Supporting information

for

# Syntheses and characterizations of $IPr^{Me}$-containing silver(I), gold(I) and gold(III) complexes

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# I. Crystallographic data

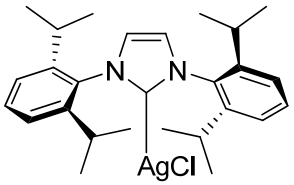
| | AgCl(IPr$^{Me}$) **3** | AuCl(IPr$^{Me}$) **4** | $AuCl_3$(IPr$^{Me}$) **5/6** |
|---|---|---|---|
| Formula | $C_{29}H_{40}N_2AgCl,CH_2Cl_2$ | $C_{29}H_{40}N_2AuCl,CH_2Cl_2$ | ($C_{29}H_{40}N_2AuCl_3$), 0.5 ($C_{29}H_{40}N_2AuCl_4$), 0.5 |
| $M_r$/g mol$^{-1}$ | 644.88 | 733.97 | 737.17 |
| Crystal habit | colorless | colorless | yellow |
| Crystal system | orthorhombic | monoclinic | monoclinic |
| Flack's *x* parameter | -0.02(3) | - | - |
| Space group | $P2_12_12_1$ | $P2_1$/m | $P2_1$/m |
| *a*/ Å | 12.203(4) | 8.795(2) | 9.4271(19) |
| *b*/ Å | 14.287(5) | 17.615(4) | 17.845(3) |
| *c*/ Å | 18.176(6) | 10.610(2) | 9.7182(18) |
| *β*/ ° | - | 99.841(6) | 110.881(5) |
| *V*/ Å$^3$ | 3169.1(19) | 1619.7(6) | 1527.5(5) |
| *Z* | 4 | 2 | 2 |
| *ρcalcd*/ g.cm$^{-3}$ | 1.352 | 1.505 | 1.603 |
| $\mu$(Mo $K_\alpha$)/ mm$^{-1}$ | 0.909 | 4.809 | 5.142 |
| *T*/ K | 93(2) | 93(2) | 93(2) |
| No of reflections | 5419 | 2802 | 2562 |
| No of unique reflections | 5709 | 3047 | 2880 |
| $R_{int}$ | 0.0843 | 0.0868 | 0.0513 |
| *R*1, w$R_2$ (I > 2$\sigma$(I)) | 0.0387, 0.0940 | 0.0553, 0.1436 | 0.0438, 0.0988 |
| *R*1, w$R_2$ (all data) | 0.0411, 0.0962 | 0.0595, 0.1490 | 0.0512, 0.1067 |
| GOF | 1.093 | 0.985 | 1.115 |

# II. SambVca calculations for AgCl(NHC) complexes

## Samb*V*ca @ MoLNaC

```
------------------------------------------------------
| |
| 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 |
| |
------------------------------------------------------
```

### *%$V_{bur}$ for AgCl(IPr)*




### Molecule from input :

```
Molecule from input :
./temp/6565104801e58aa5d253c8e677229e14.c3d1
Number of atoms : 65
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 64 65
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.056
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

### Cartesian coordinates from input :

```
C -11.57600 -29.62900 18.96100
C -13.66400 -31.75200 20.45400
C -13.99800 -32.96600 20.69700
C -14.08200 -34.01500 19.78600
C -13.72900 -33.63000 18.32200
C -13.37100 -32.37500 17.97500
C -13.60700 -30.68200 21.52700
C -14.98700 -30.63100 22.15100
C -12.61700 -30.95400 22.52000
C -13.01100 -31.95600 16.58200
C -11.83700 -32.76900 16.13000
C -14.08700 -32.67800 15.76900
C -13.34400 -31.43100 19.09200
C -13.65100 -29.01700 18.28200
C -12.86000 -27.94300 18.14800
C -10.47000 -27.49700 18.73500
C -10.22300 -27.00900 19.92600
C -8.96200 -26.15700 20.05800
C -8.24600 -25.99900 18.94100
C -8.51500 -26.47400 17.85300
C -9.68900 -27.26800 17.70900
C -11.01400 -27.16800 21.22200
```

```
C -11.72900 -26.00100 21.81800
C -10.20100 -27.93000 22.35600
C -9.98300 -27.85900 16.28400
C -10.39700 -26.87200 15.07700
C -9.07200 -29.08400 15.97700
H -14.21300 -33.17100 21.60000
H -14.33400 -34.89500 20.04000
H -13.76600 -34.29900 17.64800
H -13.40900 -29.80100 21.09900
H -14.91600 -30.30400 23.07300
H -15.55800 -30.02700 21.63300
H -15.37900 -31.53000 22.15200
H -12.66200 -31.89900 22.77600
H -11.72800 -30.75600 22.15700
H -12.78200 -30.39500 23.30600
H -12.94100 -30.97100 16.43000
H -12.12400 -33.69000 15.95400
H -11.46600 -32.38000 15.31000
H -11.15000 -32.76900 16.83000
H -14.96800 -32.31900 16.00300
H -13.92000 -32.53900 14.81300
H -14.06000 -33.63600 15.97000
H -14.58400 -29.06300 18.11700
H -13.10100 -27.10200 17.77900
H -8.70400 -25.76400 20.88300
H -7.45900 -25.47100 19.00100
H -7.94700 -26.31600 17.10800
H -11.74700 -27.80300 20.98200
H -12.29500 -25.58200 21.13700
H -12.28600 -26.30500 22.56500
H -11.07400 -25.34800 22.14500
H -9.36200 -27.45600 22.53200
H -10.73700 -27.96000 23.17800
H -10.00600 -28.84200 22.06000
H -10.85500 -28.31800 16.45300
H -9.67500 -26.22700 14.92100
H -10.55000 -27.39600 14.26400
H -11.21800 -26.39100 15.31600
H -8.13800 -28.79100 15.92600
H -9.16600 -29.74900 16.69100
H -9.33600 -29.48200 15.12200
N -12.83000 -30.03900 18.70700
N -11.61500 -28.30700 18.66100
```

## Atoms and radius in the parameter file

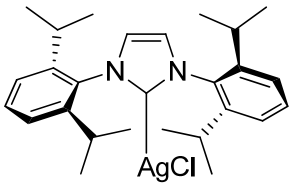
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
H -2.29573 4.44247 2.92458
```

## Results : Volumes in Angs^3

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
102.503 77.031 179.535 179.594
%V_Free %V_Bur % Tot/Ex
57.094 42.906 99.967
```

**The %V_Bur of your molecule is: 42.9**

***$\%V_{bur}^{average}$ for AgCl(IPr)***




## Molecule from input :

```
Molecule from input :
./temp/6565104801e58aa5d253c8e677229e14.c3d1
Number of atoms : 65
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 64 65
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.073
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C -11.57600 -29.62900 18.96100
C -13.66400 -31.75200 20.45400
C -13.99800 -32.96600 20.69700
C -14.08200 -34.01500 19.78600
C -13.72900 -33.63000 18.32200
C -13.37100 -32.37500 17.97500
C -13.60700 -30.68200 21.52700
C -14.98700 -30.63100 22.15100
C -12.61700 -30.95400 22.52000
C -13.01100 -31.95600 16.58200
C -11.83700 -32.76900 16.13000
C -14.08700 -32.67800 15.76900
C -13.34400 -31.43100 19.09200
C -13.65100 -29.01700 18.28200
C -12.86000 -27.94300 18.14800
C -10.47000 -27.49700 18.73500
C -10.22300 -27.00900 19.92600
C -8.96200 -26.15700 20.05800
C -8.24600 -25.99900 18.94100
C -8.51500 -26.47400 17.85300
C -9.68900 -27.26800 17.70900
C -11.01400 -27.16800 21.22200
C -11.72900 -26.00100 21.81800
C -10.20100 -27.93000 22.35600
C -9.98300 -27.85900 16.28400
C -10.39700 -26.87200 15.07700
C -9.07200 -29.08400 15.97700
H -14.21300 -33.17100 21.60000
H -14.33400 -34.89500 20.04000
H -13.76600 -34.29900 17.64800
H -13.40900 -29.80100 21.09900
H -14.91600 -30.30400 23.07300
H -15.55800 -30.02700 21.63300
H -15.37900 -31.53000 22.15200
H -12.66200 -31.89900 22.77600
H -11.72800 -30.75600 22.15700
H -12.78200 -30.39500 23.30600
H -12.94100 -30.97100 16.43000
H -12.12400 -33.69000 15.95400
H -11.46600 -32.38000 15.31000
```

