

Supporting Information

for

Flexible Cycloalkyl-substituted *N*-heterocyclic Carbenes.

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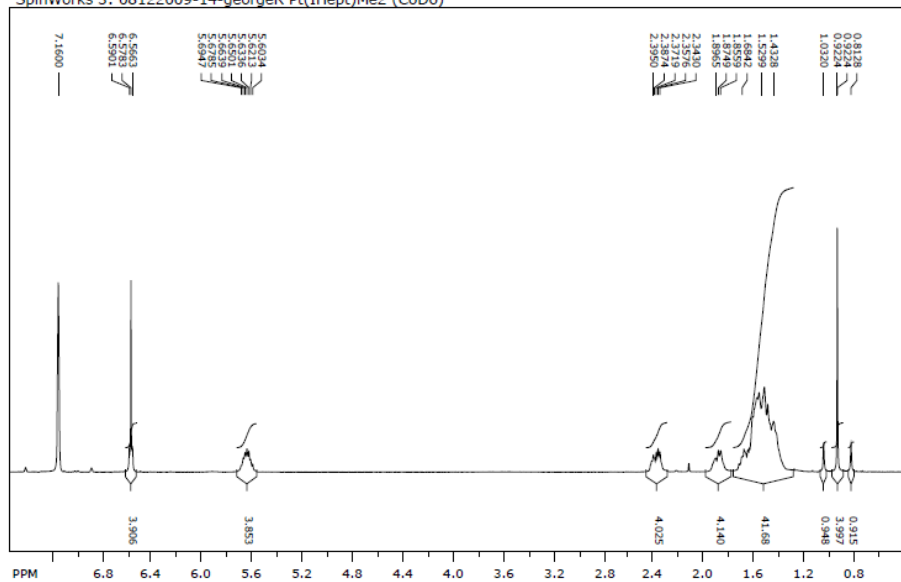
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SambVa Output	S13-S19
Crystallographic Tables	S20-S21

^1H & ^{13}C NMR

cis-Pt(ICy⁷)₂Me₂

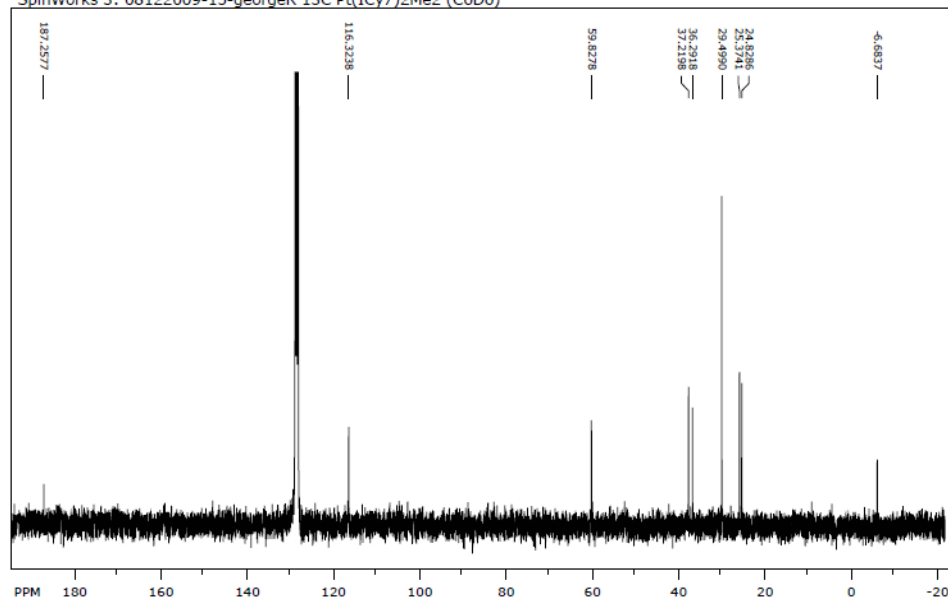
SpinWorks 3: 08122009-14-georgeR Pt(IHept)Me2 (C6D6)



file: ...rent\08122009-14-projects1R\10\fid expt: <zg>
transmitter freq.: 300.061800 MHz
time domain size: 32768 points
width: 4194.63 Hz = 13.9792 ppm = 0.128010 Hz/pt
number of scans: 16

freq. of 0 ppm: 300.060029 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 86.361 ppm/cm: 0.28781

SpinWorks 3: 08122009-15-georgeR 13C Pt(ICy7)2Me2 (C6D6)

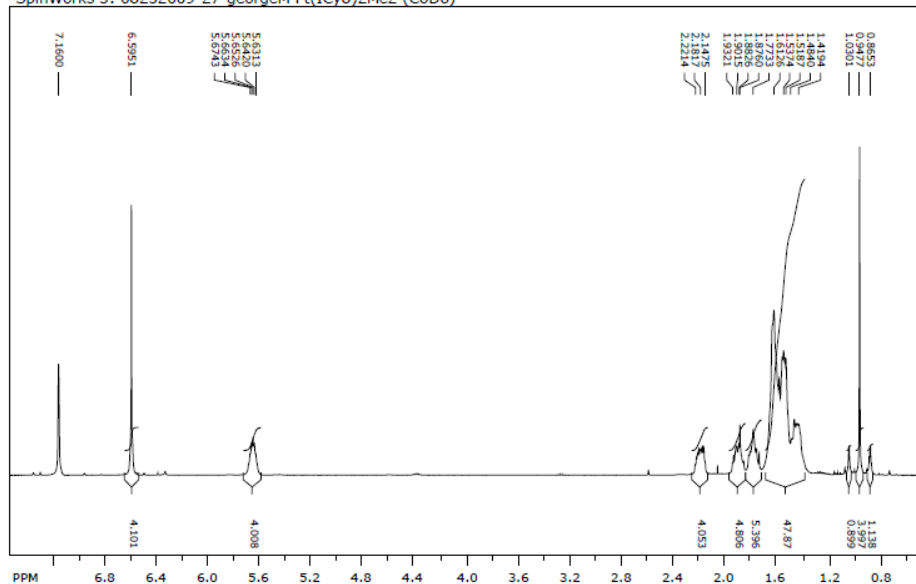


file: ...August\08122009-15-georgeR\11\fid expt: <zgpg30>
transmitter freq.: 75.457662 MHz
time domain size: 65536 points
width: 22675.74 Hz = 300.5094 ppm = 0.346004 Hz/pt
number of scans: 800

freq. of 0 ppm: 75.450100 MHz
processed size: 65536 complex points
LB: 1.000 GF: 0.0000
Hz/cm: 655.984 ppm/cm: 8.69340

cis-Pt(ICy⁸)₂Me₂

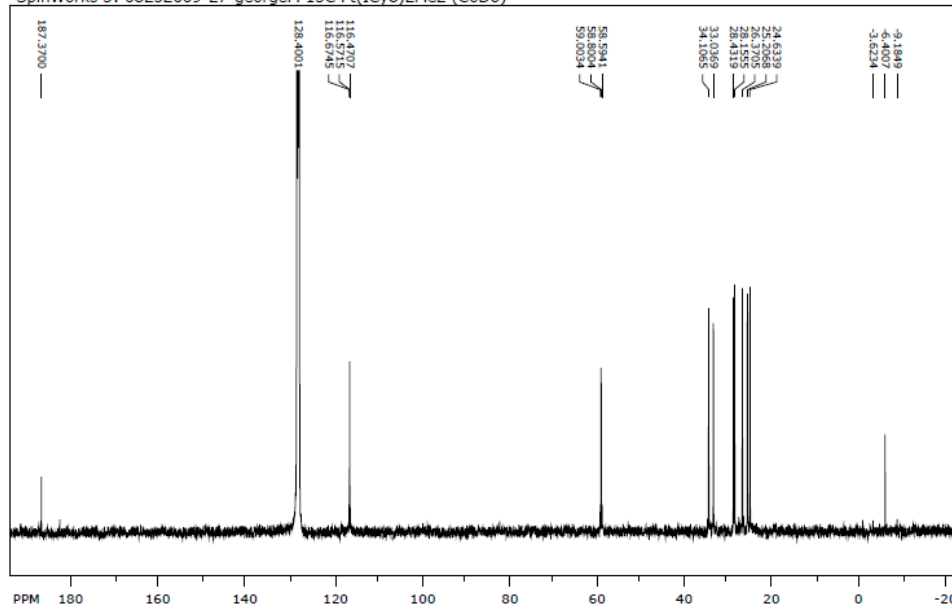
SpinWorks 3: 08252009-27-georgeM Pt(ICy8)2Me2 (C6D6)



file: ..._August\08252009-27-georgeM\10\fid exp: <zg>
transmitter freq.: 400.132401 MHz
time domain size: 65536 points
width: 5597.01 Hz = 13.9879 ppm = 0.085404 Hz/pt
number of scans: 16

freq. of 0 ppm: 400.130043 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 113.167 ppm/cm: 0.28287

SpinWorks 3: 08252009-27-georgeM 13C Pt(ICy8)2Me2 (C6D6)

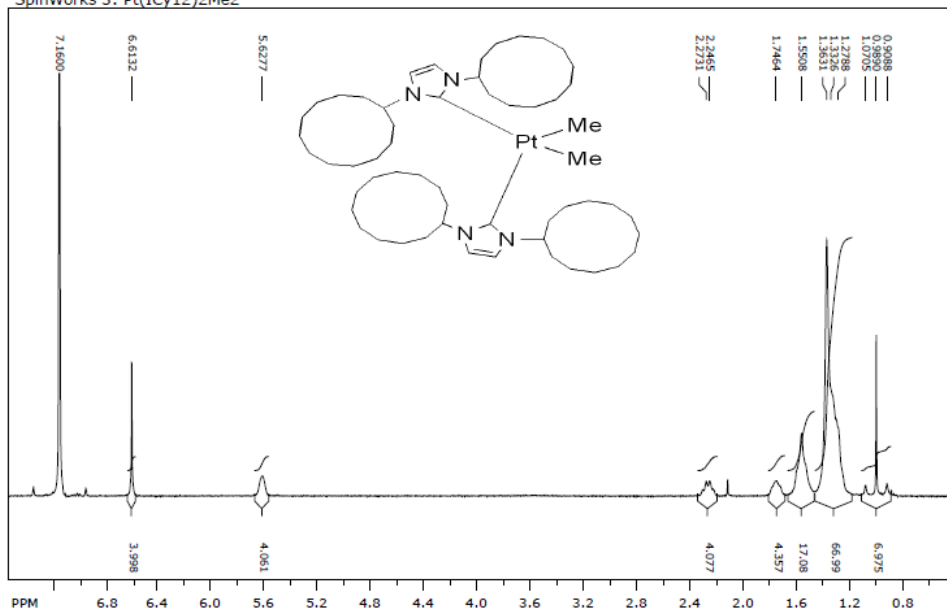


file: ..._August\08252009-27-georgeM\11\fid exp: <zgpg30>
transmitter freq.: 100.622830 MHz
time domain size: 65536 points
width: 29761.90 Hz = 295.7769 ppm = 0.454131 Hz/pt
number of scans: 800

freq. of 0 ppm: 100.612707 MHz
processed size: 32768 complex points
LB: 2.000 GF: 0.0000
Hz/cm: 871.742 ppm/cm: 8.66346

