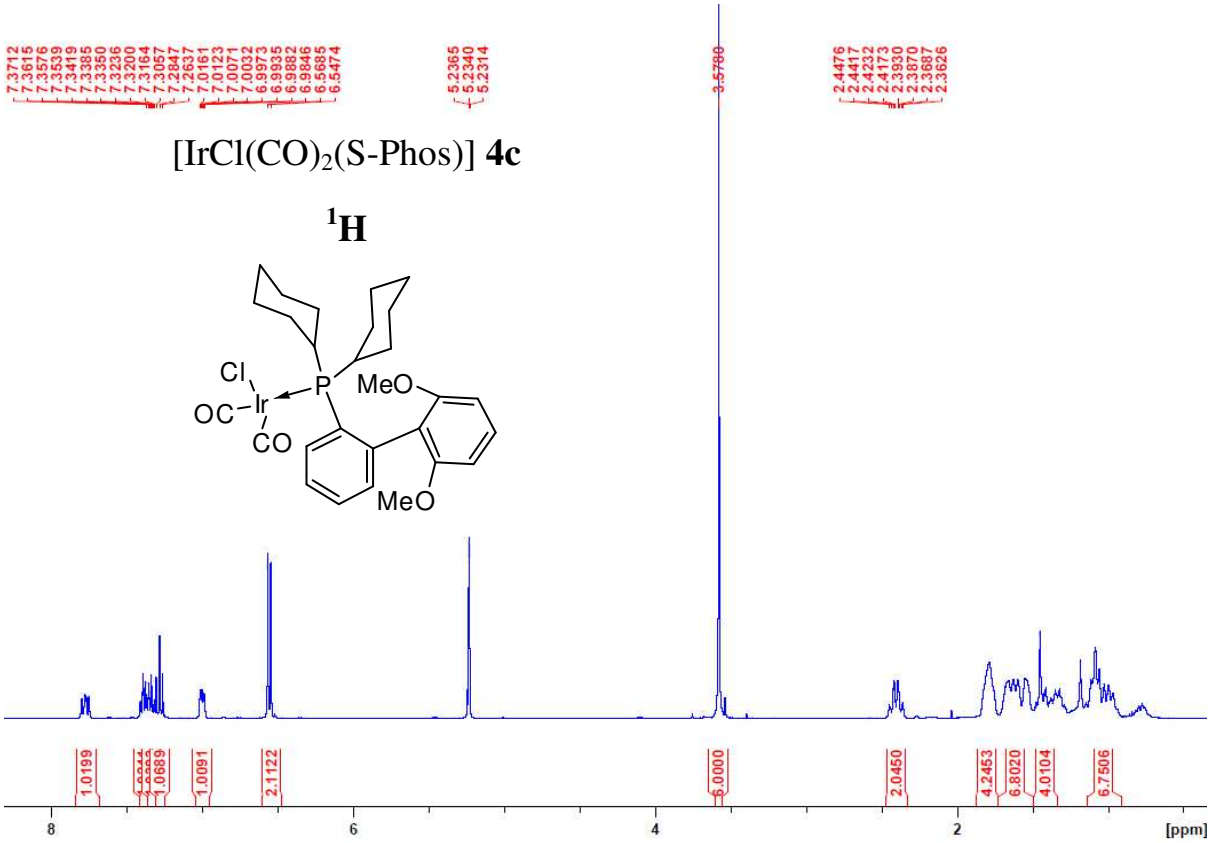
deptq





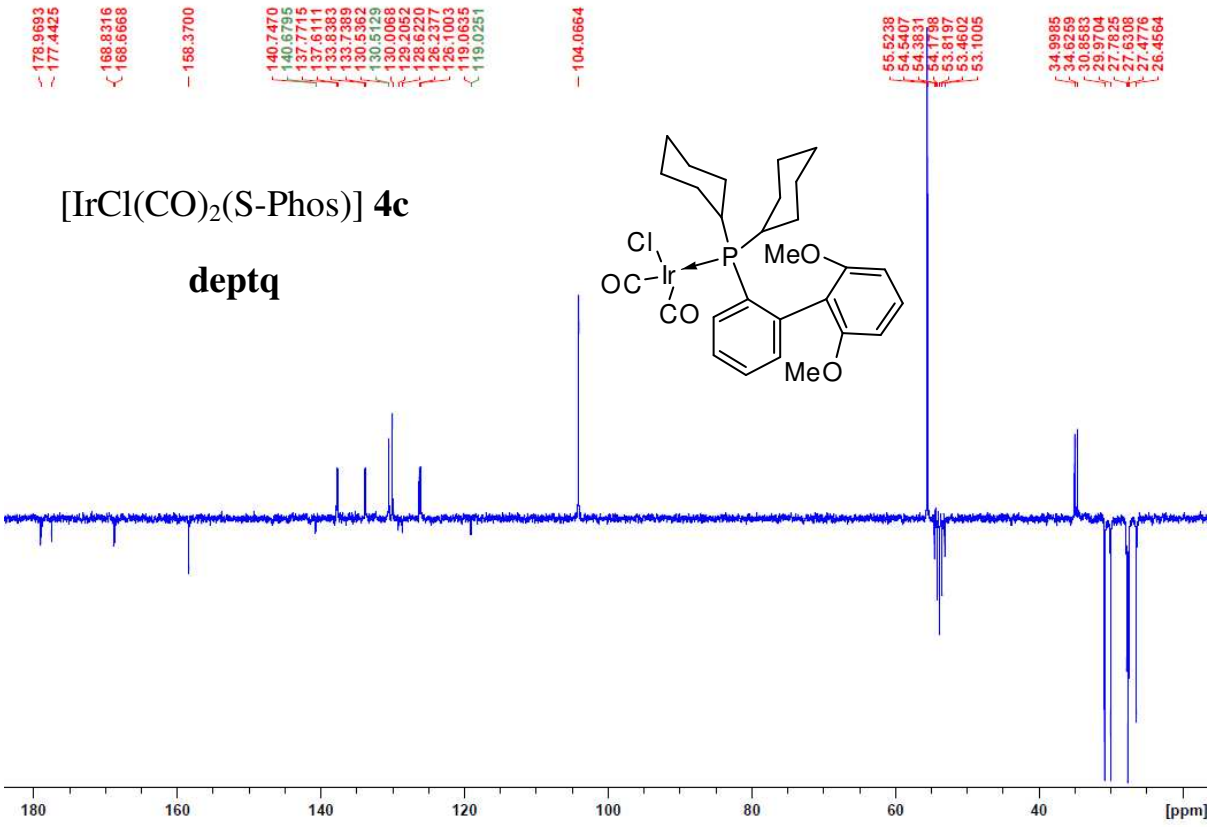
[IrCl(CO)$_2$(S-Phos)] **4c**

^{31}P-{^{1}H}



[IrCl(CO)$_2$(S-Phos)] **4c**

^{1}H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140.6795
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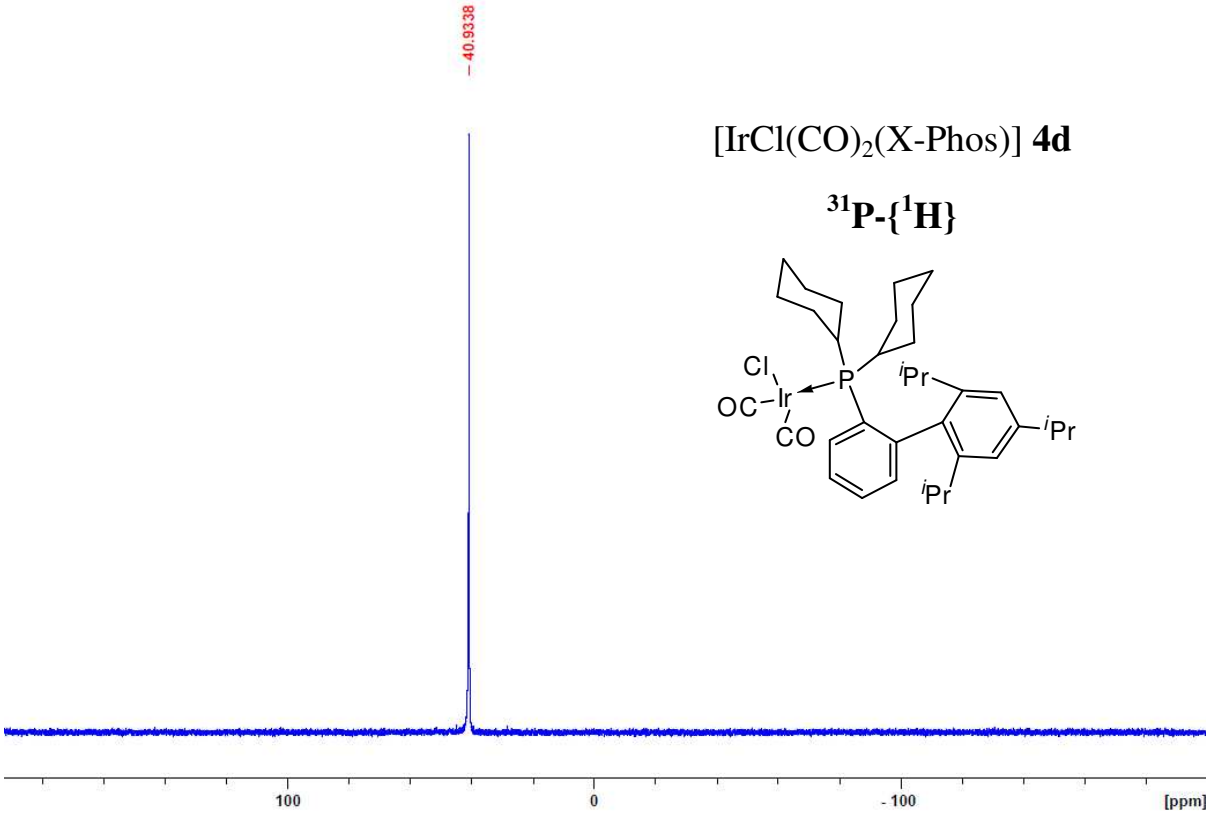
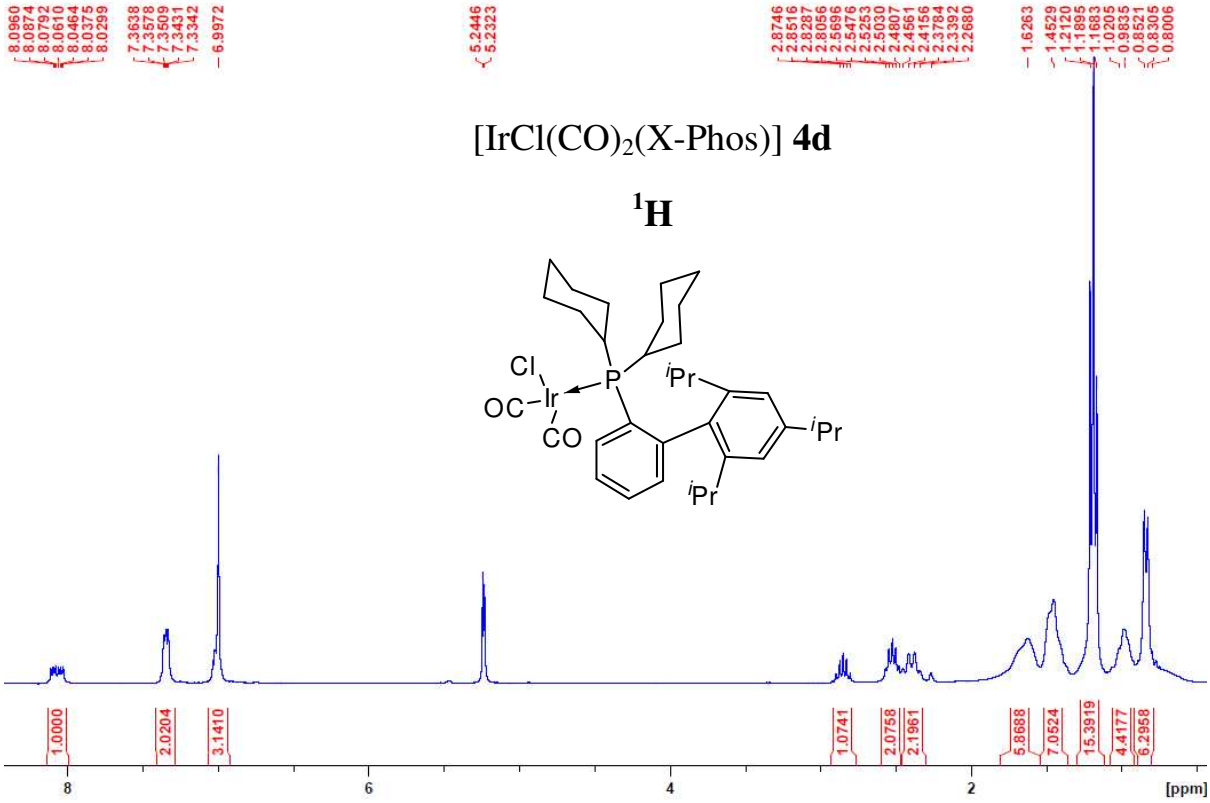
137.6111
133.8383
133.7389
130.5362
130.5129
130.0068
129.2052
128.6220
126.2377
126.1003
119.0635
119.0251
104.0664
55.5238
54.5407
54.3831
54.1798
53.8197
53.4602
53.1005
34.9985
34.6259
30.8583
29.9704
27.7825
27.6308
27.4776
26.4564
[IrCl(CO)2(S-Phos)] 4c
deptq
Cl
OC
Ir
CO
P
MeO
MeO
180
160
140
120
100
80
60
40
[ppm]


40.9338
[IrCl(CO)2(X-Phos)] 4d
31P-{1H}
Cl
OC
Ir
CO
P
iPr
iPr
iPr
100
0
- 100
[ppm]