```
H -11.15000 -32.76900 16.83000
H -14.96800 -32.31900 16.00300
H -13.92000 -32.53900 14.81300
H -14.06000 -33.63600 15.97000
H -14.58400 -29.06300 18.11700
H -13.10100 -27.10200 17.77900
H -8.70400 -25.76400 20.88300
H -7.45900 -25.47100 19.00100
H -7.94700 -26.31600 17.10800
H -11.74700 -27.80300 20.98200
H -12.29500 -25.58200 21.13700
H -12.28600 -26.30500 22.56500
H -11.07400 -25.34800 22.14500
H -9.36200 -27.45600 22.53200
H -10.73700 -27.96000 23.17800
H -10.00600 -28.84200 22.06000
H -10.85500 -28.31800 16.45300
H -9.67500 -26.22700 14.92100
H -10.55000 -27.39600 14.26400
H -11.21800 -26.39100 15.31600
H -8.13800 -28.79100 15.92600
H -9.16600 -29.74900 16.69100
H -9.33600 -29.48200 15.12200
N -12.83000 -30.03900 18.70700
N -11.61500 -28.30700 18.66100
```

## Atoms and radius in the parameter file

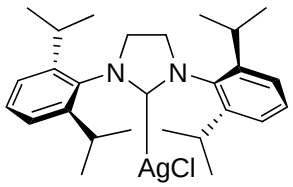
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
H -2.30884 4.45172 2.91896
```

## Results : Volumes in Angs^3

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
103.096 76.438 179.535 179.594
%V_Free %V_Bur % Tot/Ex
57.424 42.576 99.967
```

## The %V_Bur of your molecule is: 42.6

# *%$V_{bur}$ for AgCl(SIPr)*




## Molecule from input :

```
Molecule from input :
./temp/6565104801e58aa5d253c8e677229e14.c3d1
Number of atoms : 67
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 66 67
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.081
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C 29.19000 28.00600 -16.91400
C 29.93600 28.51500 -19.08600
C 28.41400 28.57100 -19.02900
C 31.60400 28.03700 -17.19300
C 32.15500 29.15900 -16.54900
C 33.41700 29.00800 -15.97100
C 34.09400 27.82100 -16.06000
C 33.58500 26.75200 -16.70500
C 32.29900 26.81900 -17.28200
C 31.68400 25.59200 -17.93900
C 32.62700 25.01100 -19.00900
C 31.29000 24.54000 -16.89400
C 31.40900 30.50800 -16.49200
C 32.18900 31.60300 -17.19500
C 31.14000 30.88600 -15.02100
C 26.74400 28.24100 -17.09800
C 26.25000 29.39500 -16.48600
C 24.92700 29.35300 -16.03400
C 24.15500 28.24500 -16.19800
C 24.67200 27.10800 -16.81600
C 25.96300 27.09400 -17.31100
C 26.51400 25.86000 -17.97700
C 26.60000 24.70600 -16.98300
C 25.68500 25.45400 -19.20000
C 27.09100 30.63300 -16.25700
C 27.28300 30.92500 -14.75200
C 26.48200 31.86400 -16.96300
H 30.25200 27.83800 -19.73500
H 30.32600 29.39600 -19.31400
H 28.01100 27.90400 -19.64000
H 28.08200 29.47200 -19.27100
H 33.81300 29.74000 -15.50900
H 34.94900 27.74900 -15.65300
H 34.09500 25.95200 -16.77200
H 30.84700 25.88400 -18.40300
H 33.49200 24.79700 -18.60100
H 32.23500 24.19700 -19.38600
H 32.75800 25.67200 -19.72200
H 30.69300 24.94600 -16.23100
H 30.82900 23.79600 -17.33600
H 32.09600 24.20400 -16.44800
H 30.53000 30.40100 -16.95600
```

```
H 32.30600 31.36600 -18.13800
H 31.69800 32.44700 -17.12900
H 33.06800 31.70000 -16.77200
H 30.57300 31.68400 -14.98700
H 30.68400 30.14300 -14.57100
H 31.99100 31.06900 -14.57000
H 24.56000 30.11500 -15.60300
H 23.25800 28.24700 -15.88800
H 24.13000 26.33400 -16.89800
H 27.44200 26.06700 -18.28900
H 25.69800 24.44700 -16.70300
H 27.04100 23.94000 -17.40900
H 27.11900 24.98700 -16.20100
H 25.67000 26.19200 -19.84500
H 26.08600 24.66400 -19.61900
H 24.76900 25.24600 -18.92000
H 27.99400 30.46900 -16.65500
H 27.76600 30.18000 -14.33600
H 27.79800 31.75100 -14.64200
H 26.40700 31.02600 -14.32600
H 25.59900 32.05500 -16.58300
H 27.06700 32.63900 -16.83000
H 26.39500 31.68100 -17.92100
N 30.25000 28.11600 -17.67200
N 28.09900 28.25600 -17.63100
```

## Atoms and radius in the parameter file

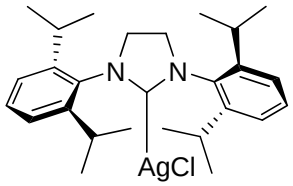
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

## Results : Volumes in Angs^3

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
100.627 78.908 179.535 179.594
%V_Free %V_Bur % Tot/Ex
56.049 43.951 99.967
```

## The %V_Bur of your molecule is: 44.0

***$\%V_{bur}^{average}$ for AgCl(IPr)***




## Molecule from input :

```
Molecule from input :
./temp/6565104801e58aa5d253c8e677229e14.c3d1
Number of atoms : 67
Atom that is coordinated : 1
```

Atoms that define the axis : 2
ID of these atoms : 66 67
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.073
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation

**Cartesian coordinates from input :**

C 29.19000 28.00600 -16.91400
C 29.93600 28.51500 -19.08600
C 28.41400 28.57100 -19.02900
C 31.60400 28.03700 -17.19300
C 32.15500 29.15900 -16.54900
C 33.41700 29.00800 -15.97100
C 34.09400 27.82100 -16.06000
C 33.58500 26.75200 -16.70500
C 32.29900 26.81900 -17.28200
C 31.68400 25.59200 -17.93900
C 32.62700 25.01100 -19.00900
C 31.29000 24.54000 -16.89400
C 31.40900 30.50800 -16.49200
C 32.18900 31.60300 -17.19500
C 31.14000 30.88600 -15.02100
C 26.74400 28.24100 -17.09800
C 26.25000 29.39500 -16.48600
C 24.92700 29.35300 -16.03400
C 24.15500 28.24500 -16.19800
C 24.67200 27.10800 -16.81600
C 25.96300 27.09400 -17.31100
C 26.51400 25.86000 -17.97700
C 26.60000 24.70600 -16.98300
C 25.68500 25.45400 -19.20000
C 27.09100 30.63300 -16.25700
C 27.28300 30.92500 -14.75200
C 26.48200 31.86400 -16.96300
H 30.25200 27.83800 -19.73500
H 30.32600 29.39600 -19.31400
H 28.01100 27.90400 -19.64000
H 28.08200 29.47200 -19.27100
H 33.81300 29.74000 -15.50900
H 34.94900 27.74900 -15.65300
H 34.09500 25.95200 -16.77200
H 30.84700 25.88400 -18.40300
H 33.49200 24.79700 -18.60100
H 32.23500 24.19700 -19.38600
H 32.75800 25.67200 -19.72200
H 30.69300 24.94600 -16.23100
H 30.82900 23.79600 -17.33600
H 32.09600 24.20400 -16.44800
H 30.53000 30.40100 -16.95600
H 32.30600 31.36600 -18.13800
H 31.69800 32.44700 -17.12900
H 33.06800 31.70000 -16.77200
H 30.57300 31.68400 -14.98700
H 30.68400 30.14300 -14.57100
H 31.99100 31.06900 -14.57000
H 24.56000 30.11500 -15.60300
H 23.25800 28.24700 -15.88800
H 24.13000 26.33400 -16.89800
H 27.44200 26.06700 -18.28900
H 25.69800 24.44700 -16.70300
H 27.04100 23.94000 -17.40900
H 27.11900 24.98700 -16.20100
H 25.67000 26.19200 -19.84500
H 26.08600 24.66400 -19.61900
H 24.76900 25.24600 -18.92000
H 27.99400 30.46900 -16.65500

```
H 27.76600 30.18000 -14.33600
H 27.79800 31.75100 -14.64200
H 26.40700 31.02600 -14.32600
H 25.59900 32.05500 -16.58300
H 27.06700 32.63900 -16.83000
H 26.39500 31.68100 -17.92100
N 30.25000 28.11600 -17.67200
N 28.09900 28.25600 -17.63100
```