cis-Pt(ICy¹²)₂Me₂

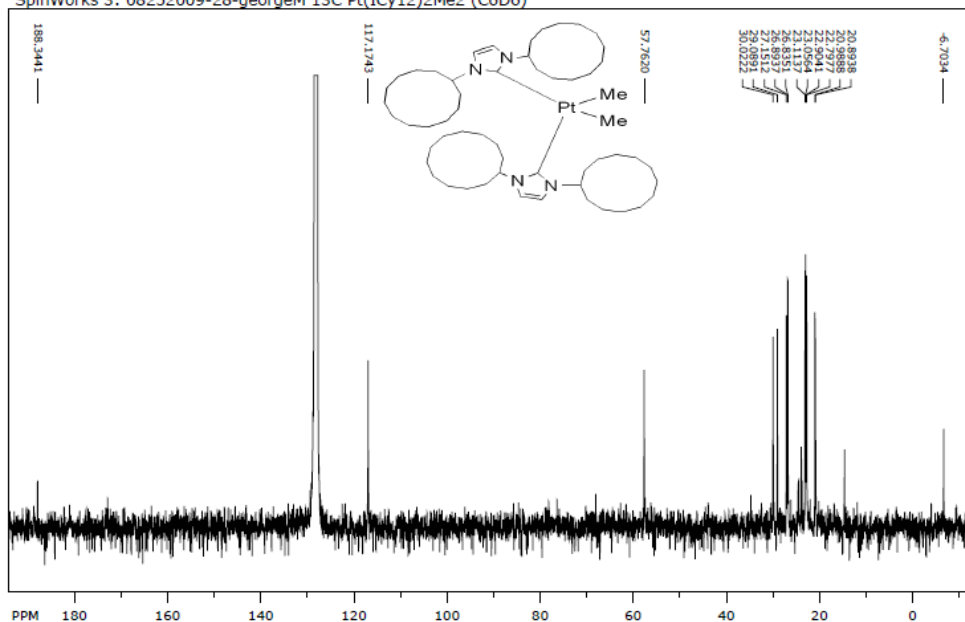
SpinWorks 3: Pt(ICy12)2Me2



file: ...October\10132009-7-georgeM\10\fid exp: <zg30>
 transmitter freq.: 400.132401 MHz
 time domain size: 65536 points
 width: 5597.01 Hz = 13.9879 ppm = 0.085404 Hz/pt
 number of scans: 8

freq. of 0 ppm: 400.130043 MHz
 processed size: 32768 complex points
 LB: 0.300 GF: 0.0000
 Hz/cm: 114.599 ppm/cm: 0.28640

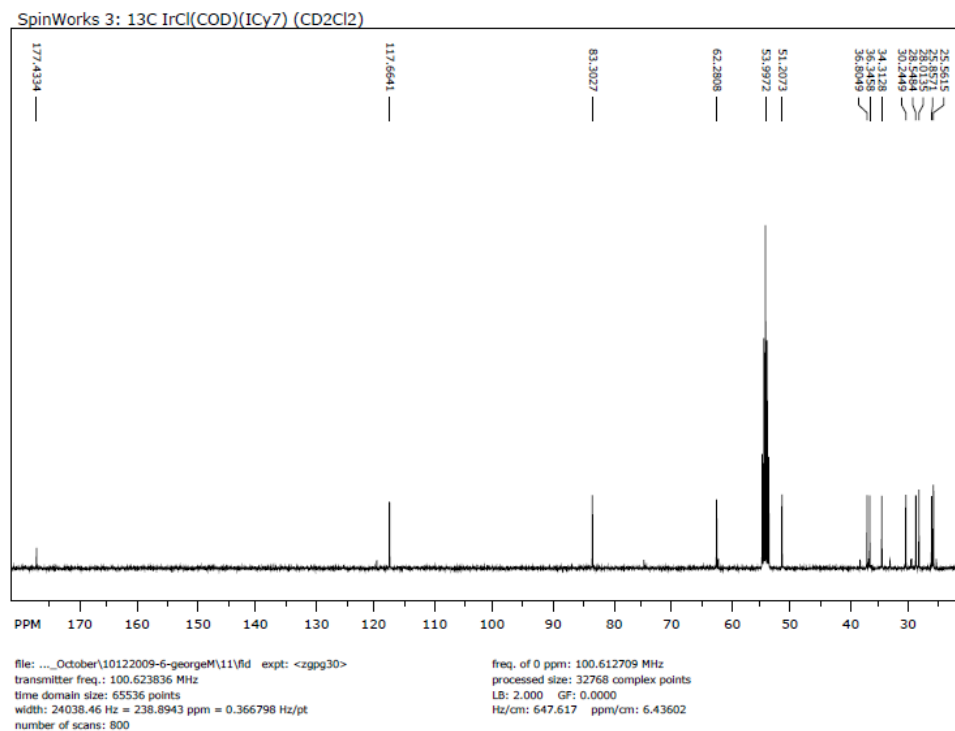
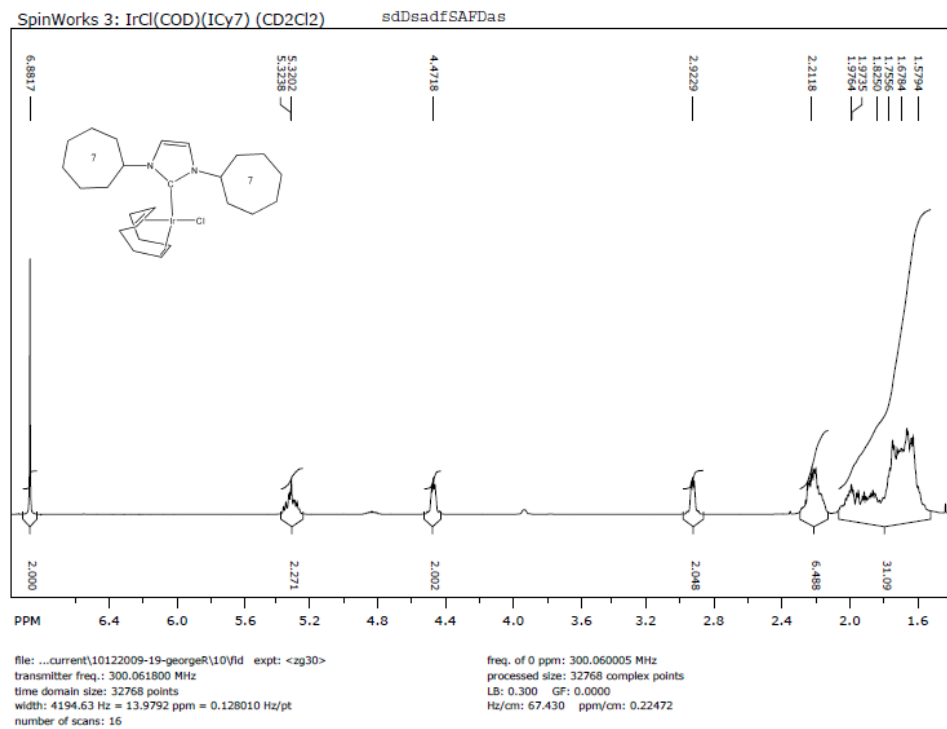
SpinWorks 3: 08252009-28-georgeM 13C Pt(ICy12)2Me2 (C6D6)



file: ...August\08252009-28-georgeM\11\fid exp: <zgpg30>
 transmitter freq.: 100.622830 MHz
 time domain size: 65536 points
 width: 29761.90 Hz = 295.7769 ppm = 0.454131 Hz/pt
 number of scans: 800

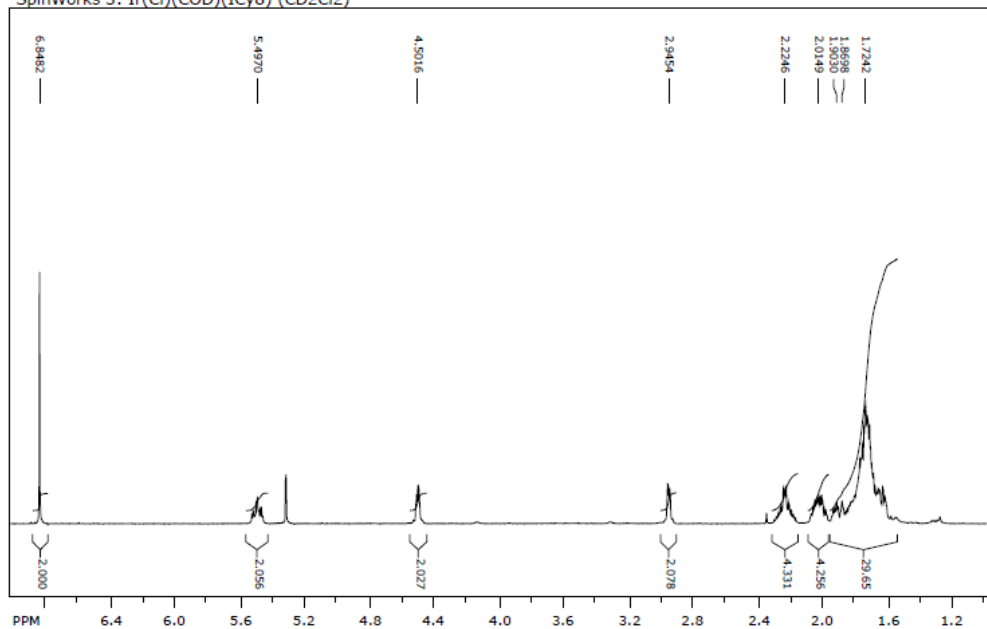
freq. of 0 ppm: 100.612707 MHz
 processed size: 32768 complex points
 LB: 2.000 GF: 0.0000
 Hz/cm: 836.951 ppm/cm: 8.31771

Ir(ICy⁷)(cod)Cl



Ir(ICy⁸)(cod)Cl

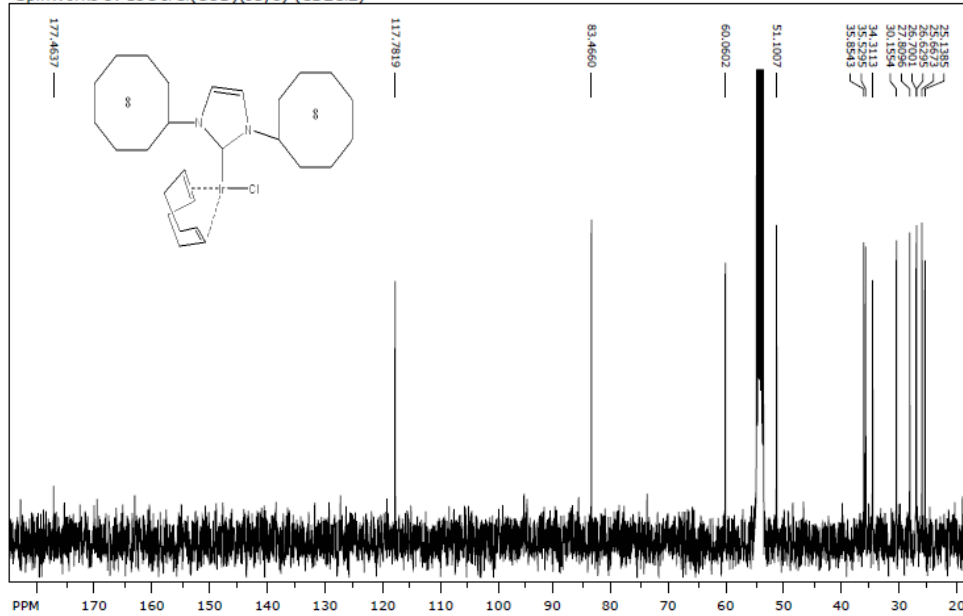
SpinWorks 3: Ir(Cl)(COD)(ICy8) (CD2Cl2)



file: ...current\10142009-30-georgeM\10\fid exp: <zg30>
transmitter freq.: 400.132401 MHz
time domain size: 65536 points
width: 5597.01 Hz = 13.9879 ppm = 0.085404 Hz/pt

freq. of 0 ppm: 400.130010 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 97.072 ppm/cm: 0.24260

SpinWorks 3: 13C IrCl(COD)(ICy8) (CD2Cl2)