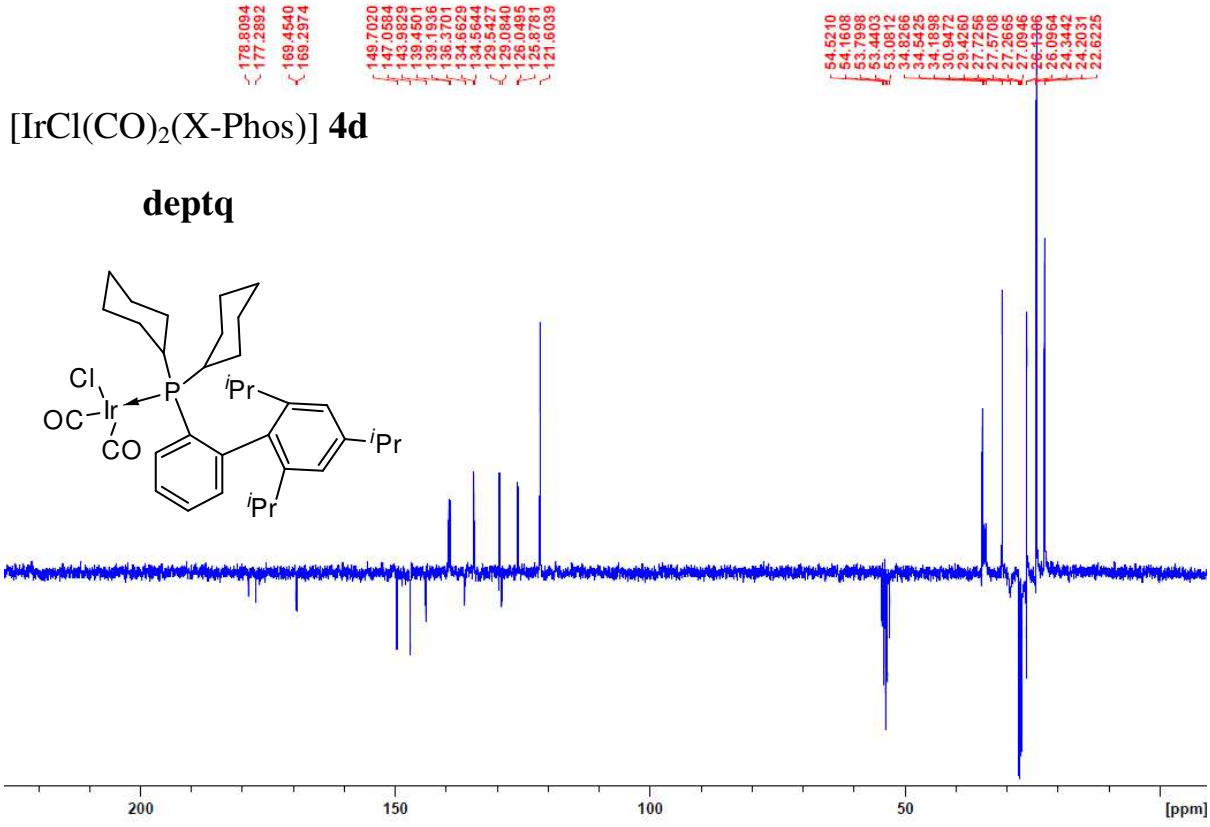
[IrCl(CO)$_2$(X-Phos)] **4d**

^{1}H

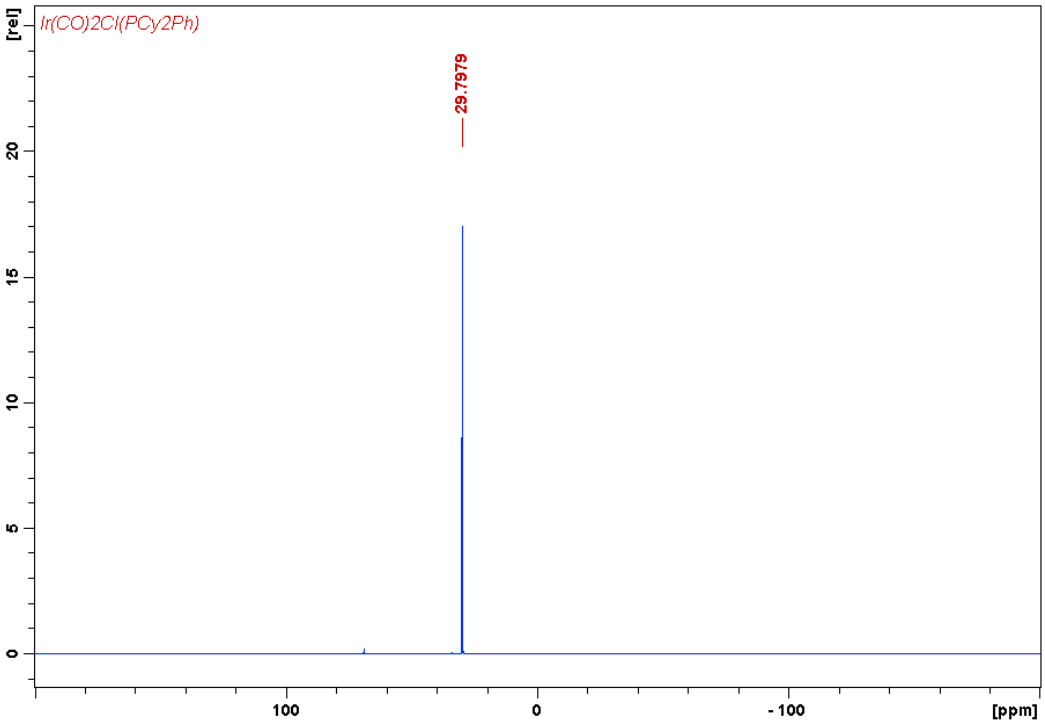


[IrCl(CO)$_2$(X-Phos)] **4d**

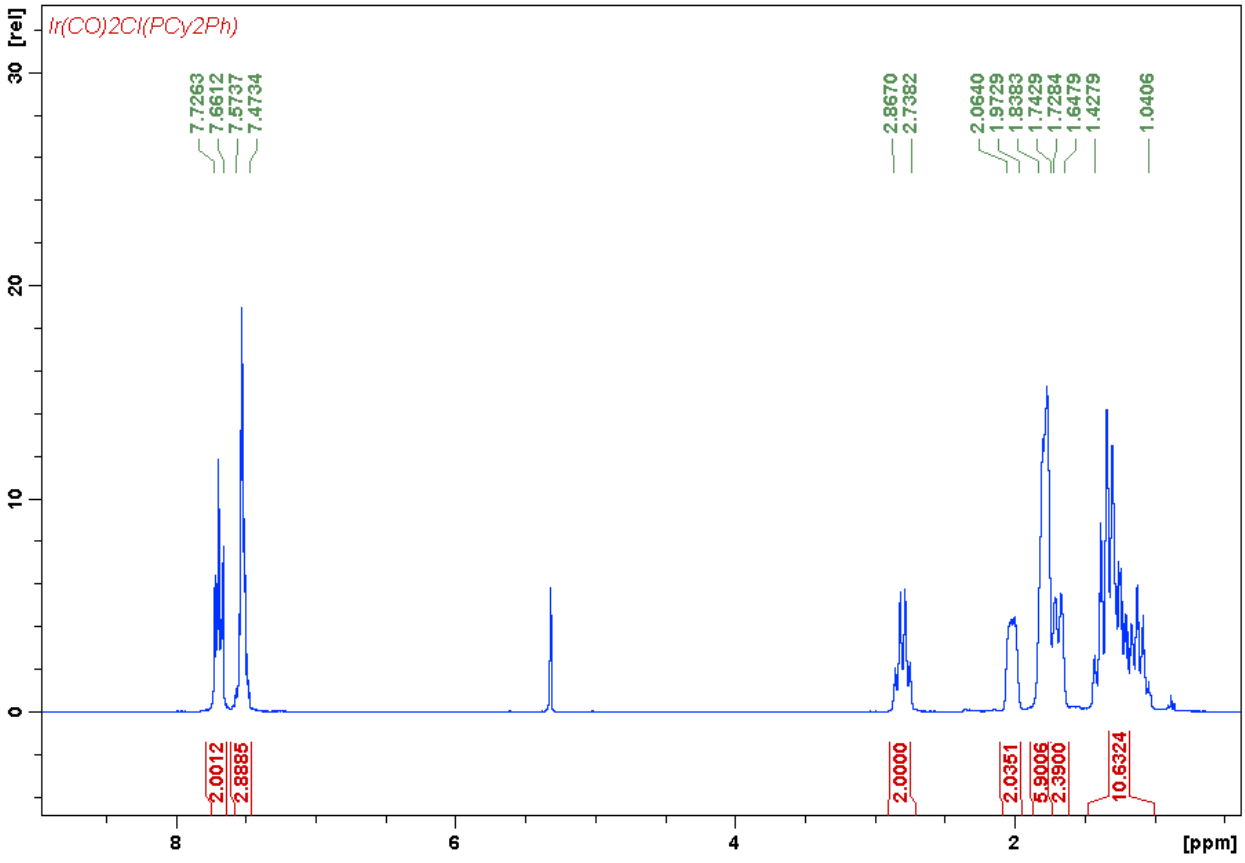
deptq



[$IrCl(CO)_2(PCy_2Ph)$] (**4g**) – ^{31}P



[$IrCl(CO)_2(PCy_2Ph)$] (**4g**)– ^{1}H



[$IrCl(CO)_2(PCy_2Ph)$] (**4g**)- ^{13}C

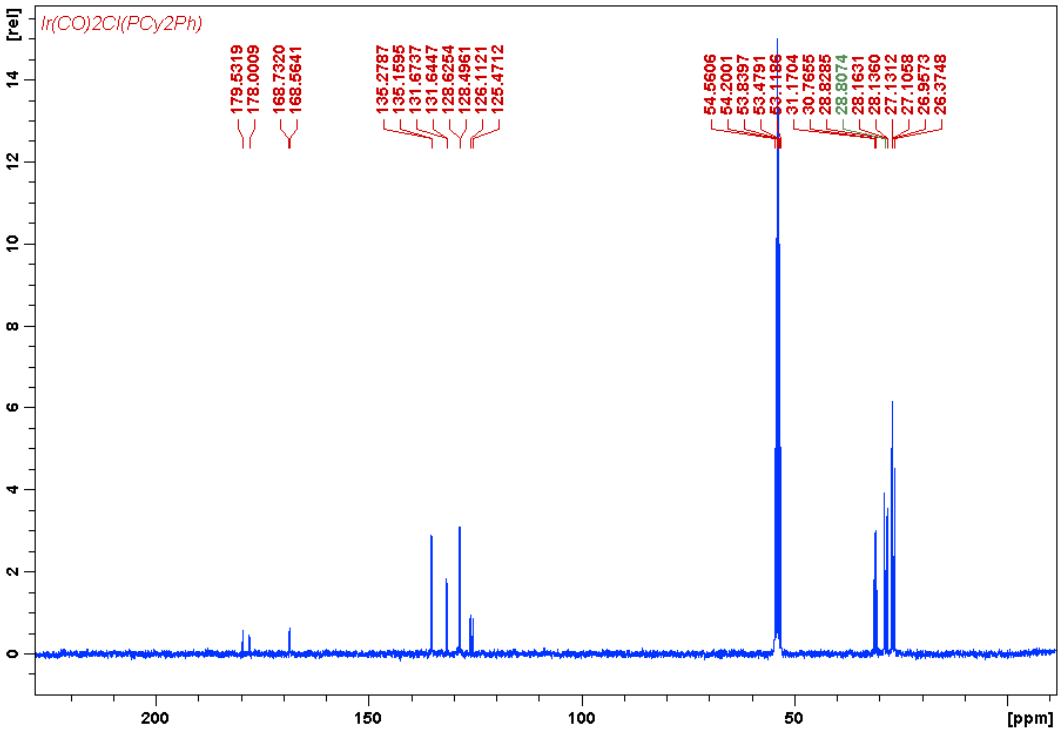


Table S1. Crystallographic Data Table.

Compound reference	3a	3b	3c	3d	4a	4b	4c	4d	4g
Chemical formula	$C_{32}H_{43}ClIrP$	$C_{35}H_{49}ClIrOP$	$C_{36}H_{51}ClIrO_3P$	$C_{41}H_{61}ClIrP$	$C_{26}H_{31}ClIrO_2P$	$C_{27}H_{33}ClIrO_2P$	$C_{28}H_{35}ClIrO_4P$	$C_{35}H_{49}ClIrO_2P$	$C_{20}H_{27}ClIrO_2P$
Formula Mass	686.28	744.36	790.39	812.52	634.13	648.15	694.18	760.36	558.04
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic
a/Å	9.1087(2)	9.7647(2)	16.0447(10)	18.787(2)	9.155(4)	9.031(3)	8.631(3)	10.8222(9)	11.050(3)
b/Å	16.9206(4)	9.8404(2)	11.3273(8)	9.3296(11)	10.415(3)	10.767(3)	20.819(6)	28.978(2)	14.534(4)
c/Å	17.9178(4)	16.6899(3)	17.9788(11)	22.156(3)	13.757(5)	13.915(4)	15.561(4)	10.5824(9)	13.029(3)
α/°	90.00	97.4660(10)	90.00	90.00	75.18(2)	75.225(14)	90.00	90.00	90.00
β/°	99.2830(10)	99.5490(10)	94.018(3)	108.885(4)	89.99(2)	88.737(15)	91.350(8)	92.147(2)	92.005(7)
γ/°	90.00	99.5550(10)	90.00	90.00	73.371(16)	71.842(14)	90.00	90.00	90.00
Unit cell volume/Å^3	2725.41(11)	1538.96(5)	3259.5(4)	3674.4(7)	1211.4(7)	1240.8(6)	2795.2(14)	3316.4(5)	2091.1(8)