**Atoms and radius in the parameter file**

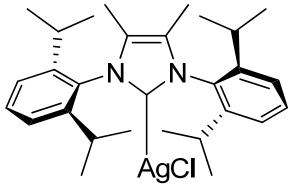
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

**Results : Volumes in Angs^3**

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
100.354 79.180 179.535 179.594
%V_Free %V_Bur % Tot/Ex
55.897 44.103 99.967
```

**The %V_Bur of your molecule is: 44.1**

# *%$V_{bur}$ for AgCl(IPr$^{Me}$)*




## Molecule from input :

```
Molecule from input :
./temp/656510480le58aa5d253c8e677229e14.c3d1
Number of atoms : 71
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 70 71
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.089
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C -33.28100 4.89100 14.38100
C -33.99600 6.49700 12.93300
C -32.69300 6.26600 12.66200
C -35.65900 5.51700 14.55500
C -36.08100 6.43900 15.51300
C -37.36700 6.26800 16.03300
C -38.17100 5.21700 15.62100
C -37.72600 4.32700 14.66700
C -36.45900 4.46900 14.08600
C -35.17400 7.54700 15.99000
C -34.34100 7.08800 17.19300
C -35.92300 8.84000 16.35800
C -36.00500 3.52800 12.97300
C -35.88800 2.09600 13.49000
C -36.93600 3.59800 11.77200
C -30.94500 4.72600 13.57400
C -29.98400 5.32500 14.38000
C -28.69000 4.80100 14.32500
C -28.38700 3.77300 13.46800
C -29.36000 3.18900 12.67400
C -30.67500 3.65000 12.71300
C -30.32400 6.42900 15.32900
C -29.30400 7.57100 15.29700
C -30.47500 5.90300 16.77000
C -31.76100 2.95800 11.91600
C -32.16200 1.64100 12.60000
C -31.37300 2.69300 10.46200
C -34.99500 7.40200 12.29500
C -31.77500 6.83700 11.63500
H -37.69500 6.88200 16.68000
H -39.03600 5.10900 15.99900
H -38.28600 3.60700 14.39900
H -34.54000 7.76300 15.24500
H -33.87200 6.25800 16.96900
H -33.68700 7.78100 17.42100
H -34.93200 6.93100 17.95900
H -36.45400 9.13900 15.58900
H -36.51700 8.66700 17.11800
H -35.27600 9.53500 16.59800
H -35.09800 3.82200 12.67500
H -35.28900 2.07800 14.26600
H -36.77300 1.77000 13.75400
```

```
H -35.52400 1.52300 12.78400
H -36.99800 4.52500 11.46000
H -36.58200 3.03400 11.05200
H -37.82600 3.27900 12.02900
H -28.01400 5.16100 14.88800
H -27.49300 3.45400 13.41900
H -29.13100 2.46900 12.09700
H -31.20700 6.80600 15.04900
H -29.20700 7.89500 14.37800
H -29.61500 8.30200 15.87200
H -28.43900 7.24400 15.62100
H -31.12600 5.17100 16.78400
H -29.60900 5.57600 17.09100
H -30.78700 6.62900 17.35100
H -32.56400 3.55500 11.91300
H -32.40900 1.82000 13.53200
H -32.92600 1.24900 12.12900
H -31.40700 1.01800 12.57500
H -31.10900 3.53600 10.03500
H -30.62200 2.06400 10.43500
H -32.13600 2.30900 9.98400
H -34.58000 7.86500 11.53700
H -35.75700 6.87600 11.97600
H -35.30500 8.06100 12.95000
H -32.23600 7.55100 11.14700
H -30.97900 7.20300 12.07400
H -31.50700 6.13300 11.00800
N -34.33500 5.65700 14.00300
N -32.28600 5.27900 13.56900
```

**Atoms and radius in the parameter file**

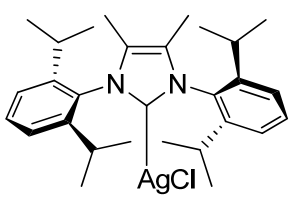
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

**Results : Volumes in Angs^3**

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
98.938 80.596 179.535 179.594
%V_Free %V_Bur % Tot/Ex
55.108 44.892 99.967
```

**The %V_Bur of your molecule is: 44.9**

***$\%V_{bur}^{average}$ for AgCl(IPr$^{Me}$)***




**Molecule from input :**

```
Molecule from input :
./temp/6565104801e58aa5d253c8e677229e14.c3d1
Number of atoms : 71
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 70 71
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.073
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

**Cartesian coordinates from input :**

```
C -33.28100 4.89100 14.38100
C -33.99600 6.49700 12.93300
C -32.69300 6.26600 12.66200
C -35.65900 5.51700 14.55500
C -36.08100 6.43900 15.51300
C -37.36700 6.26800 16.03300
C -38.17100 5.21700 15.62100
C -37.72600 4.32700 14.66700
C -36.45900 4.46900 14.08600
C -35.17400 7.54700 15.99000
C -34.34100 7.08800 17.19300
C -35.92300 8.84000 16.35800
C -36.00500 3.52800 12.97300
C -35.88800 2.09600 13.49000
C -36.93600 3.59800 11.77200
C -30.94500 4.72600 13.57400
C -29.98400 5.32500 14.38000
C -28.69000 4.80100 14.32500
C -28.38700 3.77300 13.46800
C -29.36000 3.18900 12.67400
C -30.67500 3.65000 12.71300
C -30.32400 6.42900 15.32900
C -29.30400 7.57100 15.29700
C -30.47500 5.90300 16.77000
C -31.76100 2.95800 11.91600
C -32.16200 1.64100 12.60000
C -31.37300 2.69300 10.46200
C -34.99500 7.40200 12.29500
C -31.77500 6.83700 11.63500
H -37.69500 6.88200 16.68000
H -39.03600 5.10900 15.99900
H -38.28600 3.60700 14.39900
H -34.54000 7.76300 15.24500
H -33.87200 6.25800 16.96900
H -33.68700 7.78100 17.42100
H -34.93200 6.93100 17.95900
H -36.45400 9.13900 15.58900
H -36.51700 8.66700 17.11800
H -35.27600 9.53500 16.59800
H -35.09800 3.82200 12.67500
H -35.28900 2.07800 14.26600
H -36.77300 1.77000 13.75400
H -35.52400 1.52300 12.78400
H -36.99800 4.52500 11.46000
H -36.58200 3.03400 11.05200
H -37.82600 3.27900 12.02900
H -28.01400 5.16100 14.88800
H -27.49300 3.45400 13.41900
H -29.13100 2.46900 12.09700
H -31.20700 6.80600 15.04900
H -29.20700 7.89500 14.37800
H -29.61500 8.30200 15.87200
H -28.43900 7.24400 15.62100
H -31.12600 5.17100 16.78400
H -29.60900 5.57600 17.09100
```

```
H -30.78700 6.62900 17.35100
H -32.56400 3.55500 11.91300
H -32.40900 1.82000 13.53200
H -32.92600 1.24900 12.12900
H -31.40700 1.01800 12.57500
H -31.10900 3.53600 10.03500
H -30.62200 2.06400 10.43500
H -32.13600 2.30900 9.98400
H -34.58000 7.86500 11.53700
H -35.75700 6.87600 11.97600
H -35.30500 8.06100 12.95000
H -32.23600 7.55100 11.14700
H -30.97900 7.20300 12.07400
H -31.50700 6.13300 11.00800
N -34.33500 5.65700 14.00300
N -32.28600 5.27900 13.56900
```

**Atoms and radius in the parameter file**

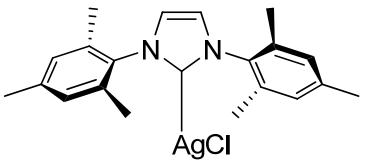
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

**Results : Volumes in Angs^3**

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
98.386 81.148 179.535 179.594
%V_Free %V_Bur % Tot/Ex
54.801 45.199 99.967
```