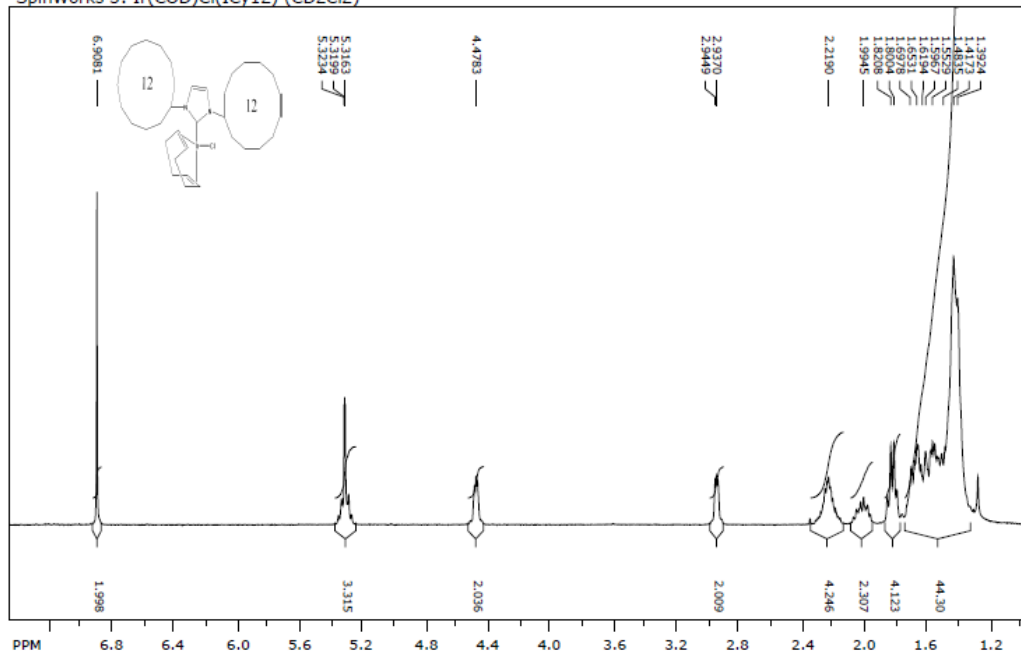


file: ...October\10142009-3-georgeM\11\fid exp: <zpg30>
transmitter freq.: 100.623836 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.8943 ppm = 0.366798 Hz/pt
number of scans: 800

freq. of 0 ppm: 100.612708 MHz
processed size: 32768 complex points
LB: 2.000 GF: 0.0000
Hz/cm: 674.807 ppm/cm: 6.70624

Ir(ICy¹²)(cod)Cl

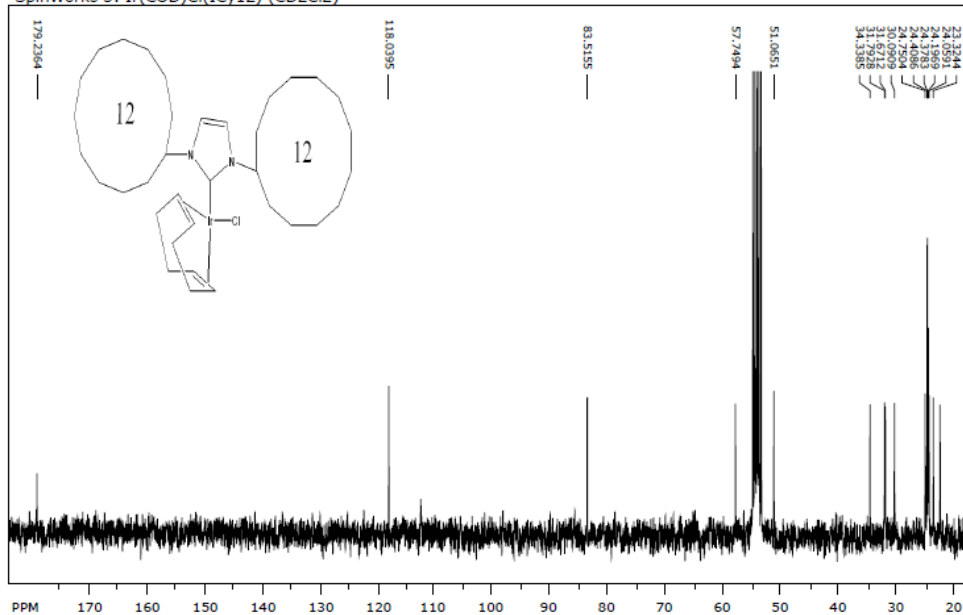
SpinWorks 3: Ir(COD)Cl(ICy12) (CD2Cl2)



file: ...October\10102009-20-georgeR\10\fid exp: <zg30>
transmitter freq.: 300.061800 MHz
time domain size: 32768 points
width: 4194.63 Hz = 13.9792 ppm = 0.128010 Hz/pt
number of scans: 16

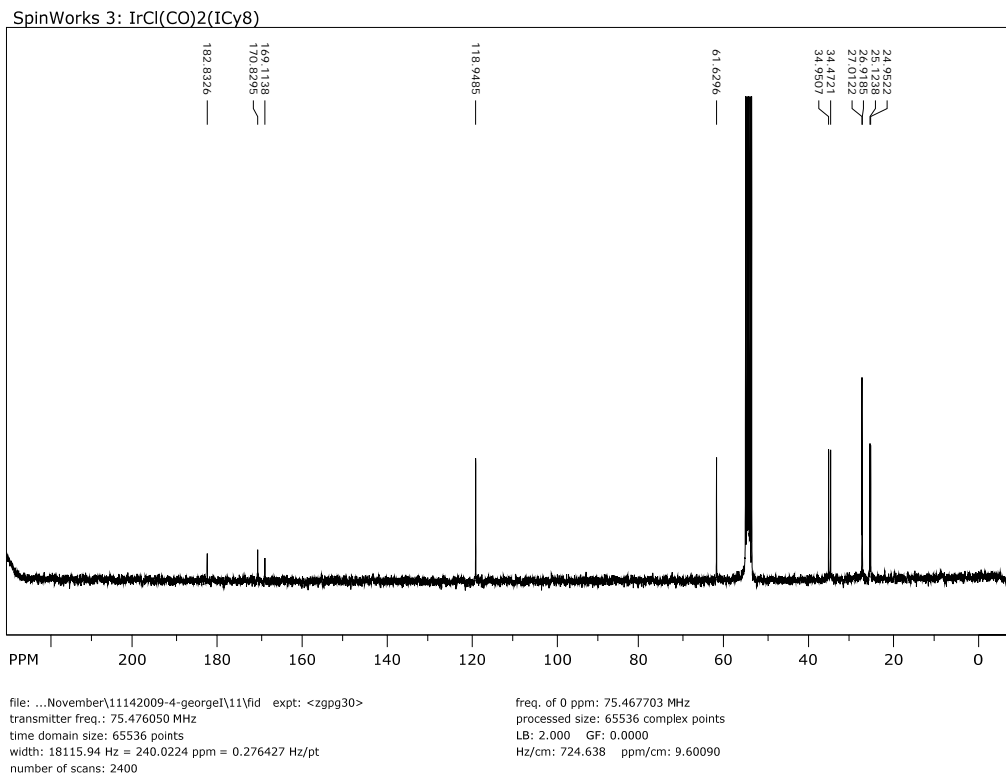
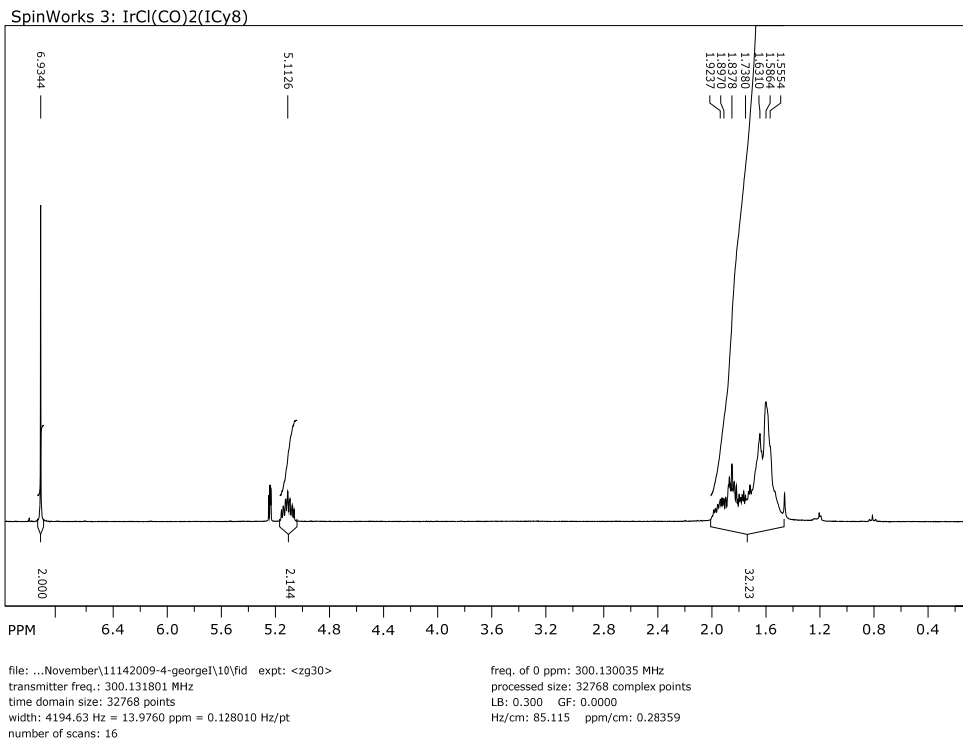
freq. of 0 ppm: 300.060007 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 78.357 ppm/cm: 0.26114

SpinWorks 3: Ir(COD)Cl(ICy12) (CD2Cl2)



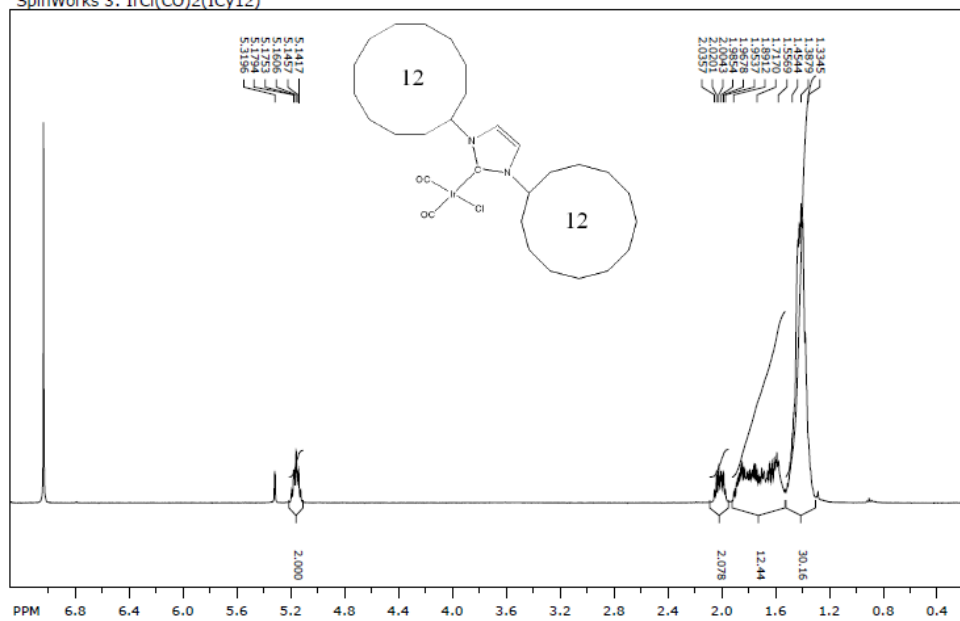
file: ...October\10102009-20-georgeR\11\fid exp: <zpg30>
transmitter freq.: 75.458417 MHz
time domain size: 65536 points
width: 18115.94 Hz = 240.0785 ppm = 0.276427 Hz/pt
number of scans: 800

freq. of 0 ppm: 75.450101 MHz
processed size: 65536 complex points
LB: 2.000 GF: 0.0000
Hz/cm: 504.204 ppm/cm: 6.68188