Temperature/K	100(2)	100(2)	100(2)	100(2)	93(2)	100(2)	93(2)	100(2)	93(2)
Space group	*P*2(1)/*n*	*P*$\bar{1}$	*P*2(1)/*c*	*P*2(1)/*c*	*P*$\bar{1}$	*P*$\bar{1}$	*Pn*	*P*2(1)/*c*	*P*2(1)/*n*
No. of formula units per unit cell, *Z*	4	2	4	4	2	2	4	4	4
No. of reflections measured	41084	36021	68232	63414	5198	29133	17374	42834	12847
No. of independent reflections	15990	15721	18378	16312	3253	12731	8741	15183	3786
R_{int}	0.0283	0.0258	0.0430	0.0657	0.0511	0.0373	0.0864	0.0458	0.0959
Final R_1 values ($I > 2\sigma(I)$)	0.0300	0.0221	0.0336	0.0707	0.0328	0.0338	0.0531	0.0436	0.0423
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0786	0.0555	0.0826	0.1608	0.0859	0.0759	0.0920	0.0918	0.1086
Final R_1 values (all data)	0.0347	0.0232	0.0463	0.0870	0.0341	0.0531	0.0657	0.0576	0.0476
Final $wR(F^2)$ values (all data)	0.0811	0.0559	0.0897	0.1681	0.0868	0.0829	0.0981	0.0964	0.1335
CCDC number	744632	744633	744634	744635	746738	744636	746738	744637	802800

Table S2. $\%V_{bur}$ calculated using shortest Ir-P and experimentally determined Ir-P distances.

Complex	Ligand	%Vbur at 2.334 Å	%Vbur exp Ir-P distance
3a	2a	35.0	34.6
3b	2b	34.1	33.6
3c	2c	30.0	30.0
3d	2d	30.2	30.0
4a	2a	33.8	33.0
4b	2b	34.4	33.9
4c	2c	31.6	30.7
4d	2d	32.4	31.7
4g	2g	30.6	29.9

Data calculated using ref 1. All values calculated keeping default values except for Ir-L distance.