**The %V_Bur of your molecule is: 45.2**

# *%$V_{bur}$ for AgCl(IMes)*




## Molecule from input :

```
Molecule from input :
./temp/6565104801e58aa5d253c8e677229e14.c3d1
Number of atoms : 47
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 46 47
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.056
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C 3.10000 47.55800 13.38800
C 0.69300 47.93800 13.22900
C 5.51900 47.62800 13.06300
C 0.15200 48.64400 14.30400
C 6.04800 46.48900 12.45500
C -0.01000 46.93300 12.56100
C 6.21500 48.35200 14.03400
C -1.28900 46.62500 13.03700
C 7.47200 47.86800 14.41200
C 0.91600 49.76200 14.97100
C 5.29500 45.75800 11.37000
C 0.58000 46.19500 11.37600
C 5.63800 49.60300 14.66400
C -1.83700 47.26100 14.12600
C 8.00600 46.72000 13.87400
C -1.10900 48.28100 14.75400
C 7.28700 46.03500 12.88500
C -3.20000 46.84300 14.65200
C 9.34200 46.19400 14.36700
C 2.45900 49.08200 11.83600
C 3.82200 48.97400 11.77000
H 1.88400 49.57600 11.39500
H 4.42100 49.36200 11.26000
H -1.79500 45.95400 12.59400
H 7.97300 48.34800 15.06100
H 1.13900 50.44700 14.30700
H 5.10700 46.37300 10.63100
H 1.74100 49.40500 15.36300
H 4.45000 45.41500 11.73200
H 0.36400 50.15900 15.67600
H 5.83700 45.01100 11.04200
H 1.30100 45.60700 11.68400
H 4.89400 49.35900 15.25400
H 0.93900 46.84200 10.73400
H 5.31300 50.20400 13.96200
H -0.11800 45.65800 10.94500
H 6.33400 50.05600 15.18600
H -1.48700 48.73100 15.50200
H 7.65600 45.24700 12.50300
H -3.82000 47.60000 14.58800
H 9.98400 46.18400 13.62600
H -3.11700 46.56600 15.58900
```

```
H 9.22800 45.28300 14.71200
H -3.53900 46.09500 14.11800
H 9.67800 46.77400 15.08300
N 2.04700 48.20900 12.83000
N 4.18300 48.03800 12.72700
```

## Atoms and radius in the parameter file

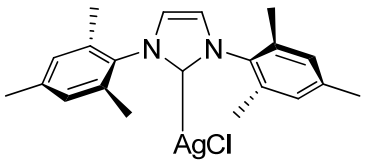
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

## Results : Volumes in Angs^3

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
116.480 63.055 179.535 179.594
%V_Free %V_Bur % Tot/Ex
64.879 35.121 99.967
```

## The %V_Bur of your molecule is: 35.1

***$\%V_{bur}^{average}$ for AgCl(IMes)***




## Molecule from input :

```
Molecule from input :
./temp/6565104801e58aa5d253c8e677229e14.c3d1
Number of atoms : 47
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 46 47
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.073
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C 3.10000 47.55800 13.38800
C 0.69300 47.93800 13.22900
C 5.51900 47.62800 13.06300
C 0.15200 48.64400 14.30400
C 6.04800 46.48900 12.45500
C -0.01000 46.93300 12.56100
C 6.21500 48.35200 14.03400
C -1.28900 46.62500 13.03700
C 7.47200 47.86800 14.41200
C 0.91600 49.76200 14.97100
```

```
C 5.29500 45.75800 11.37000
C 0.58000 46.19500 11.37600
C 5.63800 49.60300 14.66400
C -1.83700 47.26100 14.12600
C 8.00600 46.72000 13.87400
C -1.10900 48.28100 14.75400
C 7.28700 46.03500 12.88500
C -3.20000 46.84300 14.65200
C 9.34200 46.19400 14.36700
C 2.45900 49.08200 11.83600
C 3.82200 48.97400 11.77000
H 1.88400 49.57600 11.39500
H 4.42100 49.36200 11.26000
H -1.79500 45.95400 12.59400
H 7.97300 48.34800 15.06100
H 1.13900 50.44700 14.30700
H 5.10700 46.37300 10.63100
H 1.74100 49.40500 15.36300
H 4.45000 45.41500 11.73200
H 0.36400 50.15900 15.67600
H 5.83700 45.01100 11.04200
H 1.30100 45.60700 11.68400
H 4.89400 49.35900 15.25400
H 0.93900 46.84200 10.73400
H 5.31300 50.20400 13.96200
H -0.11800 45.65800 10.94500
H 6.33400 50.05600 15.18600
H -1.48700 48.73100 15.50200
H 7.65600 45.24700 12.50300
H -3.82000 47.60000 14.58800
H 9.98400 46.18400 13.62600
H -3.11700 46.56600 15.58900
H 9.22800 45.28300 14.71200
H -3.53900 46.09500 14.11800
H 9.67800 46.77400 15.08300
N 2.04700 48.20900 12.83000
N 4.18300 48.03800 12.72700
```

**Atoms and radius in the parameter file**

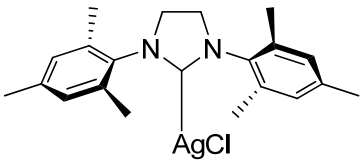
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

**Results : Volumes in Angs^3**

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
117.055 62.479 179.535 179.594
%V_Free %V_Bur % Tot/Ex
65.199 34.801 99.967
```

**The %V_Bur of your molecule is: 34.8**

# *%$V_{bur}$ for AgCl(SIMes)*




## Molecule from input :

```
Molecule from input :
./temp/6565104801e58aa5d253c8e677229e14.c3d1
Number of atoms : 49
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 48 49
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.083
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C -20.49600 -17.74600 4.07900
C -19.74500 -15.96900 2.73300
C -21.26800 -16.03600 2.66200
C -18.05600 -17.49200 3.87000
C -22.91800 -17.70500 3.64100
C -17.37700 -16.97700 4.98100
C -23.74000 -17.25600 4.68100
C -16.05300 -17.35600 5.16400
C -25.03700 -17.75000 4.74100
C -15.39600 -18.19300 4.26900
C -25.53200 -18.63700 3.79200
C -16.10100 -18.67900 3.18400
C -24.68800 -19.05600 2.78000
C -17.43900 -18.35500 2.96500
C -23.36900 -18.61500 2.68600
C -18.20100 -18.94900 1.80800
C -22.45300 -19.13500 1.60700
C -13.94200 -18.55600 4.48200
C -26.96200 -19.12700 3.86900
C -18.07400 -16.05700 5.94600
C -23.21900 -16.28300 5.70400
H -19.33700 -16.09200 1.84000
H -21.57900 -16.19000 1.73500
H -19.44000 -15.10700 3.11400
H -21.68200 -15.20600 3.00800
H -15.58100 -17.03300 5.92300
H -25.60400 -17.47300 5.45200
H -15.65900 -19.25200 2.56800
H -25.01900 -19.66200 2.12700
H -18.93000 -19.50900 2.14800
H -21.71400 -19.63100 2.01700
H -17.59600 -19.49500 1.26400
H -22.95400 -19.73000 1.01200
H -18.57300 -18.22800 1.25700
H -22.09600 -18.38300 1.09100
H -13.76400 -19.43300 4.08200
H -27.02400 -20.01400 3.45700
H -13.75100 -18.59100 5.44200
H -27.23800 -19.18200 4.80700
H -13.37200 -17.88100 4.05900
H -27.54700 -18.50200 3.39200
H -18.58900 -15.38900 5.44600
```

```
H -22.72100 -15.57000 5.25200
H -17.40900 -15.60600 6.50600
H -23.97200 -15.89400 6.19700
H -18.68000 -16.57700 6.51300
H -22.62700 -16.75000 6.32700
N -19.42000 -17.10000 3.63300
N -21.57700 -17.19400 3.53200
```

## Atoms and radius in the parameter file

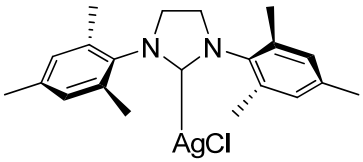
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

## Results : Volumes in Angs^3

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
117.575 61.960 179.535 179.594
%V_Free %V_Bur % Tot/Ex
65.489 34.511 99.967
```

## The %V_Bur of your molecule is: 34.5

***$\%V_{bur}^{average}$ for AgCl(SIMes)***




## Molecule from input :

```
Molecule from input :
./temp/656510480le58aa5d253c8e677229e14.c3d1
Number of atoms : 49
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 48 49
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 2.073
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C -20.49600 -17.74600 4.07900
C -19.74500 -15.96900 2.73300
C -21.26800 -16.03600 2.66200
C -18.05600 -17.49200 3.87000
C -22.91800 -17.70500 3.64100
C -17.37700 -16.97700 4.98100
C -23.74000 -17.25600 4.68100
C -16.05300 -17.35600 5.16400
C -25.03700 -17.75000 4.74100
```