Ir(ICy¹²)(CO)₂Cl

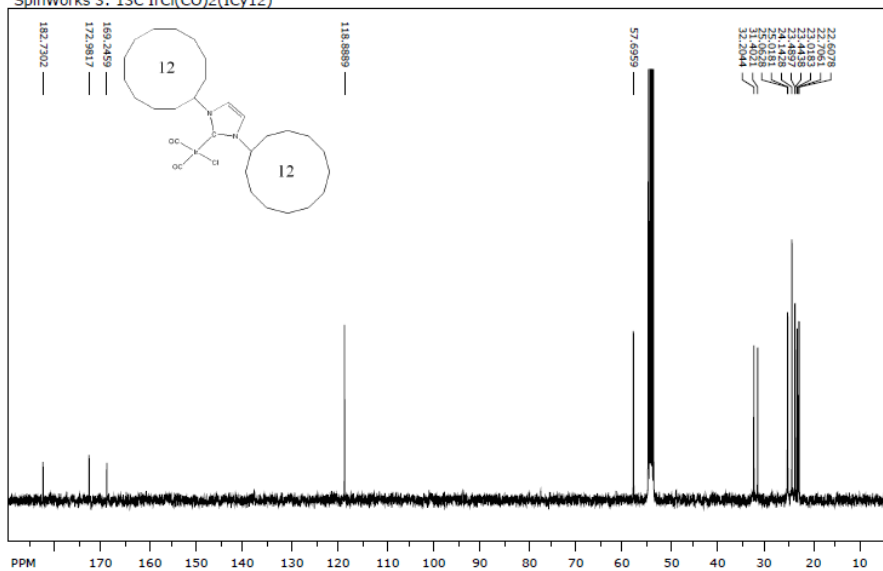
SpinWorks 3: IrCl(CO)₂(ICy12)



file: ..._October\10132009-8-georgeM\10\fd expt: <zg30>
transmitter freq.: 400.132401 MHz
time domain size: 65536 points
width: 5597.01 Hz = 13.9879 ppm = 0.085404 Hz/pt
number of scans: 8

freq. of 0 ppm: 400.130010 MHz
processed size: 32768 complex points
LB: 0.300 GF: 0.0000
Hz/cm: 114.530 ppm/cm: 0.28623

SpinWorks 3: ¹³C IrCl(CO)₂(ICy12)

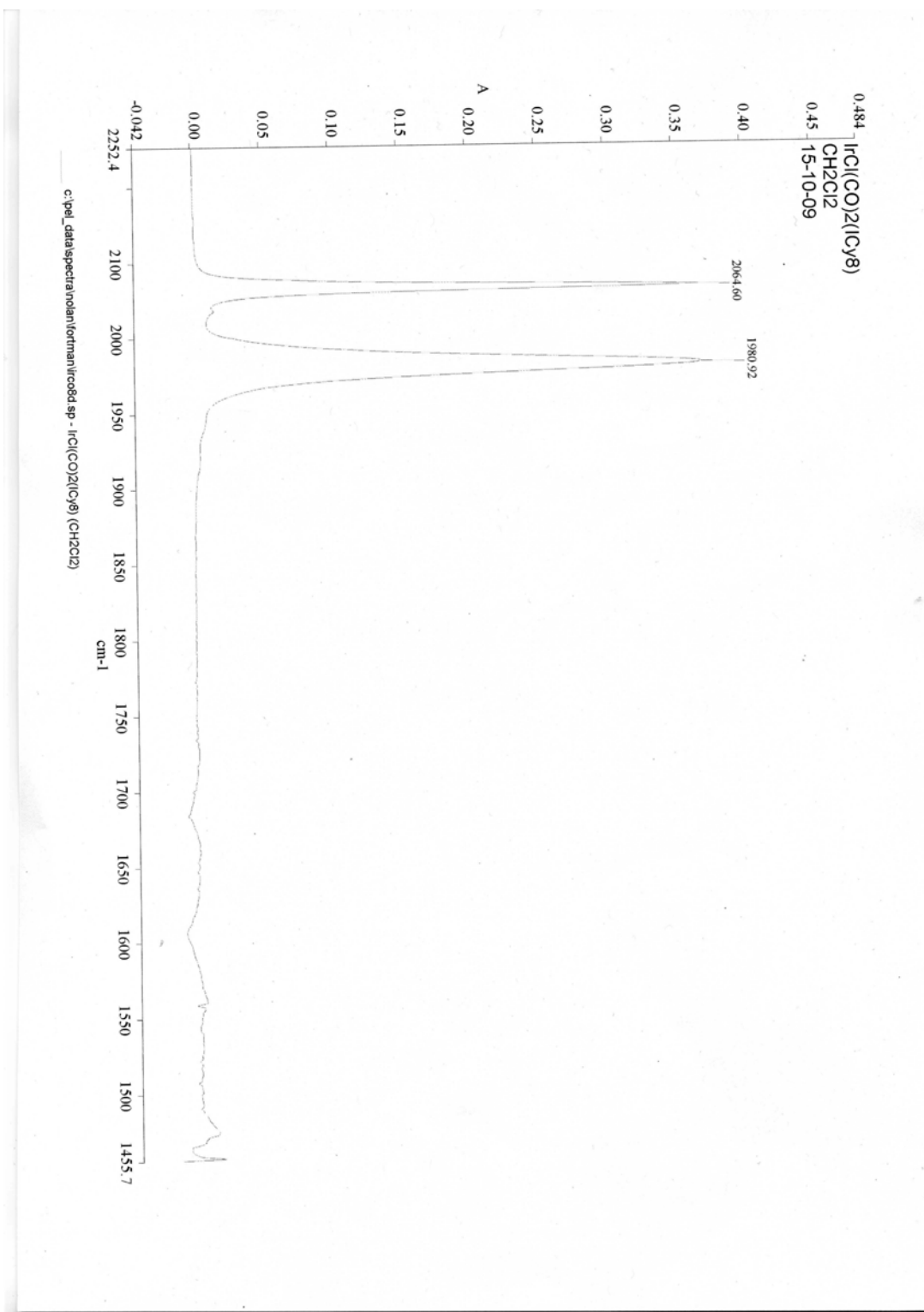


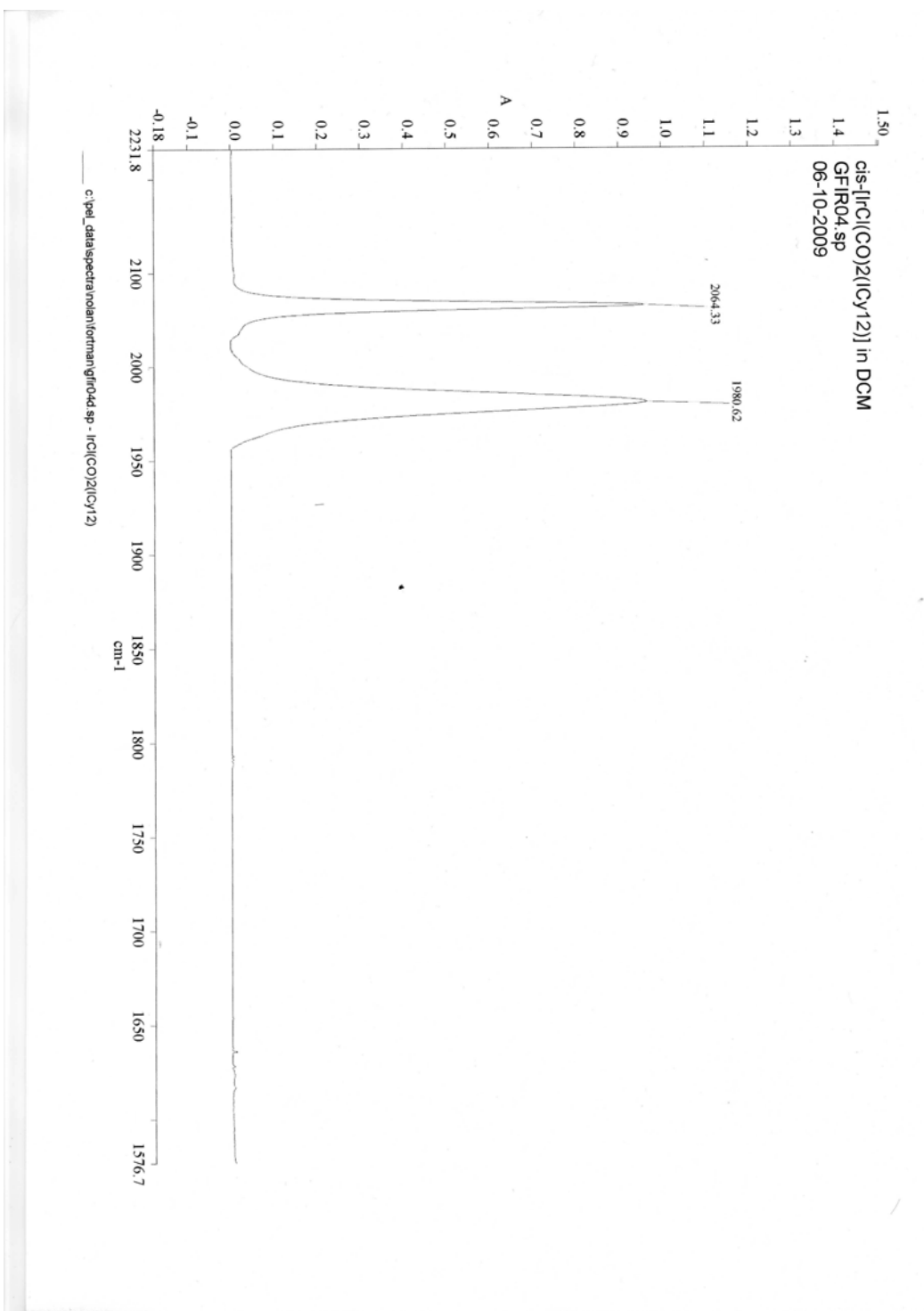
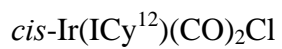
file: ..._October\10132009-8-georgeM\11\fd expt: <zpg30>
transmitter freq.: 100.623636 MHz
time domain size: 65536 points
width: 24038.46 Hz = 238.8943 ppm = 0.366798 Hz/pt
number of scans: 800

freq. of 0 ppm: 100.612708 MHz
processed size: 32768 complex points
LB: 2.000 GF: 0.0000
Hz/cm: 753.082 ppm/cm: 7.48413

FTIR

cis-Ir(ICy⁸)(CO)₂Cl





cis-Pt(ICy⁸)₂Me₂

SambVca@MOLNAC

SambVca @ MolNAC
Results page

S A M B V C A
Buzlak Volume in Italian
http://www.molnac.unina.it/DF/Tools/SambVca
S. Cavallo et al. email: scavallo@unina.it

Molecule from input :
Molecule from input :
./tmp/33136370Testand7747843a439.c3d

Number of atoms : 53
Atom that is coordinated : 3
Atom that define the axis : 3
ID of these atoms : 1 32 53
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.000
Mesh step (Angs) : 4
H atoms included in the V_Bur calculation

Cartesian coordinates from input :
Cartesian coordinates from input
Pt 1 20.40300 40.43000
C 2 20.40300 38.49300
C 3 20.40300 38.49300
C 4 20.40300 38.49300

SambVca@MOLNAC

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2 20.40300 38.49300 41.10000
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SambVca@MOLNAC

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Atoms and radius in the parameter file

Atom and radius in the parameter file

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2 3.500
3 3.500
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52 3.500
53 3.500

Coordinates exited to put the metal at the origin

Coordinates exited to put the metal at the origin

file:///C:/Documents and Settings/George Fortman/Desktop/Nolan(NH)C3PMQ2 Cal vs VBur(Free) CFF/Bur/DCL.Nml[1/22/2010 12:32:30 PM]

file:///C:/Documents and Settings/George Fortman/Desktop/Nolan(NH)C3PMQ2 Cal vs VBur(Free) CFF/Bur/DCL.Nml[1/22/2010 12:32:30 PM]

file:///C:/Documents and Settings/George Fortman/Desktop/Nolan(NH)C3PMQ2 Cal vs VBur(Free) CFF/Bur/DCL.Nml[1/22/2010 12:32:30 PM]