%Vur Data Output[1]

3a

SambVca@MoLNnaC file:///Users/gcfortman/Desktop/Nolan/Ir Buchwald/CIF iridium(...

SambVca @ MoLNaC
Results page

```
 ------------------------------------------------
|                                                |
|                S A M B V C A                   |
|                                                |
|           buried volume in salerno             |
|                                                |
|   http://www.molnac.unisa.it/OM-tools/SambVca  |
|                                                |
|    L. Cavallo et al. email: lcavallo@unisa.it  |
|                                                |
 ------------------------------------------------
```

Molecule from input :

```
  Molecule from input :

 ./temp/a32d7b4686f72d21855a24ba0d58c413.c3d1


     Number of atoms               :   25
     Atom that is coordinated      :   25
     Atoms that define the axis    :    3
     ID of these atoms             :    1  13  19

     Radius of sphere (Angs)       :    3.500
     Distance from sphere (Angs)   :    2.334
     Mesh step (Angs)              :    0.050
     H atoms omitted in the V_bur calculation
```

Cartesian coordinates from input :

```
  Cartesian coordinates from input :
C       -31.10600  -5.16700 -55.32100
C       -32.40600  -5.64300 -55.11000
C       -32.82300  -6.10500 -53.86600
C       -31.93800  -6.09700 -52.79600
C       -30.63900  -5.63600 -52.99000
C       -30.20100  -5.15700 -54.23100
C       -28.77500  -4.72300 -54.33900
```

1 of 3 12/6/10 8:49 AM

SambVca@MoLNnaC file:///Users/gcfortman/Desktop/Nolan/Ir Buchwald/CIF iridium(...

```
C       -28.41000  -3.43400 -54.74400
C       -27.07000  -3.09800 -54.92600
C       -26.07300  -4.04000 -54.67900
C       -26.42300  -5.30200 -54.20700
C       -27.76000  -5.64400 -54.03900
C       -32.00400  -5.00100 -58.13200
C       -32.14300  -6.50700 -58.41600
C       -33.35800  -6.78900 -59.29600
C       -33.26400  -6.01200 -60.61300
C       -33.12200  -4.51500 -60.35200
C       -31.92900  -4.20400 -59.45500
C       -29.10700  -5.46100 -57.40700
C       -29.12600  -6.92600 -56.91900
C       -27.75300  -7.58300 -57.11300
C       -27.30500  -7.50100 -58.58600
C       -27.31300  -6.05400 -59.05700
C       -28.69700  -5.41500 -58.88900
P       -30.64700  -4.48900 -56.97100
```

Atoms and radius in the parameter file

```
  Atoms and radius in the parameter file
H     1.29
C2    1.99
C3    1.99
C     1.99
N2    1.81
N3    1.81
N     1.81
O     1.78
F     1.72
Si    2.45
P     2.11
S     2.10
Cl    2.05
```

```
C          1.57653  -2.54853   2.68874
C          1.94153  -1.25953   2.28374
C          3.28153  -0.92353   2.10174
C          4.27853  -1.86553   2.34874
C          3.92853  -3.12753   2.82074
C          2.59153  -3.46953   2.98874
C         -1.65247  -2.82653  -1.10426
C         -1.79147  -4.33253  -1.38826
C         -3.00647  -4.61453  -2.26826
C         -2.91247  -3.83753  -3.58526
C         -2.77047  -2.34053  -3.32426
C         -1.57747  -2.02953  -2.42726
C          1.24453  -3.28653  -0.37926
C          1.22553  -4.75153   0.10874
C          2.59853  -5.40853  -0.08526
C          3.04653  -5.32653  -1.55826
C          3.03853  -3.87953  -2.02926
C          1.65453  -3.24053  -1.86126
P         -0.29547  -2.31453   0.05674
XX         0.00000   0.00000   0.00000
```

2 of 3 12/6/10 8:49 AM

SambVca@MoLNnaC file:///Users/gcfortman/Desktop/Nolan/Ir Buchwald/CIF iridium(...

Results : Volumes in Angs^3

```
  Results : volumes in Angs^3

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

   V Free   V Buried  V Total   V Exact
  116.683    62.852   179.535   179.594

  %V_Free    %V_Bur  % Tot/Ex
  64.992     35.008    99.967
```

The %V_Bur of your molecule is: 35.0

3 of 3 12/6/10 8:49 AM

3b

SambVca @ MoLNaC
Results page

```
 ------------------------------------------------------
|                                                      |
|                  S A M B V C A                       |
|                                                      |
|              Buried Volume in Salerno                |
|                                                      |
|   http://www.molnac.unisa.it/OM-tools/SambVca        |
|                                                      |
|    L. Cavallo et al. email: lcavallo@unisa.it        |
|                                                      |
 ------------------------------------------------------
```

Molecule from input :

```
 Molecule from input :

./temp/9152163785ab4314c4f70b8feb56b3cd.c3d1

     Number of atoms             :   59
     Atom that is coordinated    :   59
     Atoms that define the axis  :    3
     ID of these atoms           :    1   7  13

     Radius of sphere (Angs)     :   3.500
     Distance from sphere (Angs) :   2.334
     Mesh step (Angs)            :   0.050
     H atoms omitted in the V_bur calculation
```

Cartesian coordinates from input :

```
  Cartesian coordinates from input :
C       20.51100  -29.23800   27.01600
C       21.08600  -30.51000   26.37200
C       20.28700  -31.74000   26.82300
C       20.25100  -31.85800   28.34800
C       19.73500  -30.56900   28.98900
C       20.56800  -29.36600   28.54600
C       22.87100  -27.37500   27.12900
C       23.82700  -28.56900   27.07200
C       25.23500  -28.15300   27.51600
C       25.21500  -27.54400   28.92000
C       24.23000  -26.38400   29.00100
C       22.82400  -26.78400   28.54700
C       21.50700  -27.84300   24.59500
C       22.73100  -27.39000   24.07000
C       23.00300  -27.39200   22.70700
C       22.04500  -27.84400   21.81900
```



```
C       20.83400  -28.31300   22.30800
C       20.54100  -28.32400   23.67800
C       19.19700  -28.84400   24.06200
C       18.81000  -30.15800   23.71900
C       17.53500  -30.59100   24.08400
C       16.64100  -29.75700   24.74800
C       17.01700  -28.45200   25.05400
C       18.28600  -28.00600   24.70800
C       19.71600  -31.12100   22.97400
H       19.53800  -29.23400   26.78300
H       23.30000  -26.66900   26.56400
H       23.39500  -27.07200   24.66900
H       23.84400  -27.08400   22.38800
H       22.21300  -27.83500   20.88500
H       20.18500  -28.63700   21.69600
H       17.27100  -31.48000   23.87500
H       15.78000  -30.07600   24.99100
H       16.40900  -27.87100   25.49700
H       18.53900  -27.11300   24.91400
H       26.12200  -27.22300   29.15300
H       24.95900  -28.24000   29.57600
H       24.18900  -26.05700   29.93400
H       24.55500  -25.64100   28.43200
H       22.45000  -27.45300   29.17400
H       22.23400  -25.98900   28.55700
H       19.58100  -31.01700   22.00900
H       20.65000  -30.92800   23.19600
H       19.50100  -32.04000   23.23700
H       22.03500  -30.61700   26.63400
H       21.04500  -30.43200   25.38600
H       20.69800  -32.55500   26.44200
H       19.36100  -31.67500   26.47800
H       21.16100  -32.05000   28.68400
H       19.66300  -32.61200   28.60500
H       19.77600  -30.65200   29.97400
H       18.79000  -30.42900   28.73200
H       20.21500  -28.54100   28.96400
H       21.50700  -29.48300   28.83700
H       23.49300  -29.29100   27.66300
H       23.86300  -28.92100   26.14800
H       25.60000  -27.49100   26.87700
H       25.83000  -28.94400   27.51000
P       21.18000  -27.61800   26.40400
```

Atoms and radius in the parameter file

```
  Atoms and radius in the parameter file
H     1.29
C2    1.99
C3    1.99
C     1.99
N2    1.81
N3    1.81
N     1.81
O     1.78
F     1.72
Si    2.45
P     2.11
S     2.10
```



```
Cl    2.05
Br    2.16
```

Coordinates scaled to put the metal at the origin

```
  Coordinates scaled to put the metal at the origin

C       0.79759  -3.36165   0.09886
C       1.37259  -4.63365  -0.54514
C       0.57359  -5.86365  -0.09414
C       0.53759  -5.98165   1.43086
C       0.02159  -4.69265   2.07186
C       0.85459  -3.48965   1.62886
C       3.15759  -1.49865   0.21186
C       4.11359  -2.69265   0.15486
C       5.52159  -2.27665   0.59886
C       5.50159  -1.66765   2.00286
C       4.51659  -0.50765   2.08386
C       3.11059  -0.90765   1.62986
C       1.79359  -1.96665  -2.32214
C       3.01759  -1.51365  -2.84714
C       3.28959  -1.51565  -4.21014
C       2.33159  -1.96765  -5.09814
C       1.12059  -2.43665  -4.60914
C       0.82759  -2.44765  -3.23914
C      -0.51641  -2.96765  -2.85514
C      -0.90341  -4.28165  -3.19814
C      -2.17841  -4.71465  -2.83314
C      -3.07241  -3.88065  -2.16914
C      -2.69641  -2.57565  -1.86314
C      -1.42741  -2.12965  -2.20914
C       0.00259  -5.24465  -3.94314
H      -0.17541  -3.35765  -0.13414
H       3.58659  -0.79265  -0.35314
H       3.68159  -1.19565  -2.24814
H       4.13059  -1.20765  -4.52914
H       2.49959  -1.95865  -6.03214
H       0.47159  -2.76065  -5.22114
H      -2.44241  -5.60365  -3.04214
H      -3.93341  -4.19965  -1.92614
H      -3.30441  -1.99465  -1.42014
H      -1.17441  -1.23665  -2.00314
H       6.40859  -1.34665   2.23586
H       5.24559  -2.36365   2.65886
H       4.47559  -0.18065   3.01686
H       4.84159   0.23535   1.51486
H       2.73659  -1.57665   2.25686
H       2.52059  -0.11265   1.63986
H      -0.13241  -5.14065  -4.90814
H       0.93659  -5.05165  -3.72114
H      -0.21241  -6.16365  -3.68014
H       2.32159  -4.74065  -0.28314
H       1.33159  -4.55565  -1.53114
H       0.98459  -6.67865  -0.47514
H      -0.35241  -5.79865  -0.43914
H       1.44759  -6.17365   1.76686
```



```
H      -0.05041  -6.73565   1.68786
H       0.06259  -4.77565   3.05686
H      -0.92341  -4.55265   1.81486
H       0.50159  -2.66465   2.04686
H       1.79359  -3.60665   1.91986
H       3.77959  -3.41465   0.74586
H       4.14959  -3.04465  -0.76914
H       5.88659  -1.61465  -0.04014
H       6.11659  -3.06765   0.59286
P       1.46659  -1.74165  -0.51314
XX      0.00000   0.00000   0.00000
```