```
C -15.39600 -18.19300 4.26900
C -25.53200 -18.63700 3.79200
C -16.10100 -18.67900 3.18400
C -24.68800 -19.05600 2.78000
C -17.43900 -18.35500 2.96500
C -23.36900 -18.61500 2.68600
C -18.20100 -18.94900 1.80800
C -22.45300 -19.13500 1.60700
C -13.94200 -18.55600 4.48200
C -26.96200 -19.12700 3.86900
C -18.07400 -16.05700 5.94600
C -23.21900 -16.28300 5.70400
H -19.33700 -16.09200 1.84000
H -21.57900 -16.19000 1.73500
H -19.44000 -15.10700 3.11400
H -21.68200 -15.20600 3.00800
H -15.58100 -17.03300 5.92300
H -25.60400 -17.47300 5.45200
H -15.65900 -19.25200 2.56800
H -25.01900 -19.66200 2.12700
H -18.93000 -19.50900 2.14800
H -21.71400 -19.63100 2.01700
H -17.59600 -19.49500 1.26400
H -22.95400 -19.73000 1.01200
H -18.57300 -18.22800 1.25700
H -22.09600 -18.38300 1.09100
H -13.76400 -19.43300 4.08200
H -27.02400 -20.01400 3.45700
H -13.75100 -18.59100 5.44200
H -27.23800 -19.18200 4.80700
H -13.37200 -17.88100 4.05900
H -27.54700 -18.50200 3.39200
H -18.58900 -15.38900 5.44600
H -22.72100 -15.57000 5.25200
H -17.40900 -15.60600 6.50600
H -23.97200 -15.89400 6.19700
H -18.68000 -16.57700 6.51300
H -22.62700 -16.75000 6.32700
N -19.42000 -17.10000 3.63300
N -21.57700 -17.19400 3.53200
```

**Atoms and radius in the parameter file**

```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

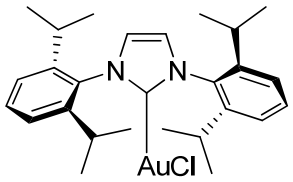
**Results : Volumes in Angs^3**

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
117.220 62.314 179.535 179.594
%V_Free %V_Bur % Tot/Ex
65.291 34.709 99.967
```

**The %V_Bur of your molecule is: 34.7**

# III. SambVca calculations for AuCl(NHC) complexes

## *%$V_{bur}$ for AuCl(IPr)*




### Molecule from input :

```
Molecule from input :
./temp/c63b235b0e5bca5b5243d9a158cf8859.c3d1
Number of atoms : 65
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 64 65
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 1.942
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

### Cartesian coordinates from input :

```
C -1.09600 29.57000 -28.72100
C 0.17900 27.70700 -29.00200
C -1.09400 27.24800 -28.91200
C 1.35000 29.97300 -28.90200
C 2.04400 30.31700 -27.86100
C 3.09600 31.08100 -27.82700
C 3.53700 31.73200 -29.15300
C 2.75500 31.38600 -30.22500
C 1.70000 30.56500 -30.28500
C 0.94100 30.28800 -31.47000
C 0.12700 31.37300 -32.02000
C 1.87800 29.64000 -32.63200
C 1.61700 29.59700 -26.45100
C 2.90500 29.13200 -25.65500
C 1.08000 30.77900 -25.54000
C -3.27600 28.42200 -28.58300
C -3.80900 28.52200 -27.45200
C -5.24700 28.53000 -27.29900
C -5.94100 28.45400 -28.52000
C -5.44300 28.35300 -29.62600
C -3.97100 28.27000 -29.90800
C -3.41100 28.23000 -31.18800
C -3.83500 27.02200 -31.93200
C -3.29500 29.52200 -31.92900
C -2.97000 28.62000 -26.08800
C -3.34500 30.02600 -25.47200
C -3.26700 27.56800 -25.20200
H 0.93100 27.17200 -29.12000
H -1.40300 26.37100 -28.95100
H 3.56300 31.22700 -27.03500
H 4.26200 32.31100 -29.21900
H 2.99300 31.78200 -31.03100
H 0.30800 29.58400 -31.21800
H -0.51200 31.65900 -31.36300
H -0.33700 31.06000 -32.80100
H 0.69200 32.11000 -32.25800
H 1.37800 29.57300 -33.44800
```

```
H 2.16800 28.76600 -32.36100
H 2.64700 30.20000 -32.77500
H 0.96200 28.87800 -26.57000
H 3.38700 29.90400 -25.34900
H 3.46600 28.61100 -26.23200
H 2.64200 28.59900 -24.90200
H 0.80900 30.43000 -24.68900
H 0.33100 31.19700 -25.97000
H 1.77800 31.42700 -25.41300
H -5.67100 28.58200 -26.47300
H -6.87000 28.48500 -28.47900
H -6.02100 28.32500 -30.35500
H -2.47300 28.02600 -30.99100
H -3.62300 26.23900 -31.41900
H -3.37600 26.98700 -32.77400
H -4.78300 27.05700 -32.08600
H -4.17200 29.88200 -32.08500
H -2.85600 29.37200 -32.76900
H -2.78300 30.14500 -31.40700
H -2.01300 28.60500 -26.29800
H -4.26600 30.02000 -25.20300
H -3.20700 30.71100 -26.12900
H -2.78900 30.19900 -24.70800
H -4.15300 27.68500 -24.85500
H -2.63600 27.57100 -24.48000
H -3.21400 26.73100 -25.67000
N 0.20200 29.14500 -28.89300
N -1.79900 28.38900 -28.75000
```

**Atoms and radius in the parameter file**

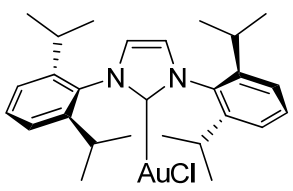
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
H -1.60993 -4.39163 -4.27936
```

**Results : Volumes in Angs^3**

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
97.598 81.936 179.535 179.594
%V_Free %V_Bur % Tot/Ex
54.362 45.638 99.967
```

**The %V_Bur of your molecule is: 45.6**

***$\%V_{bur}^{average}$ for AuCl(IPr)***




**Molecule from input :**

```
Molecule from input :
./temp/c63b235b0e5bca5b5243d9a158cf8859.c3d1
Number of atoms : 65
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 64 65
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 1.981
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

**Cartesian coordinates from input :**

```
C -1.09600 29.57000 -28.72100
C 0.17900 27.70700 -29.00200
C -1.09400 27.24800 -28.91200
C 1.35000 29.97300 -28.90200
C 2.04400 30.31700 -27.86100
C 3.09600 31.08100 -27.82700
C 3.53700 31.73200 -29.15300
C 2.75500 31.38600 -30.22500
C 1.70000 30.56500 -30.28500
C 0.94100 30.28800 -31.47000
C 0.12700 31.37300 -32.02000
C 1.87800 29.64000 -32.63200
C 1.61700 29.59700 -26.45100
C 2.90500 29.13200 -25.65500
C 1.08000 30.77900 -25.54000
C -3.27600 28.42200 -28.58300
C -3.80900 28.52200 -27.45200
C -5.24700 28.53000 -27.29900
C -5.94100 28.45400 -28.52000
C -5.44300 28.35300 -29.62600
C -3.97100 28.27000 -29.90800
C -3.41100 28.23000 -31.18800
C -3.83500 27.02200 -31.93200
C -3.29500 29.52200 -31.92900
C -2.97000 28.62000 -26.08800
C -3.34500 30.02600 -25.47200
C -3.26700 27.56800 -25.20200
H 0.93100 27.17200 -29.12000
H -1.40300 26.37100 -28.95100
H 3.56300 31.22700 -27.03500
H 4.26200 32.31100 -29.21900
H 2.99300 31.78200 -31.03100
H 0.30800 29.58400 -31.21800
H -0.51200 31.65900 -31.36300
H -0.33700 31.06000 -32.80100
H 0.69200 32.11000 -32.25800
H 1.37800 29.57300 -33.44800
H 2.16800 28.76600 -32.36100
H 2.64700 30.20000 -32.77500
H 0.96200 28.87800 -26.57000
H 3.38700 29.90400 -25.34900
H 3.46600 28.61100 -26.23200
H 2.64200 28.59900 -24.90200
H 0.80900 30.43000 -24.68900
H 0.33100 31.19700 -25.97000
H 1.77800 31.42700 -25.41300
H -5.67100 28.58200 -26.47300
H -6.87000 28.48500 -28.47900
H -6.02100 28.32500 -30.35500
H -2.47300 28.02600 -30.99100
H -3.62300 26.23900 -31.41900
H -3.37600 26.98700 -32.77400
H -4.78300 27.05700 -32.08600
H -4.17200 29.88200 -32.08500
H -2.85600 29.37200 -32.76900
```