SambVca@MOLNAC

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SambVca@MOLNAC

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53 20.40300 38.49300 41.10000

```

Results - Volume in Angs^3

Results - Volume in Angs^3

N of atoms registered : 53
Volume of model : 0.1159-05
N of Free : 53
N of Buried : 0
N of Free : 53
N of Buried : 0
N of Free : 53
N of Buried : 0

file:///C:/Documents and Settings/George Fortman/Desktop/Nolan(NH)C3PMQ2 Cal vs VBur(Free) CFF/Bur/DCL.Nml[1/22/2010 12:32:30 PM]

file:///C:/Documents and Settings/George Fortman/Desktop/Nolan(NH)C3PMQ2 Cal vs VBur(Free) CFF/Bur/DCL.Nml[1/22/2010 12:32:30 PM]

SambVca@MOLNAC

The V_Bur of your molecule is: 28.5

file:///C:/Documents and Settings/George Fortman/Desktop/Nolan(NH)C3PMQ2 Cal vs VBur(Free) CFF/Bur/DCL.Nml[1/22/2010 12:32:30 PM]

cis-Ir(ICy)(CO)₂Cl

SambVca@MoLNaC

SambVca @ MoLNaC Results page

```
-----  
S A M B V C A  
Buried Volume in Zaierno  
http://www.molnac.unina.it/09-tools/SambVca  
L. Cavallo et Al. email: l.cavallo@unina.it  
-----
```

Molecule from input :

```
Molecule from input :  
./temp/09b7707f0d3d403509b0752f3d3c747c.c3d1  
  
Number of atoms      : 41  
Atom that is coordinated : 3  
Atoms that define the axis : 2  
ID of these atoms    : 40 41  
  
Radius of sphere (Angs) : 3.550  
Distance from sphere (Angs) : 2.050  
Mask atomp (Angs)      : 0.050  
H atoms included in the V_bur calculation
```

Cartesian coordinates from input :

```
Cartesian coordinates from input :  
C  
3.52600 -2.11600 1.04600  
4.95800 -2.12100 1.08000  
2.44400 -2.20700 0.89000  
4.75300 -3.83700 6.98400  
7.52000 -3.11100 8.07900  
9.96300 -3.11100 8.07900  
9.41100 -3.73300 8.72900  
8.80700 -3.88800 5.61300  
1.71100 -3.52900 5.61300  
0.86600 -3.14800 4.71000  
-0.51600 -3.67900 6.32900  
-0.97500 -3.14800 7.70200  
-0.04500 -4.57400 8.57900  
1.37500 -4.39600 8.48000  
2.95500 -1.38400 1.07900  
5.44100 -1.39600 1.18600  
4.75300 -4.81300 1.06100  
7.44400 -2.38300 8.03400  
7.02800 -3.60900 8.89500  
9.42200 -3.23500 8.79000  
9.04200 -4.66200 8.25100  
10.51900 -3.11600 6.70200  
9.84900 -2.41100 6.41100  
9.21300 -3.73500 4.70500  
8.83200 -4.95400 3.70100  
6.62000 -3.39700 4.91400  
7.33100 -2.57600 5.44200  
1.80000 -4.88800 6.94900  
0.88200 -2.25200 6.49100  
1.13600 -3.17900 5.27100  
H  
-0.57600 -4.56600 5.93800
```

file:///C:/Documents and Settings/George Fortman/Desktop/Nolan/Ir NH2CO/Final/Vbur/ICy.htm[1/22/2010 12:13:54 PM]

SambVca@MoLNaC

```
W  
1.01821 1.47330 5.26031  
Wx  
0.00000 0.00000 0.00000
```

Results : Volumes in Angs³

```
Results : Volumes in Angs3  
# of nuclei examined : 11(2011)  
Volume of void : 8.18(215)  
V-Free V-Buried V-Total V-Empty  
137.074 84.460 177.535 37.074  
V-Free V-Buried V-Total V-Empty  
11.039 10.741 21.780 0.298
```

The %V_Bur of your molecule is: 28.9

SambVca@MoLNaC

```
H  
-1.14100 -3.10800 5.83000  
H  
-1.02500 -2.88800 8.05900  
H  
-1.46100 -2.12800 1.77100  
H  
-0.25100 -4.49900 9.52300  
H  
-0.21200 -5.03000 8.11800  
H  
1.96100 -4.73200 8.88900  
H  
1.86300 -2.44100 8.83600  
H  
5.31100 -3.28300 6.93600
```

Atoms and radius in the parameter file

```
Atoms and radius in the parameter file  
H  
1.18  
C  
1.99  
O  
1.49  
N  
1.81  
S  
1.81  
F  
1.45  
Cl  
1.72  
Br  
1.10  
I  
2.11  
Ba  
2.45  
Cs  
2.05
```

Coordinates scaled to put the metal at the origin

Coordinates scaled to put the metal at the origin

```
CO  
-0.78979 4.10220 0.37071  
CO  
0.81251 4.09230 0.40471  
-0.40379 2.81130 0.18471  
-0.45121 3.85130 0.38971  
3.05521 2.90710 1.08371  
4.96821 2.90710 1.08371  
4.51221 2.84530 1.05071  
-0.49779 2.89930 1.05071  
-0.49779 2.71130 0.44771  
-1.44479 2.72230 0.41479  
-4.80379 2.63330 0.34829  
-0.40379 2.67030 1.07571  
-4.35979 1.64430 1.96171  
-0.40379 1.22230 1.97171  
-1.23379 4.83430 6.41871  
1.16421 4.83230 0.51971  
H  
2.45821 1.49530 0.28571  
H  
3.74821 1.97930 1.54971  
H  
2.79321 2.46130 2.02971  
H  
4.07321 2.94330 2.50971  
H  
4.74721 1.55430 1.67971  
H  
4.24421 3.50530 0.60971  
H  
5.95421 3.80730 0.66429  
H  
4.96821 2.40230 1.76229  
H  
4.51721 1.04430 1.97429  
H  
4.98521 1.04430 1.97429  
H  
-0.49779 1.84230 1.03329  
H  
-0.49779 1.79030 1.04829  
H  
-1.44479 1.79630 1.04829  
H  
-1.16779 3.03330 1.40429  
H  
-4.80379 1.62430 1.97529  
H  
-0.40379 1.11030 1.04529  
H  
-0.40379 2.70030 1.02771  
H  
-4.35979 2.09030 1.05571  
H  
-4.40379 1.71930 2.07371  
H  
-4.41479 0.71230 1.84371  
H  
-2.33379 1.48830 2.21371  
H  
-0.42379 2.97130 2.02371  
H  
-1.18379 2.71130 0.45371
```

file:///C:/Documents and Settings/George Fortman/Desktop/Nolan/Ir NH2CO/Final/Vbur/ICy.htm[1/22/2010 12:13:54 PM]

file:///C:/Documents and Settings/George Fortman/Desktop/Nolan/Ir NH2CO/Final/Vbur/ICy.htm[1/22/2010 12:13:54 PM]

cis-Ir(ICy⁸)(CO)₂Cl

Sambiva@Phy.Nrc

Sambiva @ MoI.NaC Results page

 Report Name: *cis*-Ir(ICy⁸)(CO)₂Cl
<http://www.molsoft.com/moI.naC/Results.html>
 L. Caralis et al. moI.naC@molsoft.com

Molecule from Input :

Molecule from Input :
 ..femp00970379@016a44689376@hbk1.c3M

Number of atoms : 53
 Name that defines the unit :
 ID of these atoms : 52 53
 Radius of sphere (Angst) : 3.300
 Distance from sphere (Angst) : 0.100
 Work step (Angst) :
 # atoms included in the V_{surf} : 48/52/53

Cartesian coordinates from Input :

```

    Cartesian coordinates from Input :
    1  0.0000  0.0000  0.0000
    2  1.0000  0.0000  0.0000
    3  0.0000  1.0000  0.0000
    4  0.0000  0.0000  1.0000
    5  0.0000  0.0000  0.0000
    
```

Sambiva@Phy.Nrc

```

    6  0.0000  0.0000  0.0000
    7  0.0000  0.0000  0.0000
    8  0.0000  0.0000  0.0000
    9  0.0000  0.0000  0.0000
    10  0.0000  0.0000  0.0000
    11  0.0000  0.0000  0.0000
    12  0.0000  0.0000  0.0000
    13  0.0000  0.0000  0.0000
    14  0.0000  0.0000  0.0000
    15  0.0000  0.0000  0.0000
    16  0.0000  0.0000  0.0000
    17  0.0000  0.0000  0.0000
    18  0.0000  0.0000  0.0000
    19  0.0000  0.0000  0.0000
    20  0.0000  0.0000  0.0000
    21  0.0000  0.0000  0.0000
    22  0.0000  0.0000  0.0000
    23  0.0000  0.0000  0.0000
    24  0.0000  0.0000  0.0000
    25  0.0000  0.0000  0.0000
    26  0.0000  0.0000  0.0000
    27  0.0000  0.0000  0.0000
    28  0.0000  0.0000  0.0000
    29  0.0000  0.0000  0.0000
    30  0.0000  0.0000  0.0000
    31  0.0000  0.0000  0.0000
    32  0.0000  0.0000  0.0000
    33  0.0000  0.0000  0.0000
    34  0.0000  0.0000  0.0000
    35  0.0000  0.0000  0.0000
    36  0.0000  0.0000  0.0000
    37  0.0000  0.0000  0.0000
    38  0.0000  0.0000  0.0000
    39  0.0000  0.0000  0.0000
    40  0.0000  0.0000  0.0000
    41  0.0000  0.0000  0.0000
    42  0.0000  0.0000  0.0000
    43  0.0000  0.0000  0.0000
    44  0.0000  0.0000  0.0000
    45  0.0000  0.0000  0.0000
    46  0.0000  0.0000  0.0000
    47  0.0000  0.0000  0.0000
    48  0.0000  0.0000  0.0000
    49  0.0000  0.0000  0.0000
    50  0.0000  0.0000  0.0000
    51  0.0000  0.0000  0.0000
    52  0.0000  0.0000  0.0000
    53  0.0000  0.0000  0.0000
    
```

Sambiva@Phy.Nrc

Atom	X	Y	Z
1	0.0000	0.0000	0.0000
2	1.0000	0.0000	0.0000
3	0.0000	1.0000	0.0000
4	0.0000	0.0000	1.0000
5	0.0000	0.0000	0.0000
6	0.0000	0.0000	0.0000
7	0.0000	0.0000	0.0000
8	0.0000	0.0000	0.0000
9	0.0000	0.0000	0.0000
10	0.0000	0.0000	0.0000
11	0.0000	0.0000	0.0000
12	0.0000	0.0000	0.0000
13	0.0000	0.0000	0.0000
14	0.0000	0.0000	0.0000
15	0.0000	0.0000	0.0000
16	0.0000	0.0000	0.0000
17	0.0000	0.0000	0.0000
18	0.0000	0.0000	0.0000
19	0.0000	0.0000	0.0000
20	0.0000	0.0000	0.0000
21	0.0000	0.0000	0.0000
22	0.0000	0.0000	0.0000
23	0.0000	0.0000	0.0000
24	0.0000	0.0000	0.0000
25	0.0000	0.0000	0.0000
26	0.0000	0.0000	0.0000
27	0.0000	0.0000	0.0000
28	0.0000	0.0000	0.0000
29	0.0000	0.0000	0.0000
30	0.0000	0.0000	0.0000
31	0.0000	0.0000	0.0000
32	0.0000	0.0000	0.0000
33	0.0000	0.0000	0.0000
34	0.0000	0.0000	0.0000
35	0.0000	0.0000	0.0000
36	0.0000	0.0000	0.0000
37	0.0000	0.0000	0.0000
38	0.0000	0.0000	0.0000
39	0.0000	0.0000	0.0000
40	0.0000	0.0000	0.0000
41	0.0000	0.0000	0.0000
42	0.0000	0.0000	0.0000
43	0.0000	0.0000	0.0000
44	0.0000	0.0000	0.0000
45	0.0000	0.0000	0.0000
46	0.0000	0.0000	0.0000
47	0.0000	0.0000	0.0000
48	0.0000	0.0000	0.0000
49	0.0000	0.0000	0.0000
50	0.0000	0.0000	0.0000
51	0.0000	0.0000	0.0000
52	0.0000	0.0000	0.0000
53	0.0000	0.0000	0.0000

Atoms and radius in the parameter file