Results : Volumes in Angs^3

```
  Results : Volumes in Angs^3

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

   V Free   V Buried  V Total   V Exact
  118.387    61.148   179.535   179.594

 %V_Free    %V_Bur  % Tot/Ex
 65.941     34.059    99.967
```

The %V_Bur of your molecule is: 34.1

3c

SambVca @ MoLNaC
Results page

```
-------------------------------------------
|                                         |
|               S A M B V C A             |
|                                         |
|          Buried Volume in Salerno       |
|                                         |
|  http://www.molnac.unisa.it/OM-tools/SambVca |
|                                         |
|  L. Cavallo et al. email: lcavallo@unisa.it |
|                                         |
-------------------------------------------
```

Molecule from input :

Molecule from input :

./temp/a32d7b4686f72d21055aa4ba0d5ec413.c3d1

```
    Number of atoms             :   29
    Atom that is coordinated    :   29
    Atoms that define the axis  :    3
    ID of these atoms           :    1  15  21

    Radius of sphere (Angs)     :    3.500
    Distance from sphere (Angs) :    2.334
    Mesh step (Angs)            :    0.050
    H atoms omitted in the V_bur calculation
```

Cartesian coordinates from input :

Cartesian coordinates from input :

```
C      19.22200  28.01900  51.79400
C      19.84100  28.32800  53.01900
C      19.50800  27.69800  54.21700
C      18.49200  26.75300  54.21300
C      17.84600  26.44900  53.02300
C      18.19700  27.04700  51.80200
C      17.42100  26.55100  50.62800
```



```
C      16.16500  27.08300  50.31600
C      15.39000  26.56600  49.27100
C      15.88800  25.50400  48.58000
C      17.11700  24.92500  48.80700
C      17.86200  25.43400  49.90900
C      14.64900  28.87400  50.63900
C      19.63100  23.86900  49.54600
C      21.64500  28.24500  50.20000
C      21.59700  26.74900  49.87400
C      22.99200  26.22600  49.52100
C      23.99400  26.52200  50.63000
C      24.02400  28.00800  50.95500
C      22.63400  28.51300  51.34300
C      19.12400  28.62200  48.81100
C      20.04500  28.86700  47.66500
C      19.32300  28.51500  46.30200
C      18.01200  29.26300  46.13600
C      17.10900  29.04900  47.33900
C      17.83000  29.42600  48.63600
O      15.77600  28.12800  51.09400
O      19.04300  24.90100  50.33400
F      19.97000  29.01000  50.42300
```

Atoms and radius in the parameter file

Atoms and radius in the parameter file

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

```
C     -2.46288  -4.73864  -0.28835
C     -3.71888  -4.20664  -0.60035
C     -4.49388  -4.72364  -1.64535
C     -3.99588  -5.78564  -2.37635
C     -2.76688  -6.36464  -2.07935
C     -2.02188  -5.85564  -1.00735
C     -5.23488  -2.41564  -0.27735
C     -0.25288  -7.42064  -1.37035
C      1.76112  -3.04464  -0.71635
C      1.71312  -4.54064  -1.04235
C      3.10812  -5.06364  -1.39535
C      4.11012  -4.76764  -0.28635
C      4.14012  -3.28164   0.03865
C      2.75012  -2.77664   0.42665
C     -0.75988  -2.66764  -2.10535
C      0.16112  -2.42264  -3.25135
C     -0.56088  -2.77464  -4.61435
```


Results : Volumes in Angs^3

Results : Volumes in Angs^3

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

  V Free   V Buried  V Total   V Exact
 125.601    53.934   179.535   179.594

%V_Free    %V_Bur   % Tot/Ex
69.959     30.041    99.967
```

The %V_Bur of your molecule is: 30.0

3d

SambVca @ MoLNaC
Results page

```
 ------------------------------------------------------
|                                                      |
|                    S A M B V C A                     |
|                                                      |
|              Buried Volume in Salerno                |
|                                                      |
|    http://www.molnac.unisa.it/OM-tools/SambVca       |
|                                                      |
|     L. Cavallo et al. email: lcavallo@unisa.it       |
|                                                      |
 ------------------------------------------------------
```

Molecule from input :

```
  Molecule from input :

./temp/9152163785ab4314c4f70b8feb56b3cd.c3d1


      Number of atoms              :   83
      Atom that is coordinated     :   83
      Atoms that define the axis   :    3
      ID of these atoms            :    1  22  28

      Radius of sphere (Angs)      :   3.500
      Distance from sphere (Angs)  :   2.334
      Mesh step (Angs)             :   0.050
      H atoms omitted in the V_bur calculation
```

Cartesian coordinates from input :

```
  Cartesian coordinates from input :
C       56.79600   28.37500    8.90300
C       58.20500   28.45300    8.95800
C       59.04200   27.39500    8.64500
C       58.47500   26.17400    8.29500
C       57.08700   26.05000    8.27000
C       56.22400   27.11600    8.56300
C       54.75700   26.74600    8.46900
C       54.06300   26.90900    7.25300
C       52.76600   26.40400    7.11900
C       52.13400   25.73500    8.16900
C       52.83600   25.56900    9.35400
C       54.14000   26.04100    9.52800
C       54.74000   27.56000    6.06900
C       55.34700   26.47600    5.13800
C       53.81000   28.46200    5.23400
C       50.71900   25.20300    8.02600
```



```
C       49.72400   26.35600    7.85400
C       50.59900   24.17800    6.88600
C       54.87400   25.71900   10.83300
C       55.29800   24.24300   10.85700
C       54.02700   26.01300   12.08400
C       56.60600   31.17400    7.97900
C       58.08200   31.59600    8.03300
C       58.28500   32.82500    7.12300
C       57.89900   32.48700    5.68000
C       56.46000   31.97100    5.60000
C       56.22900   30.78500    6.54200
C       54.21600   29.92500    9.10500
C       53.55500   29.31200   10.34900
C       52.05000   29.13500   10.16400
C       51.38600   30.46900    9.84200
C       52.03700   31.11700    8.62400
C       53.55500   31.29400    8.81200
H       58.60000   29.27500    9.22500
H       59.98500   27.50000    8.67000
H       59.02700   25.43200    8.07400
H       56.70900   25.20800    8.04600
H       52.30600   26.51900    6.29500
H       52.41200   25.12000   10.07700
H       55.48900   28.12500    6.39000
H       50.48900   24.73300    8.87700
H       55.69900   26.28100   10.87600
H       56.09700   32.01500    8.15100
H       54.03000   29.32100    8.32900
H       56.02600   25.97400    5.63500
H       55.76100   26.90000    4.35800
H       54.64100   25.86500    4.84000
H       53.10200   27.92100    4.83000
H       54.32400   28.91100    4.53100
H       53.40800   29.13300    5.82500
H       49.77700   26.95200    8.63100
H       48.81500   25.99600    7.78200
H       49.94100   26.85800    7.04100
H       50.93600   24.57300    6.05500
H       49.65900   23.92600    6.77200
H       51.12700   23.38100    7.10500
H       54.51900   23.67700   10.67500
H       55.66200   24.02200   11.73900
H       55.98100   24.08900   10.17300
H       53.66000   26.91900   12.02200
H       54.58900   25.94100   12.88300
H       53.29300   25.96600   12.14000
H       58.65800   30.85100    7.72800
H       58.33300   31.82300    8.96400
H       57.72800   33.57600    7.44800
H       59.23300   33.10800    7.15400
H       58.51600   31.79900    5.32600
H       57.99000   33.29600    5.11700
H       56.26300   31.69400    4.67100
H       55.83700   32.70300    5.83900
H       56.78000   30.01600    6.24900
H       55.27800   30.51400    6.50900
H       53.96700   28.43000   10.53600
H       53.72200   29.89800   11.12900
H       51.88000   28.49600    9.42900
H       51.65700   28.76200   10.99400
H       51.46700   31.07600   10.62300
H       50.42300   30.32700    9.66600
```



```
H       51.62200   32.00300    8.46500
H       51.87000   30.55400    7.82700
H       53.72700   31.91400    9.56400
H       53.94900   31.68700    7.99300
P       56.06000   30.01300    9.33000
```

Atoms and radius in the parameter file

```
  Atoms and radius in the parameter file
H     1.29
C2    1.99
C3    1.99
C     1.99
N2    1.81
N3    1.81
N     1.81
O     1.78
F     1.72
Si    2.45
P     2.11
S     2.10
Cl    2.05
Br    2.16
```

Coordinates scaled to put the metal at the origin