```
H -2.78300 30.14500 -31.40700
H -2.01300 28.60500 -26.29800
H -4.26600 30.02000 -25.20300
H -3.20700 30.71100 -26.12900
H -2.78900 30.19900 -24.70800
H -4.15300 27.68500 -24.85500
H -2.63600 27.57100 -24.48000
H -3.21400 26.73100 -25.67000
N 0.20200 29.14500 -28.89300
N -1.79900 28.38900 -28.75000
```

## Atoms and radius in the parameter file

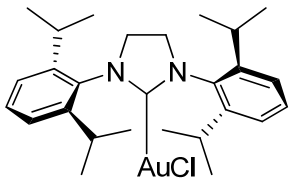
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
H -1.59647 -4.42795 -4.28391
```

## Results : Volumes in Angs^3

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
98.959 80.576 179.535 179.594
%V_Free %V_Bur % Tot/Ex
55.120 44.880 99.967
```

## The %V_Bur of your molecule is: 44.9

# *%$V_{bur}$ for AuCl(SIPr)*




## Molecule from input :

```
Molecule from input :
./temp/c63b235b0e5bca5b5243d9a158cf8859.c3d1
Number of atoms : 67
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 66 67
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 1.982
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C 8.86800 -10.84100 -28.87300
C 9.04300 -9.79400 -30.96900
C 10.16400 -10.83500 -30.83200
C 7.26500 -9.04100 -29.28600
C 10.65200 -12.51000 -28.95900
C 7.50700 -7.85500 -28.58300
C 10.22300 -13.83000 -29.14900
C 6.39500 -7.09700 -28.20700
C 10.98300 -14.84000 -28.55200
C 5.11700 -7.48000 -28.55700
C 12.13200 -14.55000 -27.84700
C 4.90900 -8.63600 -29.28600
C 12.55400 -13.24100 -27.70800
C 5.98000 -9.45000 -29.65700
C 11.81500 -12.18900 -28.25100
C 12.24900 -10.75500 -28.02500
C 5.72900 -10.75300 -30.38900
C 11.97500 -10.33600 -26.57700
C 5.13300 -11.79500 -29.43800
C 13.70700 -10.52900 -28.39900
C 4.85400 -10.56300 -31.61900
C 8.90000 -7.38500 -28.22400
C 8.99300 -14.18400 -29.95500
C 9.16700 -7.52700 -26.71900
C 7.85100 -14.66800 -29.05000
C 9.15700 -5.95200 -28.68300
C 9.29600 -15.21600 -31.03700
H 8.42100 -10.03000 -31.70100
H 11.05600 -10.40600 -30.84300
H 9.41100 -8.89000 -31.13300
H 10.11800 -11.50800 -31.55600
H 6.52100 -6.30400 -27.70000
H 10.70200 -15.74400 -28.63400
H 4.37600 -6.94600 -28.29500
H 12.63600 -15.25400 -27.45500
H 4.02600 -8.87900 -29.53800
H 13.35700 -13.05500 -27.23700
H 6.61500 -11.09900 -30.70000
H 11.69200 -10.17400 -28.61800
H 12.56200 -10.83800 -25.97500
H 4.23100 -11.51700 -29.17400
H 12.14800 -9.37700 -26.47700
```

```
H 5.08800 -12.66200 -29.89100
H 11.04000 -10.52500 -26.35400
H 5.69800 -11.87100 -28.64200
H 13.85200 -10.80700 -29.32600
H 5.25700 -9.89100 -32.20600
H 13.92400 -9.57700 -28.30600
H 4.77800 -11.41400 -32.10100
H 14.28200 -11.05400 -27.80500
H 3.96200 -10.26300 -31.34300
H 9.55000 -7.97600 -28.70200
H 8.68200 -13.35000 -30.41100
H 9.03600 -8.46000 -26.45000
H 7.64500 -13.97700 -28.38700
H 10.08800 -7.25600 -26.52300
H 7.05700 -14.84800 -29.59400
H 8.54700 -6.95400 -26.22200
H 8.12500 -15.48900 -28.59000
H 8.54000 -5.34600 -28.22200
H 9.59300 -16.05100 -30.61900
H 10.08000 -5.70300 -28.47000
H 8.48500 -15.38500 -31.56200
H 9.01700 -5.88900 -29.65100
H 10.00100 -14.87600 -31.62700
N 8.37700 -9.87400 -29.64600
N 9.87100 -11.44200 -29.51100
```

**Atoms and radius in the parameter file**

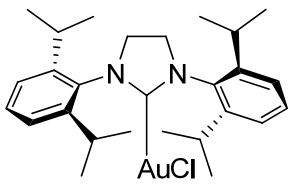
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

**Results : Volumes in Angs^3**

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
94.456 85.079 179.535 179.594
%V_Free %V_Bur % Tot/Ex
52.611 47.389 99.967
```

**The %V_Bur of your molecule is: 47.4**

***$\%V_{bur}^{average}$ for AuCl(SIPr)***




**Molecule from input :**

```
Molecule from input :
./temp/bf8bd1d07000506acaa6690ac92a3217.c3d1
Number of atoms : 67
```

```
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 66 67
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 1.981
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

**Cartesian coordinates from input :**

```
C 8.86800 -10.84100 -28.87300
C 9.04300 -9.79400 -30.96900
C 10.16400 -10.83500 -30.83200
C 7.26500 -9.04100 -29.28600
C 10.65200 -12.51000 -28.95900
C 7.50700 -7.85500 -28.58300
C 10.22300 -13.83000 -29.14900
C 6.39500 -7.09700 -28.20700
C 10.98300 -14.84000 -28.55200
C 5.11700 -7.48000 -28.55700
C 12.13200 -14.55000 -27.84700
C 4.90900 -8.63600 -29.28600
C 12.55400 -13.24100 -27.70800
C 5.98000 -9.45000 -29.65700
C 11.81500 -12.18900 -28.25100
C 12.24900 -10.75500 -28.02500
C 5.72900 -10.75300 -30.38900
C 11.97500 -10.33600 -26.57700
C 5.13300 -11.79500 -29.43800
C 13.70700 -10.52900 -28.39900
C 4.85400 -10.56300 -31.61900
C 8.90000 -7.38500 -28.22400
C 8.99300 -14.18400 -29.95500
C 9.16700 -7.52700 -26.71900
C 7.85100 -14.66800 -29.05000
C 9.15700 -5.95200 -28.68300
C 9.29600 -15.21600 -31.03700
H 8.42100 -10.03000 -31.70100
H 11.05600 -10.40600 -30.84300
H 9.41100 -8.89000 -31.13300
H 10.11800 -11.50800 -31.55600
H 6.52100 -6.30400 -27.70000
H 10.70200 -15.74400 -28.63400
H 4.37600 -6.94600 -28.29500
H 12.63600 -15.25400 -27.45500
H 4.02600 -8.87900 -29.53800
H 13.35700 -13.05500 -27.23700
H 6.61500 -11.09900 -30.70000
H 11.69200 -10.17400 -28.61800
H 12.56200 -10.83800 -25.97500
H 4.23100 -11.51700 -29.17400
H 12.14800 -9.37700 -26.47700
H 5.08800 -12.66200 -29.89100
H 11.04000 -10.52500 -26.35400
H 5.69800 -11.87100 -28.64200
H 13.85200 -10.80700 -29.32600
H 5.25700 -9.89100 -32.20600
H 13.92400 -9.57700 -28.30600
H 4.77800 -11.41400 -32.10100
H 14.28200 -11.05400 -27.80500
H 3.96200 -10.26300 -31.34300
H 9.55000 -7.97600 -28.70200
H 8.68200 -13.35000 -30.41100
H 9.03600 -8.46000 -26.45000
H 7.64500 -13.97700 -28.38700
H 10.08800 -7.25600 -26.52300
H 7.05700 -14.84800 -29.59400
H 8.54700 -6.95400 -26.22200
```