```

    Atom and radius in the parameter file
    1  Ir  0.0000
    2  Cl  0.0000
    3  C  0.0000
    4  N  0.0000
    5  O  0.0000
    6  S  0.0000
    7  P  0.0000
    8  D  0.0000
    9  H  0.0000
    10  F  0.0000
    11  Br  0.0000
    12  I  0.0000
    
```

Coordinates scaled to put the metal at the origin

File: [C:\Documents and Settings\George Fortman\Desktop\files\H\CCDC\Final\Nrc\08-9-sambiva_result.php.html\0202010 12:12:47 PM] Sambiva@Phy.Nrc

```

    1  0.0000  0.0000  0.0000
    2  1.0000  0.0000  0.0000
    3  0.0000  1.0000  0.0000
    4  0.0000  0.0000  1.0000
    5  0.0000  0.0000  0.0000
    6  0.0000  0.0000  0.0000
    7  0.0000  0.0000  0.0000
    8  0.0000  0.0000  0.0000
    9  0.0000  0.0000  0.0000
    10  0.0000  0.0000  0.0000
    11  0.0000  0.0000  0.0000
    12  0.0000  0.0000  0.0000
    13  0.0000  0.0000  0.0000
    14  0.0000  0.0000  0.0000
    15  0.0000  0.0000  0.0000
    16  0.0000  0.0000  0.0000
    17  0.0000  0.0000  0.0000
    18  0.0000  0.0000  0.0000
    19  0.0000  0.0000  0.0000
    20  0.0000  0.0000  0.0000
    21  0.0000  0.0000  0.0000
    22  0.0000  0.0000  0.0000
    23  0.0000  0.0000  0.0000
    24  0.0000  0.0000  0.0000
    25  0.0000  0.0000  0.0000
    26  0.0000  0.0000  0.0000
    27  0.0000  0.0000  0.0000
    28  0.0000  0.0000  0.0000
    29  0.0000  0.0000  0.0000
    30  0.0000  0.0000  0.0000
    31  0.0000  0.0000  0.0000
    32  0.0000  0.0000  0.0000
    33  0.0000  0.0000  0.0000
    34  0.0000  0.0000  0.0000
    35  0.0000  0.0000  0.0000
    36  0.0000  0.0000  0.0000
    37  0.0000  0.0000  0.0000
    38  0.0000  0.0000  0.0000
    39  0.0000  0.0000  0.0000
    40  0.0000  0.0000  0.0000
    41  0.0000  0.0000  0.0000
    42  0.0000  0.0000  0.0000
    43  0.0000  0.0000  0.0000
    44  0.0000  0.0000  0.0000
    45  0.0000  0.0000  0.0000
    46  0.0000  0.0000  0.0000
    47  0.0000  0.0000  0.0000
    48  0.0000  0.0000  0.0000
    49  0.0000  0.0000  0.0000
    50  0.0000  0.0000  0.0000
    51  0.0000  0.0000  0.0000
    52  0.0000  0.0000  0.0000
    53  0.0000  0.0000  0.0000
    
```

Sambiva@Phy.Nrc

```

    1  0.0000  0.0000  0.0000
    2  1.0000  0.0000  0.0000
    3  0.0000  1.0000  0.0000
    4  0.0000  0.0000  1.0000
    5  0.0000  0.0000  0.0000
    6  0.0000  0.0000  0.0000
    7  0.0000  0.0000  0.0000
    8  0.0000  0.0000  0.0000
    9  0.0000  0.0000  0.0000
    10  0.0000  0.0000  0.0000
    11  0.0000  0.0000  0.0000
    12  0.0000  0.0000  0.0000
    13  0.0000  0.0000  0.0000
    14  0.0000  0.0000  0.0000
    15  0.0000  0.0000  0.0000
    16  0.0000  0.0000  0.0000
    17  0.0000  0.0000  0.0000
    18  0.0000  0.0000  0.0000
    19  0.0000  0.0000  0.0000
    20  0.0000  0.0000  0.0000
    21  0.0000  0.0000  0.0000
    22  0.0000  0.0000  0.0000
    23  0.0000  0.0000  0.0000
    24  0.0000  0.0000  0.0000
    25  0.0000  0.0000  0.0000
    26  0.0000  0.0000  0.0000
    27  0.0000  0.0000  0.0000
    28  0.0000  0.0000  0.0000
    29  0.0000  0.0000  0.0000
    30  0.0000  0.0000  0.0000
    31  0.0000  0.0000  0.0000
    32  0.0000  0.0000  0.0000
    33  0.0000  0.0000  0.0000
    34  0.0000  0.0000  0.0000
    35  0.0000  0.0000  0.0000
    36  0.0000  0.0000  0.0000
    37  0.0000  0.0000  0.0000
    38  0.0000  0.0000  0.0000
    39  0.0000  0.0000  0.0000
    40  0.0000  0.0000  0.0000
    41  0.0000  0.0000  0.0000
    42  0.0000  0.0000  0.0000
    43  0.0000  0.0000  0.0000
    44  0.0000  0.0000  0.0000
    45  0.0000  0.0000  0.0000
    46  0.0000  0.0000  0.0000
    47  0.0000  0.0000  0.0000
    48  0.0000  0.0000  0.0000
    49  0.0000  0.0000  0.0000
    50  0.0000  0.0000  0.0000
    51  0.0000  0.0000  0.0000
    52  0.0000  0.0000  0.0000
    53  0.0000  0.0000  0.0000
    
```

Sambiva@Phy.Nrc

```

    1  0.0000  0.0000  0.0000
    2  1.0000  0.0000  0.0000
    3  0.0000  1.0000  0.0000
    4  0.0000  0.0000  1.0000
    5  0.0000  0.0000  0.0000
    6  0.0000  0.0000  0.0000
    7  0.0000  0.0000  0.0000
    8  0.0000  0.0000  0.0000
    9  0.0000  0.0000  0.0000
    10  0.0000  0.0000  0.0000
    11  0.0000  0.0000  0.0000
    12  0.0000  0.0000  0.0000
    13  0.0000  0.0000  0.0000
    14  0.0000  0.0000  0.0000
    15  0.0000  0.0000  0.0000
    16  0.0000  0.0000  0.0000
    17  0.0000  0.0000  0.0000
    18  0.0000  0.0000  0.0000
    19  0.0000  0.0000  0.0000
    20  0.0000  0.0000  0.0000
    21  0.0000  0.0000  0.0000
    22  0.0000  0.0000  0.0000
    23  0.0000  0.0000  0.0000
    24  0.0000  0.0000  0.0000
    25  0.0000  0.0000  0.0000
    26  0.0000  0.0000  0.0000
    27  0.0000  0.0000  0.0000
    28  0.0000  0.0000  0.0000
    29  0.0000  0.0000  0.0000
    30  0.0000  0.0000  0.0000
    31  0.0000  0.0000  0.0000
    32  0.0000  0.0000  0.0000
    33  0.0000  0.0000  0.0000
    34  0.0000  0.0000  0.0000
    35  0.0000  0.0000  0.0000
    36  0.0000  0.0000  0.0000
    37  0.0000  0.0000  0.0000
    38  0.0000  0.0000  0.0000
    39  0.0000  0.0000  0.0000
    40  0.0000  0.0000  0.0000
    41  0.0000  0.0000  0.0000
    42  0.0000  0.0000  0.0000
    43  0.0000  0.0000  0.0000
    44  0.0000  0.0000  0.0000
    45  0.0000  0.0000  0.0000
    46  0.0000  0.0000  0.0000
    47  0.0000  0.0000  0.0000
    48  0.0000  0.0000  0.0000
    49  0.0000  0.0000  0.0000
    50  0.0000  0.0000  0.0000
    51  0.0000  0.0000  0.0000
    52  0.0000  0.0000  0.0000
    53  0.0000  0.0000  0.0000
    
```

Sambiva@Phy.Nrc

The V_{surf} of your molecule is: 30.7

File: [C:\Documents and Settings\George Fortman\Desktop\files\H\CCDC\Final\Nrc\08-9-sambiva_result.php.html\0202010 12:12:47 PM] Sambiva@Phy.Nrc

cis-Ir(ICy¹²)(CO)₂Cl

SambVca@Phd.tusc

SambVca @ MolNaC Results page

S A M B V C A
Buried Volume Calculator
<http://www.uclouvain.be/~s11/09-1003/3ambVca>
L. Cavalari et al. email: inveval@uclouvain.be

Molecule from input :
Molecule from input :
../tmp/9C5372437948L1Caas0a00977a6h3c1_001

Number of atoms : 77
Atom type : 14
Atom that define the unit :
ID of these atoms : 76 77

Radius of sphere (Angst) : 3.200
Extension from sphere (Angst) : 2.000
Mean atmp (Angst) : 3.000
atoms included in the V_{Bur} calculation :

Cartesian coordinates from input :
Cartesian coordinates from input :
C1 0.244000 +1.493000
C2 0.207000
C3 -0.810100 -2.341000
C4 -0.114300 +2.394000

SambVca@Phd.tusc

```
C1 0.244000 +1.493000
C2 0.207000 +1.493000
C3 -0.810100 -2.341000
C4 -0.114300 +2.394000
C5 0.244000 +1.493000
C6 0.207000 +1.493000
C7 -0.810100 -2.341000
C8 -0.114300 +2.394000
C9 0.244000 +1.493000
C10 0.207000 +1.493000
C11 -0.810100 -2.341000
C12 -0.114300 +2.394000
C13 0.244000 +1.493000
C14 0.207000 +1.493000
C15 -0.810100 -2.341000
C16 -0.114300 +2.394000
C17 0.244000 +1.493000
C18 0.207000 +1.493000
C19 -0.810100 -2.341000
C20 -0.114300 +2.394000
C21 0.244000 +1.493000
C22 0.207000 +1.493000
C23 -0.810100 -2.341000
C24 -0.114300 +2.394000
C25 0.244000 +1.493000
C26 0.207000 +1.493000
C27 -0.810100 -2.341000
C28 -0.114300 +2.394000
C29 0.244000 +1.493000
C30 0.207000 +1.493000
C31 -0.810100 -2.341000
C32 -0.114300 +2.394000
C33 0.244000 +1.493000
C34 0.207000 +1.493000
C35 -0.810100 -2.341000
C36 -0.114300 +2.394000
C37 0.244000 +1.493000
C38 0.207000 +1.493000
C39 -0.810100 -2.341000
C40 -0.114300 +2.394000
C41 0.244000 +1.493000
C42 0.207000 +1.493000
C43 -0.810100 -2.341000
C44 -0.114300 +2.394000
C45 0.244000 +1.493000
C46 0.207000 +1.493000
C47 -0.810100 -2.341000
C48 -0.114300 +2.394000
C49 0.244000 +1.493000
C50 0.207000 +1.493000
C51 -0.810100 -2.341000
C52 -0.114300 +2.394000
C53 0.244000 +1.493000
C54 0.207000 +1.493000
C55 -0.810100 -2.341000
C56 -0.114300 +2.394000
C57 0.244000 +1.493000
C58 0.207000 +1.493000
C59 -0.810100 -2.341000
C60 -0.114300 +2.394000
C61 0.244000 +1.493000
C62 0.207000 +1.493000
C63 -0.810100 -2.341000
C64 -0.114300 +2.394000
C65 0.244000 +1.493000
C66 0.207000 +1.493000
C67 -0.810100 -2.341000
C68 -0.114300 +2.394000
C69 0.244000 +1.493000
C70 0.207000 +1.493000
C71 -0.810100 -2.341000
C72 -0.114300 +2.394000
C73 0.244000 +1.493000
C74 0.207000 +1.493000
C75 -0.810100 -2.341000
C76 -0.114300 +2.394000
C77 0.244000 +1.493000
```

SambVca@Phd.tusc