```
  Coordinates scaled to put the metal at the origin
C        0.12752  -2.24973  -2.59566
C        1.53652  -2.17173  -2.54066
C        2.37352  -3.22973  -2.85366
C        1.80652  -4.45073  -3.20366
C        0.41852  -4.57473  -3.22866
C       -0.44448  -3.50873  -2.93566
C       -1.91148  -3.87873  -3.02966
C       -2.60548  -3.71573  -4.24566
C       -3.90248  -4.22073  -4.37966
C       -4.53448  -4.88973  -3.32966
C       -3.83248  -5.05573  -2.14466
C       -2.52848  -4.58373  -1.97066
C       -1.92848  -3.06473  -5.44966
C       -1.32148  -4.14873  -6.26066
C       -2.85848  -2.16273  -6.26466
C       -5.94948  -5.42173  -3.47266
C       -6.94448  -4.26873  -3.64466
C       -6.06948  -6.44673  -4.61266
C       -1.79448  -4.90573  -0.66566
C       -1.37048  -6.38173  -0.64166
C       -2.64148  -4.61173   0.58534
C       -0.06248   0.54927  -3.51966
C        1.41352   0.97127  -3.46566
C        1.61652   2.20027  -4.37566
C        1.23052   1.86227  -5.81866
```



```
C       -0.20848   1.34627  -5.89866
C       -0.43948   0.16027  -4.95666
C       -2.45248  -0.49973  -2.39366
C       -3.11348  -1.31273  -1.14966
C       -4.41848  -1.48973  -1.33466
C       -5.28248  -0.15573  -1.65466
H       -4.43148   0.49227  -2.87466
C       -3.11348   0.66927  -2.68666
H        1.93152  -1.34973  -2.27366
H        3.31652  -3.12473  -2.82866
H        2.35852  -5.19273  -3.42466
H        0.84052  -5.41673  -3.45266
H       -4.36248  -4.10573  -5.20366
H       -4.25648  -5.50473  -1.42166
H       -1.17948  -2.49973  -5.10866
H       -6.17948  -5.89173  -2.62166
H       -0.90748  -4.24373  -0.62266
H       -0.57148   1.39027  -3.24766
H       -2.63848  -1.30373  -3.16966
H       -0.64248  -4.65073  -5.86366
H       -0.90748  -3.72473  -7.14066
H       -2.02748  -4.75973  -6.65866
H       -3.54648  -2.70373  -6.66866
H       -2.34448  -1.71373  -6.96766
H       -3.20048  -1.49173  -5.67366
H       -6.89148  -3.67273  -2.86766
H       -7.85348  -4.62873  -3.71666
H       -6.72748  -3.76673  -4.45766
H       -5.73248  -6.05173  -5.44366
H       -7.00948  -6.69873  -4.72666
H       -5.54148  -7.24373  -4.39366
H       -2.14948  -6.94773  -0.82366
H       -1.06648  -6.60273   0.24034
H       -0.68748  -6.53573  -1.32566
H       -3.00848  -5.70573   0.52334
H       -2.07948  -4.68373   1.38434
H       -3.37548  -5.25873   0.64134
H        1.98352   0.22627  -3.77066
H        1.66452   1.19827  -2.53466
H        1.05952   2.95127  -4.05066
H        2.54652   2.48327  -4.34466
H        1.84752   1.17427  -6.17266
H        1.32152   2.67127  -6.38166
H       -0.40548   1.06927  -6.82766
H       -0.81148   2.07827  -5.65966
H        0.11152  -0.60873  -5.24966
H       -1.39048  -0.11073  -4.98966
H       -2.70148  -2.19473  -0.96266
H       -2.94648  -0.72673  -0.36966
H       -4.78848  -2.12873  -2.06966
H       -5.61148  -1.86273  -0.50466
H       -5.20148   0.45127  -0.87566
H       -6.24548  -0.29773  -1.83266
H       -5.04648   1.37827  -3.03266
H       -4.79848  -0.07073  -3.67166
H       -2.94148   1.28927  -1.93466
H       -2.17948   1.06227  -3.50566
P       -0.60948  -0.61173  -2.16866
XX       0.00000   0.00000   0.00000
```


Results : Volumes in Angs^3

```
 Results : Volumes in Angs^3

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

   V_Free    V_Buried  V_Total   V_Exact
  125.238     54.296   179.535   179.594

 %V_Free     %V_Bur   % Tot/Ex
  69.757      30.243     99.967
```

The %V_Bur of your molecule is: 30.2

4a

SambVca @ MoLNaC
Results page

```
┌──────────────────────────────────────────────┐
│                                              │
│                 S A M B V C A                │
│                                              │
│              Buried Volume in Salerno        │
│                                              │
│    http://www.molnac.unisa.it/OM-tools/SambVca   │
│                                              │
│    L. Cavallo et al. email: lcavallo@unisa.it    │
│                                              │
└──────────────────────────────────────────────┘
```

Molecule from input :

Molecule from input :

./temp/a32d7b4686f72d21855aa4ba0d5ec413.c3dl

```
    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) :    2.334
    Mesh step (Angs)            :    0.050
    H atoms omitted in the V_bur calculation
```

Cartesian coordinates from input :

Cartesian coordinates from input :

```
C     -47.62000  22.57700   3.16400
C     -48.46500  22.22700   1.92700
C     -49.90200  22.66900   2.15700
C     -50.01900  24.13800   2.45900
C     -49.10600  24.53200   3.62900
C     -47.66300  24.08500   3.39300
C     -45.06300  22.23500   1.55900
```



```
C     -44.96400  23.72500   1.22400
C     -43.93800  23.93100   0.09900
C     -44.32700  23.14300  -1.12400
C     -44.54700  21.64800  -0.82100
C     -45.53700  21.43500   0.32700
C     -44.95000  22.54400   4.46800
C     -45.43400  22.78600   5.77900
C     -44.59400  23.39400   6.70600
C     -43.28300  23.74100   6.40700
C     -42.80200  23.46300   5.13700
C     -43.62100  22.89400   4.20400
C     -46.79500  22.37900   6.27100
C     -47.17200  21.05600   6.36300
C     -48.39500  20.69900   6.91300
C     -49.25600  21.67600   7.35600
C     -48.88900  23.01600   7.26700
C     -47.66400  23.35400   6.74500
P     -45.95400  21.78800   3.12300
```

Atoms and radius in the parameter file

Atoms and radius in the parameter file

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

```
C       1.15652   2.75665  -1.77038
C       1.25552   4.24665  -2.10538
C       2.28152   4.45265  -3.23038
C       1.89252   3.66465  -4.45338
C       1.67252   2.16965  -4.15038
C       0.68252   1.95665  -3.00238
C       1.26952   3.06565   1.13862
C       0.78552   3.30765   2.44962
C       1.62552   3.91565   3.37662
C       2.93652   4.26265   3.07762
C       3.41752   3.98465   1.80762
C       2.59852   3.41565   0.87462
C      -0.57548   2.90065   2.94162
C      -0.95248   1.57765   3.03362
C      -2.17548   1.22065   3.58362
C      -3.03648   2.19765   4.02662
C      -2.66948   3.53765   3.93762
C      -1.44448   3.87565   3.41562
P       0.26552   2.30965  -0.20638
XX      0.00000   0.00000   0.00000
```


Results : Volumes in Angs^3

Results : Volumes in Angs^3

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

  V Free   V Buried  V Total   V Exact
 118.866    60.669   179.535   179.594

%V_Free    %V_Bur   % Tot/Ex
 66.208    33.792    99.967
```

The %V_Bur of your molecule is: 33.8

4b

Samb*V*ca @ MoLNaC
Results page

```
 ------------------------------------------------------
|                                                      |
|                  S A M B V C A                       |
|                                                      |
|              Buried Volume in Salerno                |
|                                                      |
|     http://www.molnac.unisa.it/OM-tools/SambVca      |
|                                                      |
|      L. Cavallo et al. email: lcavallo@unisa.it      |
|                                                      |
 ------------------------------------------------------
```

Molecule from input :

Molecule from input :

./temp/9152163785ab4314c4f70b8feb56b3cd.c3d1

Number of atoms	:	59
Atom that is coordinated	:	59
Atoms that define the axis	:	3
ID of these atoms	:	1 14 20
Radius of sphere (Angs)	:	3.500
Distance from sphere (Angs)	:	2.334
Mesh step (Angs)	:	0.050

H atoms omitted in the V_bur calculation

Cartesian coordinates from input :

Cartesian coordinates from input :

C	33.05200	19.05400	47.41900
C	32.32700	17.95100	46.96600
C	31.09000	17.64600	47.46800
C	30.52800	18.42800	48.45300
C	31.21600	19.52800	48.91000
C	32.45900	19.86500	48.40800
C	33.05300	21.11200	48.94200
C	33.38900	21.24000	50.30100
C	33.88800	22.45800	50.74200
C	34.01500	23.52500	49.88900
C	33.65700	23.40600	48.55600
C	33.17600	22.19800	48.09400
C	33.22000	20.16300	51.31300
C	35.84700	19.83400	47.95500
C	37.28800	19.92300	47.45900
C	38.13700	20.60600	48.52900

C	38.07700	19.84700	49.84000
C	36.64600	19.62900	50.30300
C	35.81300	18.97800	49.21400
C	35.14300	17.83800	45.78200
C	35.40300	16.65300	46.70100
C	35.51600	15.38700	45.85300
C	36.61700	15.51600	44.82800
C	36.41900	16.73000	43.95000
C	36.28900	17.99400	44.77900
H	34.35200	24.35200	50.21400
H	33.74100	24.14800	47.96800
H	32.92700	22.11000	47.18100
H	33.99800	20.15100	51.90900
H	32.40900	20.33100	51.83600
H	33.14300	19.29800	50.85900
H	35.60500	20.75800	48.24800
H	37.63800	19.01500	47.27800
H	37.32200	20.44400	46.61800
H	37.81100	21.53000	48.66900
H	39.07700	20.65600	48.22100
H	38.52200	18.97000	49.73000
H	38.57000	20.35400	50.53300
H	36.24400	20.49900	50.55000
H	36.64600	19.05100	51.10700
H	36.16900	18.07700	49.01500
H	34.87800	18.87900	49.52500
H	34.34900	17.57500	45.23400
H	36.24200	16.79600	47.20700
H	34.66100	16.56000	47.35000
H	34.65500	15.22100	45.39300
H	35.70300	14.61300	46.44100
H	37.48800	15.58600	45.29100
H	36.63500	14.70300	44.26300
H	37.18900	16.81900	43.33400
H	35.60200	16.61000	43.40300
H	37.13600	18.16500	45.26200
H	36.11000	18.76600	44.18500
H	32.70100	17.39600	46.29100
H	30.61800	16.89200	47.13600
H	29.67600	18.21000	48.81200
H	30.82600	20.07000	49.58500
H	34.14600	22.55500	51.65100
P	34.65700	19.40400	46.61700