```
H 8.12500 -15.48900 -28.59000
H 8.54000 -5.34600 -28.22200
H 9.59300 -16.05100 -30.61900
H 10.08000 -5.70300 -28.47000
H 8.48500 -15.38500 -31.56200
H 9.01700 -5.88900 -29.65100
H 10.00100 -14.87600 -31.62700
N 8.37700 -9.87400 -29.64600
N 9.87100 -11.44200 -29.51100
```

## Atoms and radius in the parameter file

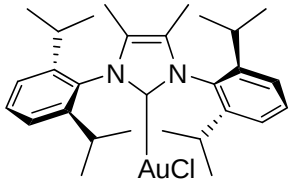
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

## Results : Volumes in Angs^3

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
94.418 85.117 179.535 179.594
%V_Free %V_Bur % Tot/Ex
52.590 47.410 99.967
```

## The %V_Bur of your molecule is: 47.4

# *%$V_{bur}$ for AuCl(IPr$^{Me}$)*




## Molecule from input :

```
Molecule from input :
./temp/c63b235b0e5bca5b5243d9a158cf8859.c3d1
Number of atoms : 71
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 70 71
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 1.997
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C -31.62900 -18.04400 26.81600
C -31.88400 -15.83900 26.48100
C -30.57500 -16.11300 26.37000
C -33.95500 -17.15400 27.02400
C -29.14000 -18.16100 26.61900
C -34.82400 -17.31600 25.94400
C -28.59300 -18.61900 25.41900
C -27.37300 -19.23500 25.49700
C -36.15800 -17.39800 26.23700
C -26.73300 -19.40500 26.70500
C -36.61100 -17.34000 27.53700
C -35.74000 -17.19100 28.58500
C -27.29200 -18.95700 27.87400
C -34.38200 -17.07800 28.34700
C -28.51200 -18.30500 27.85200
C -33.40300 -16.88100 29.51300
C -29.13100 -17.77400 29.15300
C -33.78300 -15.68000 30.36700
C -28.17400 -16.85200 29.89400
C -33.35300 -18.18000 30.37800
C -29.55500 -18.97300 30.05900
C -34.33400 -17.41500 24.51800
C -29.30300 -18.46700 24.09500
C -34.32200 -18.84100 24.04700
C -29.95700 -19.75300 23.67900
C -35.09100 -16.52300 23.56600
C -28.41700 -17.91800 23.00400
C -32.63900 -14.54400 26.39200
C -29.39100 -15.22300 26.11900
H -26.95900 -19.55100 24.70300
H -36.78500 -17.49600 25.53000
H -25.88900 -19.84200 26.72800
H -37.54300 -17.40500 27.70900
H -26.84200 -19.09400 28.69900
H -36.06900 -17.16400 29.47600
H -32.49200 -16.72100 29.13400
H -29.95200 -17.25200 28.92000
H -33.80600 -14.87600 29.80700
H -27.92200 -16.10600 29.31100
H -33.11800 -15.56200 31.07900
H -28.61300 -16.50400 30.69900
H -34.66500 -15.82800 30.76500
```

```
H -27.37200 -17.35200 30.15100
H -33.09900 -18.93900 29.81200
H -30.17700 -19.54900 29.56600
H -34.23300 -18.34500 30.77200
H -28.76200 -19.48800 30.31100
H -32.69000 -18.07000 31.09200
H -29.99600 -18.63300 30.86500
H -33.38400 -17.10100 24.51600
H -30.03700 -17.80100 24.23400
H -33.81600 -19.38900 24.68200
H -30.53000 -20.07600 24.40500
H -33.89900 -18.88900 23.16400
H -30.50000 -19.60000 22.87800
H -35.24100 -19.17300 23.98800
H -29.26800 -20.42200 23.48500
H -35.07300 -15.60100 23.89800
H -28.01400 -17.07700 23.30400
H -36.02000 -16.82900 23.50100
H -27.71000 -18.56600 22.80200
H -34.67200 -16.56000 22.68100
H -28.95300 -17.75600 22.20000
H -32.00500 -13.80000 26.33100
H -29.67800 -14.28600 26.13500
H -33.19500 -14.43400 27.19200
H -28.71700 -15.37000 26.81500
H -33.21000 -14.55200 25.59700
H -29.00700 -15.43100 25.24300
N -32.50900 -17.04000 26.75300
N -30.44400 -17.47100 26.57900
```

**Atoms and radius in the parameter file**

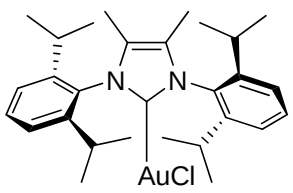
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

**Results : Volumes in Angs^3**

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
99.653 79.881 179.535 179.594
%V_Free %V_Bur % Tot/Ex
55.506 44.494 99.967
```

**The %V_Bur of your molecule is: 44.5**

***$\%V_{bur}^{average}$ for AuCl(IPr$^{Me}$)***




**Molecule from input :**

```
Molecule from input :
./temp/bf8bd1d07000506acaa6690ac92a3217.c3d1
Number of atoms : 71
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 70 71
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 1.981
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

**Cartesian coordinates from input :**

```
C -31.62900 -18.04400 26.81600
C -31.88400 -15.83900 26.48100
C -30.57500 -16.11300 26.37000
C -33.95500 -17.15400 27.02400
C -29.14000 -18.16100 26.61900
C -34.82400 -17.31600 25.94400
C -28.59300 -18.61900 25.41900
C -27.37300 -19.23500 25.49700
C -36.15800 -17.39800 26.23700
C -26.73300 -19.40500 26.70500
C -36.61100 -17.34000 27.53700
C -35.74000 -17.19100 28.58500
C -27.29200 -18.95700 27.87400
C -34.38200 -17.07800 28.34700
C -28.51200 -18.30500 27.85200
C -33.40300 -16.88100 29.51300
C -29.13100 -17.77400 29.15300
C -33.78300 -15.68000 30.36700
C -28.17400 -16.85200 29.89400
C -33.35300 -18.18000 30.37800
C -29.55500 -18.97300 30.05900
C -34.33400 -17.41500 24.51800
C -29.30300 -18.46700 24.09500
C -34.32200 -18.84100 24.04700
C -29.95700 -19.75300 23.67900
C -35.09100 -16.52300 23.56600
C -28.41700 -17.91800 23.00400
C -32.63900 -14.54400 26.39200
C -29.39100 -15.22300 26.11900
H -26.95900 -19.55100 24.70300
H -36.78500 -17.49600 25.53000
H -25.88900 -19.84200 26.72800
H -37.54300 -17.40500 27.70900
H -26.84200 -19.09400 28.69900
H -36.06900 -17.16400 29.47600
H -32.49200 -16.72100 29.13400
H -29.95200 -17.25200 28.92000
H -33.80600 -14.87600 29.80700
H -27.92200 -16.10600 29.31100
H -33.11800 -15.56200 31.07900
H -28.61300 -16.50400 30.69900
H -34.66500 -15.82800 30.76500
H -27.37200 -17.35200 30.15100
H -33.09900 -18.93900 29.81200
H -30.17700 -19.54900 29.56600
H -34.23300 -18.34500 30.77200
H -28.76200 -19.48800 30.31100
H -32.69000 -18.07000 31.09200
H -29.99600 -18.63300 30.86500
H -33.38400 -17.10100 24.51600
H -30.03700 -17.80100 24.23400
H -33.81600 -19.38900 24.68200
H -30.53000 -20.07600 24.40500
H -33.89900 -18.88900 23.16400
H -30.50000 -19.60000 22.87800
```

```
H -35.24100 -19.17300 23.98800
H -29.26800 -20.42200 23.48500
H -35.07300 -15.60100 23.89800
H -28.01400 -17.07700 23.30400
H -36.02000 -16.82900 23.50100
H -27.71000 -18.56600 22.80200
H -34.67200 -16.56000 22.68100
H -28.95300 -17.75600 22.20000
H -32.00500 -13.80000 26.33100
H -29.67800 -14.28600 26.13500
H -33.19500 -14.43400 27.19200
H -28.71700 -15.37000 26.81500
H -33.21000 -14.55200 25.59700
H -29.00700 -15.43100 25.24300
N -32.50900 -17.04000 26.75300
N -30.44400 -17.47100 26.57900
```

**Atoms and radius in the parameter file**

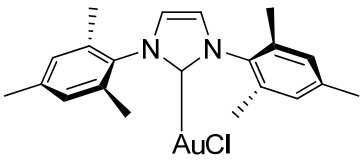
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