```
O1 0.244000 +1.493000
O2 0.207000 +1.493000
O3 -0.810100 -2.341000
O4 -0.114300 +2.394000
O5 0.244000 +1.493000
O6 0.207000 +1.493000
O7 -0.810100 -2.341000
O8 -0.114300 +2.394000
O9 0.244000 +1.493000
O10 0.207000 +1.493000
O11 -0.810100 -2.341000
O12 -0.114300 +2.394000
O13 0.244000 +1.493000
O14 0.207000 +1.493000
O15 -0.810100 -2.341000
O16 -0.114300 +2.394000
O17 0.244000 +1.493000
O18 0.207000 +1.493000
O19 -0.810100 -2.341000
O20 -0.114300 +2.394000
O21 0.244000 +1.493000
O22 0.207000 +1.493000
O23 -0.810100 -2.341000
O24 -0.114300 +2.394000
O25 0.244000 +1.493000
O26 0.207000 +1.493000
O27 -0.810100 -2.341000
O28 -0.114300 +2.394000
O29 0.244000 +1.493000
O30 0.207000 +1.493000
O31 -0.810100 -2.341000
O32 -0.114300 +2.394000
O33 0.244000 +1.493000
O34 0.207000 +1.493000
O35 -0.810100 -2.341000
O36 -0.114300 +2.394000
O37 0.244000 +1.493000
O38 0.207000 +1.493000
O39 -0.810100 -2.341000
O40 -0.114300 +2.394000
O41 0.244000 +1.493000
O42 0.207000 +1.493000
O43 -0.810100 -2.341000
O44 -0.114300 +2.394000
O45 0.244000 +1.493000
O46 0.207000 +1.493000
O47 -0.810100 -2.341000
O48 -0.114300 +2.394000
O49 0.244000 +1.493000
O50 0.207000 +1.493000
O51 -0.810100 -2.341000
O52 -0.114300 +2.394000
O53 0.244000 +1.493000
O54 0.207000 +1.493000
O55 -0.810100 -2.341000
O56 -0.114300 +2.394000
O57 0.244000 +1.493000
O58 0.207000 +1.493000
O59 -0.810100 -2.341000
O60 -0.114300 +2.394000
O61 0.244000 +1.493000
O62 0.207000 +1.493000
O63 -0.810100 -2.341000
O64 -0.114300 +2.394000
O65 0.244000 +1.493000
O66 0.207000 +1.493000
O67 -0.810100 -2.341000
O68 -0.114300 +2.394000
O69 0.244000 +1.493000
O70 0.207000 +1.493000
O71 -0.810100 -2.341000
O72 -0.114300 +2.394000
O73 0.244000 +1.493000
O74 0.207000 +1.493000
O75 -0.810100 -2.341000
O76 -0.114300 +2.394000
O77 0.244000 +1.493000
```

SambVca@Phd.tusc

```
C1 0.244000 +1.493000
C2 0.207000 +1.493000
C3 -0.810100 -2.341000
C4 -0.114300 +2.394000
```

Atoms and radius in the parameter file
Atom and radius in the parameter file

Atom	radius
C	1.70
O	1.52
N	1.55
H	0.93
Cl	1.75
Ir	1.43
Co	1.43
Ni	1.43
Cr	1.43
Mn	1.43
Fe	1.43
Co	1.43
Ni	1.43
Cr	1.43
Mn	1.43
Fe	1.43

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

C	-0.1144	1.9962
O	0.2440	-0.4568
N	0.2070	-0.4568
H	0.2440	-0.4568
Cl	0.2070	-0.4568
Ir	0.0000	0.0000
Co	-0.1144	1.9962
Ni	-0.1144	1.9962
Cr	-0.1144	1.9962
Mn	-0.1144	1.9962
Fe	-0.1144	1.9962
Co	-0.1144	1.9962
Ni	-0.1144	1.9962
Cr	-0.1144	1.9962
Mn	-0.1144	1.9962
Fe	-0.1144	1.9962

SambVca@Phd.tusc

```
C1 0.244000 +1.493000
C2 0.207000 +1.493000
C3 -0.810100 -2.341000
C4 -0.114300 +2.394000
C5 0.244000 +1.493000
C6 0.207000 +1.493000
C7 -0.810100 -2.341000
C8 -0.114300 +2.394000
C9 0.244000 +1.493000
C10 0.207000 +1.493000
C11 -0.810100 -2.341000
C12 -0.114300 +2.394000
C13 0.244000 +1.493000
C14 0.207000 +1.493000
C15 -0.810100 -2.341000
C16 -0.114300 +2.394000
C17 0.244000 +1.493000
C18 0.207000 +1.493000
C19 -0.810100 -2.341000
C20 -0.114300 +2.394000
C21 0.244000 +1.493000
C22 0.207000 +1.493000
C23 -0.810100 -2.341000
C24 -0.114300 +2.394000
C25 0.244000 +1.493000
C26 0.207000 +1.493000
C27 -0.810100 -2.341000
C28 -0.114300 +2.394000
C29 0.244000 +1.493000
C30 0.207000 +1.493000
C31 -0.810100 -2.341000
C32 -0.114300 +2.394000
C33 0.244000 +1.493000
C34 0.207000 +1.493000
C35 -0.810100 -2.341000
C36 -0.114300 +2.394000
C37 0.244000 +1.493000
C38 0.207000 +1.493000
C39 -0.810100 -2.341000
C40 -0.114300 +2.394000
C41 0.244000 +1.493000
C42 0.207000 +1.493000
C43 -0.810100 -2.341000
C44 -0.114300 +2.394000
C45 0.244000 +1.493000
C46 0.207000 +1.493000
C47 -0.810100 -2.341000
C48 -0.114300 +2.394000
C49 0.244000 +1.493000
C50 0.207000 +1.493000
C51 -0.810100 -2.341000
C52 -0.114300 +2.394000
C53 0.244000 +1.493000
C54 0.207000 +1.493000
C55 -0.810100 -2.341000
C56 -0.114300 +2.394000
C57 0.244000 +1.493000
C58 0.207000 +1.493000
C59 -0.810100 -2.341000
C60 -0.114300 +2.394000
C61 0.244000 +1.493000
C62 0.207000 +1.493000
C63 -0.810100 -2.341000
C64 -0.114300 +2.394000
C65 0.244000 +1.493000
C66 0.207000 +1.493000
C67 -0.810100 -2.341000
C68 -0.114300 +2.394000
C69 0.244000 +1.493000
C70 0.207000 +1.493000
C71 -0.810100 -2.341000
C72 -0.114300 +2.394000
C73 0.244000 +1.493000
C74 0.207000 +1.493000
C75 -0.810100 -2.341000
C76 -0.114300 +2.394000
C77 0.244000 +1.493000
```

SambVca@Phd.tusc