Atoms and radius in the parameter file

Atoms and radius in the parameter file

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

Cl	2.05
Br	2.16

Coordinates scaled to put the metal at the origin

Coordinates scaled to put the metal at the origin

C	-1.52126	-2.10260	2.34113
C	-2.24626	-3.20560	1.88813
C	-3.48326	-3.51060	2.39013
C	-4.04526	-2.72860	3.37513
C	-3.35726	-1.62860	3.83213
C	-2.11426	-1.29160	3.33013
C	-1.52026	-0.04460	3.86413
C	-1.18426	0.08340	5.22313
C	-0.68526	1.30140	5.66413
C	-0.55826	2.36840	4.81113
C	-0.91626	2.24940	3.47813
C	-1.39726	1.04140	3.01613
C	-1.35326	-0.99360	6.23513
C	1.27374	-1.32260	2.87713
C	2.71474	-1.23360	2.38113
C	3.56374	-0.55060	3.45113
C	3.50374	-1.30960	4.76213
C	2.07274	-1.52760	5.22513
C	1.23974	-2.17860	4.13613
C	0.56974	-3.31860	0.70413
C	0.82974	-4.50360	1.62313
C	0.94274	-5.76960	0.77513
C	2.04374	-5.64060	-0.24987
C	1.84574	-4.42660	-1.12787
C	1.71574	-3.16260	-0.29887
H	-0.22126	3.19540	5.13613
H	-0.83226	2.99140	2.89013
H	-1.64626	0.95340	2.10313
H	-0.57526	-1.00560	6.83113
H	-2.16426	-0.82560	6.75813
H	-1.43026	-1.85860	5.78113
H	1.03174	-0.39860	3.17013
H	3.06474	-2.14160	2.20013
H	2.74874	-0.71260	1.54013
H	3.23774	0.37340	3.59113
H	4.50374	-0.50060	3.14313
H	3.94874	-2.18660	4.65213
H	3.99674	-0.80260	5.45513
H	1.67074	-0.65760	5.47213
H	2.07274	-2.10560	6.02913
H	1.59574	-3.07960	3.93713
H	0.30474	-2.27760	4.44713
H	-0.22426	-3.58160	0.15613
H	1.66874	-4.36060	2.12913
H	0.08774	-4.59660	2.27213
H	0.08174	-5.93560	0.31513
H	1.12974	-6.54360	1.36313
H	2.91474	-5.57060	0.21313
H	2.06174	-6.45360	-0.81487

H	2.61574	-4.33760	-1.74387
H	1.02874	-4.54660	-1.67487
H	2.56274	-2.99160	0.18413
H	1.53674	-2.39060	-0.89287
H	-1.87226	-3.76060	1.21313
H	-3.95526	-4.26460	2.05813
H	-4.89726	-2.94660	3.73413
H	-3.74726	-1.08660	4.50713
H	-0.42726	1.39840	6.57313
P	0.08374	-1.75260	1.53913
XX	0.00000	0.00000	0.00000

Results : Volumes in Angs^3

Results : Volumes in Angs^3

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

V Free	V Buried	V Total	V Exact
117.735	61.799	179.535	179.594

%V_Free	%V_Bur	% Tot/Ex
65.578	34.422	99.967

The %V_Bur of your molecule is: 34.4

4c

SambVca @ MoLNaC
Results page

```
-------------------------------------------------
|                                               |
|                 S A M B V C A                 |
|                                               |
|            Buried Volume in Salerno           |
|                                               |
|   http://www.molnac.unisa.it/OM-tools/SambVca |
|                                               |
|    L. Cavallo et al. email: lcavallo@unisa.it |
|                                               |
-------------------------------------------------
```

Molecule from input :

Molecule from input :

./temp/a32d7b4686f72d21855aa4ba0d5ec413.c3d1

```
    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) :    2.334
    Mesh step (Angs)            :    0.050
    H atoms omitted in the V_bur calculation
```

Cartesian coordinates from input :

Cartesian coordinates from input :

```
C      62.68400  20.19600  14.41400
C      62.22600  19.39600  15.63500
C      60.88600  19.90500  16.11000
C      60.93300  21.37600  16.47000
C      61.42700  22.21700  15.26000
C      62.79400  21.71000  14.74900
C      64.44500  20.55000  12.08600
```



```
C      63.08700  20.72600  11.30600
C      63.36600  21.47000  10.00400
C      64.39000  20.82200   9.11700
C      65.69100  20.60300   9.90700
C      65.45700  19.80500  11.16800
C      65.54000  19.91300  14.80300
C      66.48900  20.91500  14.89900
C      67.31500  21.04300  16.00700
C      67.19400  20.19000  17.16300
C      66.24600  19.16300  17.05900
C      65.50100  19.02000  15.96300
C      66.83700  21.87900  13.78400
C      66.27900  23.19500  13.76800
C      66.58800  24.08600  12.73100
C      67.49800  23.70100  11.78800
C      68.11200  22.45400  11.79200
C      67.76900  21.51800  12.82900
C      64.77500  24.78300  14.79300
C      69.07500  19.73300  11.85400
O      65.43700  23.49900  14.79600
O      68.29800  20.25700  12.94800
F      64.23000  19.54400  13.62000
```

Atoms and radius in the parameter file

Atoms and radius in the parameter file

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

```
C      0.19145   3.27882  -1.00364
C     -1.16655   3.45482  -1.78364
C     -0.88755   4.19882  -3.08564
C      0.13645   3.55082  -3.97264
C      1.43745   3.33182  -3.10264
C      1.20345   2.53382  -1.92164
C      1.28645   2.64182   1.74336
C      2.23545   3.64382   1.80936
C      3.06145   3.77182   2.91736
C      2.94045   2.91882   4.07336
C      1.99245   1.89182   3.96936
C      1.24745   1.74882   2.87336
C      2.58345   4.60782   0.69436
C      2.02545   5.92382   0.67836
C      2.33445   6.81482  -0.35864
C      3.24445   6.42982  -1.30164
C      3.85845   5.18282  -1.29764
```


Results : Volumes in Angs^3

Results : Volumes in Angs^3

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

  V_Free   V_Buried  V_Total   V_Exact
 122.803    56.732   179.535   179.594

%V_Free    %V_Bur   % Tot/Ex
68.401     31.599    99.967
```

The %V_Bur of your molecule is: 31.6

4d

Samb*V*ca @ MoLNaC
Results page

```
 ----------------------------------------------------
|                                                    |
|                  S A M B V C A                     |
|                                                    |
|             Buried Volume in Salerno               |
|                                                    |
|   http://www.molnac.unisa.it/OM-tools/SambVca      |
|                                                    |
|    L. Cavallo et al. email: lcavallo@unisa.it      |
|                                                    |
 ----------------------------------------------------
```

Molecule from input :

```
  Molecule from input :

 ./temp/9152163785ab4314c4f70b8feb56b3cd.c3d1


     Number of atoms              :   82
     Atom that is coordinated     :   82
     Atoms that define the axis   :    3
     ID of these atoms            :    1  22  28

     Radius of sphere (Angs)      :    3.500
     Distance from sphere (Angs)  :    2.334
     Mesh step (Angs)             :    0.050
     H atoms omitted in the V_bur calculation
```

Cartesian coordinates from input :

```
  Cartesian coordinates from input :
C     -79.04100 -20.02900  -9.02500
C     -80.39400 -20.35900  -9.22300
C     -81.12100 -19.91200 -10.31200
C     -80.49000 -19.10200 -11.25400
C     -79.18500 -18.68200 -11.02400
C     -78.44300 -19.10600  -9.91100
C     -77.11900 -18.40900  -9.74400
C     -76.00200 -18.79000 -10.50600
C     -74.98600 -17.78200 -10.52300
C     -75.00000 -16.62900  -9.73500
C     -76.13300 -16.36500  -8.98300
C     -77.03500 -17.25800  -8.92000
C     -76.04000 -19.98800 -11.44800
C     -75.99300 -19.52100 -12.90500
C     -74.90800 -20.98600 -11.17800
C     -73.78000 -15.72800  -9.65700
```



```
C     -72.91000 -15.74200 -10.91400
C     -72.90300 -16.14600  -8.50400
C     -78.23800 -16.78200  -8.11800
C     -79.13700 -15.88100  -8.96200
C     -77.87700 -16.06000  -6.81800
C     -76.48500 -20.63400  -7.53600
C     -75.61400 -21.84500  -7.15600
C     -74.14100 -21.43100  -7.04500
C     -73.92700 -20.28000  -6.07100
C     -74.79200 -19.08600  -6.46200
C     -76.26700 -19.49700  -6.52700
C     -78.41500 -22.76300  -8.25400
C     -77.93800 -22.94500  -9.70200
C     -77.90900 -24.42700 -10.08600
C     -79.26600 -25.09700  -9.85500
C     -79.71200 -24.91800  -8.40700
C     -79.78400 -23.42900  -8.05200
H     -80.82500 -20.91100  -8.58200
H     -82.03500 -20.15200 -10.41600
H     -80.94700 -18.84000 -12.04500
H     -78.78100 -18.08500 -11.64300
H     -74.25200 -17.90500 -11.11200
H     -76.23200 -15.54000  -8.52400
H     -76.90700 -20.46300 -11.30500
H     -78.77200 -17.59100  -7.87200
H     -76.18000 -20.31000  -8.43100
H     -77.77400 -23.28500  -7.69000
H     -76.03100 -20.30000 -13.50000
H     -75.16300 -19.02700 -13.06400
H     -74.04700 -20.56700 -11.38600
H     -75.02900 -21.77800 -11.74100
H     -74.92400 -21.24900 -10.23400
H     -74.09000 -14.78900  -9.50000
H     -72.15400 -15.13700 -10.79400
H     -73.44500 -15.45900 -11.68200
H     -73.12600 -16.05300 -11.58500
H     -72.16600 -15.50600  -8.41200
H     -72.54700 -17.03800  -8.67100
H     -73.29900 -15.95700  -7.48300
H     -79.96100 -15.68800  -8.46900
H     -79.35700 -16.33400  -9.80300
H     -78.66800 -15.04200  -9.15600
H     -77.43100 -15.21300  -7.02800
H     -77.27700 -16.62200  -6.28800
H     -78.69400 -15.88100  -6.30700
H     -75.91900 -22.21400  -6.29000
H     -75.71000 -22.55000  -7.84300
H     -73.60700 -22.21000  -6.74700
H     -73.81200 -21.16300  -7.94000
H     -72.97300 -20.01500  -6.07500
H     -74.15900 -20.57400  -5.15400
H     -74.50400 -18.74100  -7.34400
H     -74.67700 -18.36100  -5.79600
H     -76.81400 -18.71500  -6.78900
H     -76.56500 -19.79200  -5.63000
H     -78.54600 -22.45700 -10.31300
H     -77.03200 -22.56100  -9.80200
H     -77.65900 -24.51400 -11.03900
H     -77.22000 -24.89100  -9.54800
H     -79.93900 -24.69800 -10.46000
H     -79.19700 -26.06300 -10.06200
H     -79.07300 -25.37300  -7.80300
```



```
H     -80.60300 -25.33200  -8.28000
H     -80.06600 -23.32700  -7.10900
H     -80.45600 -22.98400  -8.62400
P     -78.29700 -21.00900  -7.65800
```

Atoms and radius in the parameter file

```
  Atoms and radius in the parameter file
H     1.29
C2    1.99
C3    1.99
C     1.99
N2    1.81
N3    1.81
N     1.81
O     1.78
F     1.72
Si    2.45
P     2.11
S     2.10
Cl    2.05
Br    2.16
```

Coordinates scaled to put the metal at the origin

```
  Coordinates scaled to put the metal at the origin

C        0.30699   0.53859  -3.40370
C       -1.04601   0.20859  -3.60170
C       -1.77301   0.65559  -4.69070
C       -1.14201   1.46559  -5.63270
C        0.16299   1.88559  -5.40270
C        0.90499   1.46159  -4.28970
C        2.22899   2.15859  -4.12270
C        3.34599   1.77759  -4.88470
C        4.36199   2.78559  -4.90170
C        4.34799   3.93859  -4.11370
C        3.21499   4.20259  -3.36170
C        2.31299   3.30959  -3.29870
C        3.30799   0.57959  -5.82670
C        3.35499   1.04659  -7.28370
C        4.43999  -0.41841  -5.55670
C        5.56799   4.83959  -4.03570
C        6.43799   4.82559  -5.29270
C        6.44499   4.42159  -2.88270
C        1.10999   3.78559  -2.49670
C        0.21099   4.68659  -3.34070
C        1.47099   4.50759  -1.19670
C        2.86299  -0.06641  -1.91470
C        3.73399  -1.27741  -1.53470
C        5.20699  -0.86341  -1.42370
C        5.42099   0.28759  -0.44970
C        4.55599   1.48159  -0.84070
```



```
C        3.08099   1.07059  -0.90570
C        0.93299  -2.19541  -2.63270
C        1.40999  -2.37741  -4.08070
C        1.43899  -3.85941  -4.46470
C        0.08199  -4.52941  -4.23370
C       -0.36401  -4.35041  -2.78570
C       -0.43601  -2.86141  -2.43070
H       -1.47701  -0.34341  -2.96070
H       -2.68701   0.41559  -4.79470
H       -1.59901   1.72759  -6.42370
H        0.56699   2.48259  -6.02170
H        5.09599   2.66259  -5.49070
H        3.11599   5.02759  -2.90270
H        2.44099   0.10459  -5.68370
H        0.57599   2.97659  -2.25070
H        3.16799   0.25759  -2.80970
H        1.57399  -2.71741  -2.06870
H        3.31699   0.26759  -7.87870
H        4.18499   1.54059  -7.44270
H        5.30099   0.00059  -5.76470
H        4.31899  -1.21041  -6.11970
H        4.42399  -0.68141  -4.61270
H        5.25799   5.77859  -3.87870
H        7.19399   5.43059  -5.17270
H        5.90299   5.10859  -6.06070
H        6.22199   4.51459  -5.96370
H        7.18199   5.06159  -2.79070
H        6.80099   3.52959  -3.04970
H        6.04899   4.61059  -1.86170
H       -0.61301   4.87959  -2.84770
H       -0.00901   4.23359  -4.18170
H        0.67999   5.52559  -3.53470
H        1.91699   5.35459  -1.40670
H        2.07099   3.94559  -0.66670
H        0.65399   4.68659  -0.68570
H        3.42899  -1.64641  -0.66870
H        3.63799  -1.98241  -2.22170
H        5.74099  -1.64241  -1.12570
H        5.53599  -0.59541  -2.31870
H        6.37499   0.55259  -0.45370
H        5.18899  -0.00641   0.46730
H        4.84399   1.82659  -1.72270
H        4.67099   2.20659  -0.17470
H        2.53399   1.85259  -1.16770
H        2.78299   0.77559  -0.00870
H        0.80199  -1.88941  -4.69170
H        2.31599  -1.99341  -4.18070
H        1.68899  -3.94641  -5.41770
H        2.12799  -4.32341  -3.92670
H       -0.59101  -4.13041  -4.83870
H        0.15099  -5.49541  -4.44070
H        0.27499  -4.80541  -2.18170
H       -1.25501  -4.76441  -2.65870
H       -0.71801  -2.75941  -1.48770
H       -1.10801  -2.41641  -3.00270
P        1.05099  -0.44141  -2.03670
XX       0.00000   0.00000   0.00000
```


Results : Volumes in Angs^3

```
  Results : Volumes in Angs^3

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

   V Free   V Buried  V Total   V Exact
  121.330    58.205   179.535   179.594

  %V_Free    %V_Bur  % Tot/Ex
  67.580     32.420    99.967
```

The %V_Bur of your molecule is: 32.4

4g

SambVca @ MoLNaC
Results page

```
 ------------------------------------------------
|                                                |
|                  S A M B V C A                 |
|                                                |
|              Buried Volume in Salerno          |
|                                                |
|    http://www.molnac.unisa.it/OM-tools/SambVca |
|                                                |
|    L. Cavallo et al. email: lcavallo@unisa.it  |
|                                                |
 ------------------------------------------------
```

Molecule from input :

Molecule from input :

./temp/40124c17775afe13906b0f8d66028ada.c3d1

```
    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) :    2.334
    Mesh step (Angs)            :    0.050
    H atoms omitted in the V_bur calculation
```

Cartesian coordinates from input :

Cartesian coordinates from input :

```
C      -56.24300   24.05400   14.42400
C      -55.57100   24.66500   13.33600
C      -54.41500   25.41800   13.55500
C      -53.92500   25.59300   14.86600
C      -54.60800   25.02600   15.92800
C      -55.75600   24.27100   15.71400
C      -59.14500   24.10700   14.32600
C      -59.19300   24.72400   15.74900
C      -60.42400   25.62900   15.89600
C      -60.45200   26.72300   14.81800
C      -60.41300   26.07500   13.40500
C      -59.18700   25.18800   13.23500
C      -57.64900   22.39800   12.44600
C      -58.93700   21.66700   12.07000
C      -58.87900   21.17000   10.61300
C      -57.65000   20.30100   10.35500
```



```
C      -56.37700   21.01600   10.73400
C      -56.43500   21.49900   12.21900
P      -57.69000   22.98200   14.19200
```

Atoms and radius in the parameter file

Atoms and radius in the parameter file

```
H     1.29
C2    1.99
C3    1.99
C     1.99
N2    1.81
N3    1.81
N     1.81
O     1.78
P     1.72
Si    2.65
P     2.11
S     2.10
Cl    2.05
Br    2.16
```

Coordinates scaled to put the metal at the origin

Coordinates scaled to put the metal at the origin

```
C       1.48328   2.84529  -1.28513
C       2.15528   3.45629  -2.37313
C       3.31128   4.20929  -2.15413
C       3.80128   4.38429  -0.84313
C       3.11828   3.81729   0.21887
C       1.97028   3.06229   0.00487
C      -1.41872   2.89829  -1.38313
C      -1.46672   3.51529   0.03987
C      -2.69772   4.42029   0.18687
C      -2.72572   5.51429  -0.89113
C      -2.68672   4.86629  -2.30413
C      -1.46072   3.97929  -2.47413
C       0.07728   1.18929  -3.26313
C      -1.21072   0.45829  -3.63913
C      -1.15272  -0.03871  -5.09613
C       0.07628  -0.90771  -5.35413
C       1.34928  -0.19271  -4.97513
C       1.29128   0.29029  -3.49013
P       0.03628   1.77329  -1.51713
XX      0.00000   0.00000   0.00000
```

Results : Volumes in Angs^3

Results : Volumes in Angs^3

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

  V_Free    V_Buried  V_Total   V_Exact
 124.595     54.939   179.535   179.534

%V_Free    %V_Bur  % Tot/Ex
 69.399     30.601    99.947
```

The %V_Bur of your molecule is: 30.6

References

1. Poater, A.; Cosenza, B.; Correa, A.; Giudice, S.; Ragone, F.; Scarano, V.; Cavallo, L., *Eur. J. Inorg. Chem.* **2009**, 1759-1766. (b) Poater, A.; Cosenza, B.; Correa, A.; Giudice, S.; Ragone, F.; Scarano, V.; Cavallo, L. SambVca: A Web Application for the Calculation of the Buried Volume of N-Heterocyclic Carbene Ligands. https://www.molnac.unisa.it/OMtools/sambvca.php (accessed October 26 2009).