```
O1 0.244000 +1.493000
O2 0.207000 +1.493000
O3 -0.810100 -2.341000
O4 -0.114300 +2.394000
O5 0.244000 +1.493000
O6 0.207000 +1.493000
O7 -0.810100 -2.341000
O8 -0.114300 +2.394000
O9 0.244000 +1.493000
O10 0.207000 +1.493000
O11 -0.810100 -2.341000
O12 -0.114300 +2.394000
O13 0.244000 +1.493000
O14 0.207000 +1.493000
O15 -0.810100 -2.341000
O16 -0.114300 +2.394000
O17 0.244000 +1.493000
O18 0.207000 +1.493000
O19 -0.810100 -2.341000
O20 -0.114300 +2.394000
O21 0.244000 +1.493000
O22 0.207000 +1.493000
O23 -0.810100 -2.341000
O24 -0.114300 +2.394000
O25 0.244000 +1.493000
O26 0.207000 +1.493000
O27 -0.810100 -2.341000
O28 -0.114300 +2.394000
O29 0.244000 +1.493000
O30 0.207000 +1.493000
O31 -0.810100 -2.341000
O32 -0.114300 +2.394000
O33 0.244000 +1.493000
O34 0.207000 +1.493000
O35 -0.810100 -2.341000
O36 -0.114300 +2.394000
O37 0.244000 +1.493000
O38 0.207000 +1.493000
O39 -0.810100 -2.341000
O40 -0.114300 +2.394000
O41 0.244000 +1.493000
O42 0.207000 +1.493000
O43 -0.810100 -2.341000
O44 -0.114300 +2.394000
O45 0.244000 +1.493000
O46 0.207000 +1.493000
O47 -0.810100 -2.341000
O48 -0.114300 +2.394000
O49 0.244000 +1.493000
O50 0.207000 +1.493000
O51 -0.810100 -2.341000
O52 -0.114300 +2.394000
O53 0.244000 +1.493000
O54 0.207000 +1.493000
O55 -0.810100 -2.341000
O56 -0.114300 +2.394000
O57 0.244000 +1.493000
O58 0.207000 +1.493000
O59 -0.810100 -2.341000
O60 -0.114300 +2.394000
O61 0.244000 +1.493000
O62 0.207000 +1.493000
O63 -0.810100 -2.341000
O64 -0.114300 +2.394000
O65 0.244000 +1.493000
O66 0.207000 +1.493000
O67 -0.810100 -2.341000
O68 -0.114300 +2.394000
O69 0.244000 +1.493000
O70 0.207000 +1.493000
O71 -0.810100 -2.341000
O72 -0.114300 +2.394000
O73 0.244000 +1.493000
O74 0.207000 +1.493000
O75 -0.810100 -2.341000
O76 -0.114300 +2.394000
O77 0.244000 +1.493000
```

SambVca@Phd.tusc

Results : Volume in Angs^3

Results : Volume in Angs^3

N of voxels examined :	1436277		
Volume of voxel :	0.1256-03		
V Free	V Buried	V Total	V Empty
109.683	70.473	179.550	179.594

VV Free	VV Bur	% Tot/Free
60.634	39.364	99.997

The VV_Bur of your molecule is: 39.4

File:///C:/Documents and Settings/George Fortman/Desktop/Naica/1/NC/CF/Naica/Naica/1/1 - sambVca_result.php.htm(12/20/2010 12:13:30 PM)

cis-Ir(IMes)(CO)₂Cl

SambVca@Mol.NaC

SambVca @ Mol.NaC
Results page

S A M B V C A
Results Volume in Parameter
http://www.molnac.univ-lille.fr/~SambVca
L. Cavalie et al., email: lorcavalie@univ-lille.fr

Molecule from input :
Molecule from input :
-rsmpt076.777258338555867512635749c.csd

Number of atoms : 47
Atom type in formula defined : 5
Atom type within the mol : 5
ID of these atoms : 44 47

Radius of sphere (Angst) : 3.500
Distance from sphere (Angst) : 2.000
Mesh step (Angst) : 0.250
N atoms included in the V_Bur calculation

Cartesian coordinates from input :
Cartesian coordinates from input :
C1 1.488400 -4.300000
C2 2.160200 0.700000 -4.460000
C3 -1.441000 0.300000 -4.430000
C4 2.388000

file:///C:/Documents and Settings/George Fortman/Desktop/NaCv/ NCC/CE/NaCv/NaCv.htm#(12/20/03 12:14:47 PM)

SambVca@Mol.NaC

C1	1.488400	-4.300000	-0.700000
C2	2.160200	0.700000	-4.460000
C3	-1.441000	0.300000	-4.430000
C4	2.388000		
C5	1.199400	-5.740000	
C6	1.101000	-1.200000	-4.220000
C7	2.428000		
C8	-1.589000	-4.480000	
C9	1.199400	-5.740000	-4.690000
C10	1.101000	-1.200000	-4.690000
C11	2.428000		
C12	0.387000	-7.430000	
C13	1.747000	-4.470000	-4.690000
C14	1.192000	1.800000	-4.460000
C15	2.109000		
C16	1.192000	-7.430000	-4.690000
C17	1.747000	-4.470000	-4.690000
C18	2.109000		
C19	0.387000	-7.430000	-4.690000
C20	1.747000	-4.470000	-4.690000
C21	2.109000		
C22	1.192000	1.800000	-4.460000
C23	1.192000	-7.430000	-4.690000
C24	1.747000	-4.470000	-4.690000
C25	2.109000		
C26	1.192000	1.800000	-4.460000
C27	1.192000	-7.430000	-4.690000
C28	1.747000	-4.470000	-4.690000
C29	2.109000		
C30	1.192000	1.800000	-4.460000
C31	1.192000	-7.430000	-4.690000
C32	1.747000	-4.470000	-4.690000
C33	2.109000		
C34	1.192000	1.800000	-4.460000
C35	1.192000	-7.430000	-4.690000
C36	1.747000	-4.470000	-4.690000
C37	2.109000		
C38	1.192000	1.800000	-4.460000
C39	1.192000	-7.430000	-4.690000
C40	1.747000	-4.470000	-4.690000
C41	2.109000		
C42	1.192000	1.800000	-4.460000
C43	1.192000	-7.430000	-4.690000
C44	1.747000	-4.470000	-4.690000
C45	2.109000		
C46	1.192000	1.800000	-4.460000
C47	1.192000	-7.430000	-4.690000

file:///C:/Documents and Settings/George Fortman/Desktop/NaCv/ NCC/CE/NaCv/NaCv.htm#(12/20/03 12:14:47 PM)

SambVca@Mol.NaC

C1	1.488400	-4.300000	-0.700000
C2	2.160200	0.700000	-4.460000
C3	-1.441000	0.300000	-4.430000
C4	2.388000		
C5	1.199400	-5.740000	
C6	1.101000	-1.200000	-4.220000
C7	2.428000		
C8	-1.589000	-4.480000	
C9	1.199400	-5.740000	-4.690000
C10	1.101000	-1.200000	-4.690000
C11	2.428000		
C12	0.387000	-7.430000	
C13	1.747000	-4.470000	-4.690000
C14	1.192000	1.800000	-4.460000
C15	2.109000		
C16	1.192000	-7.430000	-4.690000
C17	1.747000	-4.470000	-4.690000
C18	2.109000		
C19	0.387000	-7.430000	-4.690000
C20	1.747000	-4.470000	-4.690000
C21	2.109000		
C22	1.192000	1.800000	-4.460000
C23	1.192000	-7.430000	-4.690000
C24	1.747000	-4.470000	-4.690000
C25	2.109000		
C26	1.192000	1.800000	-4.460000
C27	1.192000	-7.430000	-4.690000
C28	1.747000	-4.470000	-4.690000
C29	2.109000		
C30	1.192000	1.800000	-4.460000
C31	1.192000	-7.430000	-4.690000
C32	1.747000	-4.470000	-4.690000
C33	2.109000		
C34	1.192000	1.800000	-4.460000
C35	1.192000	-7.430000	-4.690000
C36	1.747000	-4.470000	-4.690000
C37	2.109000		
C38	1.192000	1.800000	-4.460000
C39	1.192000	-7.430000	-4.690000
C40	1.747000	-4.470000	-4.690000
C41	2.109000		
C42	1.192000	1.800000	-4.460000
C43	1.192000	-7.430000	-4.690000
C44	1.747000	-4.470000	-4.690000
C45	2.109000		
C46	1.192000	1.800000	-4.460000
C47	1.192000	-7.430000	-4.690000

file:///C:/Documents and Settings/George Fortman/Desktop/NaCv/ NCC/CE/NaCv/NaCv.htm#(12/20/03 12:14:47 PM)

SambVca@Mol.NaC

C1	1.488400	-4.300000	-0.700000
C2	2.160200	0.700000	-4.460000
C3	-1.441000	0.300000	-4.430000
C4	2.388000		
C5	1.199400	-5.740000	
C6	1.101000	-1.200000	-4.220000
C7	2.428000		
C8	-1.589000	-4.480000	
C9	1.199400	-5.740000	-4.690000
C10	1.101000	-1.200000	-4.690000
C11	2.428000		
C12	0.387000	-7.430000	
C13	1.747000	-4.470000	-4.690000
C14	1.192000	1.800000	-4.460000
C15	2.109000		
C16	1.192000	-7.430000	-4.690000
C17	1.747000	-4.470000	-4.690000
C18	2.109000		
C19	0.387000	-7.430000	-4.690000
C20	1.747000	-4.470000	-4.690000
C21	2.109000		
C22	1.192000	1.800000	-4.460000
C23	1.192000	-7.430000	-4.690000
C24	1.747000	-4.470000	-4.690000
C25	2.109000		
C26	1.192000	1.800000	-4.460000
C27	1.192000	-7.430000	-4.690000
C28	1.747000	-4.470000	-4.690000
C29	2.109000		
C30	1.192000	1.800000	-4.460000
C31	1.192000	-7.430000	-4.690000
C32	1.747000	-4.470000	-4.690000
C33	2.109000		
C34	1.192000	1.800000	-4.460000
C35	1.192000	-7.430000	-4.690000
C36	1.747000	-4.470000	-4.690000
C37	2.109000		
C38	1.192000	1.800000	-4.460000
C39	1.192000	-7.430000	-4.690000
C40	1.747000	-4.470000	-4.690000
C41	2.109000		
C42	1.192000	1.800000	-4.460000
C43	1.192000	-7.430000	-4.690000
C44	1.747000	-4.470000	-4.690000
C45	2.109000		
C46	1.192000	1.800000	-4.460000
C47	1.192000	-7.430000	-4.690000

file:///C:/Documents and Settings/George Fortman/Desktop/NaCv/ NCC/CE/NaCv/NaCv.htm#(12/20/03 12:14:47 PM)

SambVca@Mol.NaC

C1	1.488400	-4.300000	-0.700000
C2	2.160200	0.700000	-4.460000
C3	-1.441000	0.300000	-4.430000
C4	2.388000		
C5	1.199400	-5.740000	
C6	1.101000	-1.200000	-4.220000
C7	2.428000		
C8	-1.589000	-4.480000	
C9	1.199400	-5.740000	-4.690000
C10	1.101000	-1.200000	-4.690000
C11	2.428000		
C12	0.387000	-7.430000	
C13	1.747000	-4.470000	-4.690000
C14	1.192000	1.800000	-4.460000
C15	2.109000		
C16	1.192000	-7.430000	-4.690000
C17	1.747000	-4.470000	-4.690000
C18	2.109000		
C19	0.387000	-7.430000	-4.690000
C20	1.747000	-4.470000	-4.690000
C21	2.109000		
C22	1.192000	1.800000	-4.460000
C23	1.192000	-7.430000	-4.690000
C24	1.747000	-4.470000	-4.690000
C25	2.109000		
C26	1.192000	1.800000	-4.460000
C27	1.192000	-7.430000	-4.690000
C28	1.747000	-4.470000	-4.690000
C29	2.109000		
C30	1.192000	1.800000	-4.460000
C31	1.192000	-7.430000	-4.690000
C32	1.747000	-4.470000	-4.690000
C33	2.109000		
C34	1.192000	1.800000	-4.460000
C35	1.192000	-7.430000	-4.690000
C36	1.747000	-4.470000	-4.690000
C37	2.109000		
C38	1.192000	1.800000	-4.460000
C39	1.192000	-7.430000	-4.690000
C40	1.747000	-4.470000	-4.690000
C41	2.109000		
C42	1.192000	1.800000	-4.460000
C43	1.192000	-7.430000	-4.690000
C44	1.747000	-4.470000	-4.690000
C45	2.109000		
C46	1.192000	1.800000	-4.460000
C47	1.192000	-7.430000	-4.690000

file:///C:/Documents and Settings/George Fortman/Desktop/NaCv/ NCC/CE/NaCv/NaCv.htm#(12/20/03 12:14:47 PM)

Table S1. Crystallographic data for *cis*-Pt(NHC)₂Me₂ (NHC = ICy⁷, ICy⁸, ICy¹²) complexes.

Compound reference	<i>cis</i> -Pt(ICy ⁷) ₂ Me ₂ (3e)	<i>cis</i> -Pt(ICy ⁸) ₂ Me ₂ (3f)	<i>cis</i> -Pt(ICy ¹²) ₂ Me ₂ (3g)
Chemical formula	C ₃₆ H ₆₂ N ₄ Pt	C ₄₀ H ₇₀ N ₄ Pt	C ₅₆ H ₁₀₂ N ₄ Pt•C ₄ H ₈ O ₂
Formula Mass	745.99	802.09	1114.61
CCDC number	762962	762961	762963
Crystal system	Orthorhombic	Orthorhombic	Monoclinic
<i>a</i> /Å	19.481(4)	12.924(3)	17.712(5)
<i>b</i> /Å	15.267(3)	14.532(3)	15.351(4)
<i>c</i> /Å	22.882(5)	19.717(4)	23.005(7)
α /°	90.00	90.00	90.00
β /°	90.00	90.00	111.436(7)
γ /°	90.00	90.00	90.00
Unit cell volume/Å ³	6806(2)	3703.3(14)	5822(3)
Temperature/K	93(2)	93(2)	93(2)
Space group	<i>Pbca</i>	<i>P2(1)2(1)2(1)</i>	<i>P2(1)/n</i>
No. of formula units per unit cell, <i>Z</i>	8	4	4
Absorption coefficient, μ /mm ⁻¹	4.153	3.822	2.453
No. of reflections measured	41103	23569	36606
No. of independent reflections	6210	6756	10549
<i>R</i> _{int}	0.1494	0.0764	0.1599
Final <i>R</i> _{<i>I</i>} values (<i>I</i> > 2σ(<i>I</i>))	0.0582	0.0408	0.0641
Final <i>wR</i> (<i>F</i> ²) values (<i>I</i> > 2σ(<i>I</i>))	0.1034	0.0651	0.1005
Final <i>R</i> _{<i>I</i>} values (all data)	0.1082	0.0486	0.1321
Final <i>wR</i> (<i>F</i> ²) values (all data)	0.1191	0.0680	0.1192

Table S2. Crystallographic data for *cis*-Ir(NHC)(CO)₂Cl (NHC = ICy⁸, ICy¹²) complexes.

Compound reference	<i>cis</i> -Ir(ICy ⁸)(CO) ₂ Cl (6f)	<i>cis</i> -Ir(ICy ¹²)(CO) ₂ Cl (6g)
Chemical formula	C ₂₁ H ₃₂ ClIrN ₂ O ₂	C ₂₉ H ₄₈ ClIrN ₂ O ₂
Formula Mass	572.14	684.34
CCDC number	762964	762965
Crystal system	Orthorhombic	Triclinic
<i>a</i> /Å	17.878(6)	7.815(4)
<i>b</i> /Å	19.052(6)	9.552(5)
<i>c</i> /Å	13.392(4)	20.760(9)
<i>α</i> /°	90.00	92.160(9)
<i>β</i> /°	90.00	92.229(10)
<i>γ</i> /°	90.00	111.059(15)
Unit cell volume/Å ³	4561(2)	1442.8(12)
Temperature/K	93(2)	93(2)
Space group	<i>Pccn</i>	<i>P1</i>
No. of formula units per unit cell, <i>Z</i>	8	2
Absorption coefficient, <i>μ</i> /mm ⁻¹	5.988	4.747
No. of reflections measured	27093	9296
No. of independent reflections	4135	5089
<i>R</i> _{int}	0.1448	0.0837
Final <i>R</i> _{<i>I</i>} values (<i>I</i> > 2σ(<i>I</i>))	0.0821	0.0681
Final <i>wR</i> (<i>F</i> ²) values (<i>I</i> > 2σ(<i>I</i>))	0.1559	0.1215
Final <i>R</i> _{<i>I</i>} values (all data)	0.1330	0.1059
Final <i>wR</i> (<i>F</i> ²) values (all data)	0.1745	0.1375