**Results : Volumes in Angs^3**

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
99.099 80.435 179.535 179.594
%V_Free %V_Bur % Tot/Ex
55.198 44.802 99.967
```

**The %V_Bur of your molecule is: 44.8**

# *%$V_{bur}$ for AuCl(IMes)*




## Molecule from input :

```
Molecule from input :
./temp/c63b235b0e5bca5b5243d9a158cf8859.c3d1
Number of atoms : 47
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 46 47
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 1.999
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C -44.01600 -7.11900 31.09500
C -44.69300 -5.38600 29.85700
C -43.32900 -5.36800 29.88800
C -46.43900 -6.92800 30.83100
C -41.59100 -6.81600 31.01200
C -47.11500 -6.49000 31.96700
C -40.91700 -7.73800 30.21500
C -48.38300 -7.03800 32.22800
C -39.65200 -8.17400 30.64500
C -39.07500 -7.65400 31.80300
C -48.96200 -7.94700 31.34300
C -39.76200 -6.71200 32.54100
C -48.27200 -8.32400 30.20900
C -46.99200 -7.83600 29.92300
C -41.04000 -6.27300 32.17500
C -46.51200 -5.47100 32.89800
C -41.51800 -8.26400 28.93900
C -37.72100 -8.14400 32.26200
C -50.31800 -8.53900 31.64400
C -46.25000 -8.28600 28.69900
C -41.78000 -5.27200 33.01300
H -45.31100 -4.74000 29.39500
H -42.70700 -4.71700 29.43900
H -48.91600 -6.69200 32.98200
H -39.15500 -8.74300 30.10100
H -39.39500 -6.39900 33.23800
H -48.64000 -8.87100 29.67600
H -46.30700 -4.69200 32.46600
H -41.71900 -7.59200 28.35200
H -45.53700 -5.70900 33.08000
H -42.49500 -8.51200 29.09800
H -46.98300 -5.26300 33.55800
H -41.04900 -8.81600 28.52000
H -41.18800 -4.92000 33.76600
H -46.84300 -8.87200 28.11100
H -37.67500 -8.93600 32.36600
H -50.36800 -8.90600 32.35400
H -37.43600 -7.81200 33.03900
H -50.60400 -9.15700 31.06700
H -37.14600 -8.01900 31.64800
H -50.89100 -7.91800 31.73400
H -45.46600 -9.00700 28.90400
H -42.56800 -5.70700 33.61900
```

```
H -45.90700 -7.55200 28.20600
H -42.11800 -4.55700 32.49000
N -45.08800 -6.48400 30.60900
N -42.94000 -6.45100 30.66600
```

## Atoms and radius in the parameter file

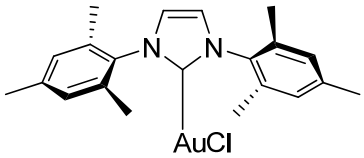
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

## Results : Volumes in Angs^3

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
113.939 65.595 179.535 179.594
%V_Free %V_Bur % Tot/Ex
63.464 36.536 99.967
```

## The %V_Bur of your molecule is: 36.5

***$\%V_{bur}^{average}$ for AuCl(IMes)***




## Molecule from input :

```
Molecule from input :
./temp/c63b235b0e5bca5b5243d9a158cf8859.c3d1
Number of atoms : 47
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 46 47
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 1.981
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C -44.01600 -7.11900 31.09500
C -44.69300 -5.38600 29.85700
C -43.32900 -5.36800 29.88800
C -46.43900 -6.92800 30.83100
C -41.59100 -6.81600 31.01200
C -47.11500 -6.49000 31.96700
C -40.91700 -7.73800 30.21500
C -48.38300 -7.03800 32.22800
C -39.65200 -8.17400 30.64500
C -39.07500 -7.65400 31.80300
C -48.96200 -7.94700 31.34300
C -39.76200 -6.71200 32.54100
```

```
C -48.27200 -8.32400 30.20900
C -46.99200 -7.83600 29.92300
C -41.04000 -6.27300 32.17500
C -46.51200 -5.47100 32.89800
C -41.51800 -8.26400 28.93900
C -37.72100 -8.14400 32.26200
C -50.31800 -8.53900 31.64400
C -46.25000 -8.28600 28.69900
C -41.78000 -5.27200 33.01300
H -45.31100 -4.74000 29.39500
H -42.70700 -4.71700 29.43900
H -48.91600 -6.69200 32.98200
H -39.15500 -8.74300 30.10100
H -39.39500 -6.39900 33.23800
H -48.64000 -8.87100 29.67600
H -46.30700 -4.69200 32.46600
H -41.71900 -7.59200 28.35200
H -45.53700 -5.70900 33.08000
H -42.49500 -8.51200 29.09800
H -46.98300 -5.26300 33.55800
H -41.04900 -8.81600 28.52000
H -41.18800 -4.92000 33.76600
H -46.84300 -8.87200 28.11100
H -37.67500 -8.93600 32.36600
H -50.36800 -8.90600 32.35400
H -37.43600 -7.81200 33.03900
H -50.60400 -9.15700 31.06700
H -37.14600 -8.01900 31.64800
H -50.89100 -7.91800 31.73400
H -45.46600 -9.00700 28.90400
H -42.56800 -5.70700 33.61900
H -45.90700 -7.55200 28.20600
H -42.11800 -4.55700 32.49000
N -45.08800 -6.48400 30.60900
N -42.94000 -6.45100 30.66600
```

## Atoms and radius in the parameter file

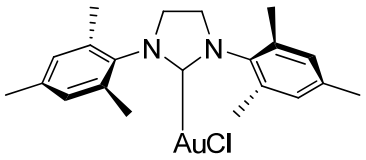
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

## Results : Volumes in Angs^3

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
113.326 66.208 179.535 179.594
%V_Free %V_Bur % Tot/Ex
63.122 36.878 99.967
```

## The %V_Bur of your molecule is: 36.9

## *%$V_{bur}$ for AuCl(SIMes)*




### Molecule from input :

```
Molecule from input :
./temp/c63b235b0e5bca5b5243d9a158cf8859.c3d1
Number of atoms : 49
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 48 49
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 1.983
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

### Cartesian coordinates from input :

```
C 21.16700 45.51000 12.90000
C 19.05000 46.25800 12.26700
C 19.11100 44.74800 12.08200
C 20.87200 47.96700 12.74500
C 20.72200 48.71400 13.90100
C 21.05300 50.07200 13.84500
C 21.50200 50.67200 12.68600
C 21.65100 49.88700 11.55700
C 21.38100 48.52700 11.56200
C 21.67600 47.67100 10.36000
C 21.84100 52.15000 12.64500
C 20.25300 48.09400 15.20500
C 20.95400 43.06800 12.63700
C 21.87000 42.67100 11.64700
C 22.37000 41.37100 11.71500
C 21.97100 40.47600 12.69800
C 21.01900 40.88900 13.61200
C 20.48600 42.18100 13.60900
C 19.43300 42.57000 14.61600
C 22.56400 39.09100 12.77300
C 22.28600 43.59600 10.53200
H 18.38900 46.50700 12.96000
H 18.81800 46.71400 11.41900
H 19.03900 44.50000 11.12600
H 18.39200 44.29400 12.59100
H 20.96600 50.59800 14.63100
H 21.94800 50.29300 10.75100
H 22.45100 47.10200 10.54600
H 20.89900 47.10800 10.16100
H 21.86900 48.24500 9.58900
H 22.47700 52.35900 13.36100
H 22.24200 52.36900 11.77800
H 21.02500 52.67500 12.76800
H 21.02900 47.78300 15.71500
H 19.76500 48.76400 15.72800
H 19.66300 47.33600 15.01200
H 23.00500 41.08800 11.06800
H 20.71500 40.27200 14.26700
H 18.54400 42.38900 14.24600
H 19.55800 42.05000 15.43700
H 19.51300 43.52600 14.81800
H 21.85200 38.43800 12.94000
H 23.00800 38.88000 11.92600
H 23.21700 39.05400 13.50300
```

```
H 22.75700 43.08400 9.84200
H 21.49100 44.01600 10.14200
H 22.88100 44.28900 10.88800
N 20.42200 46.59200 12.69300
N 20.44500 44.41600 12.62400
```

## Atoms and radius in the parameter file

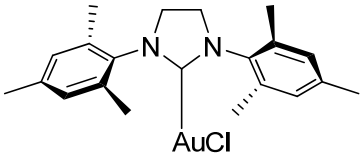
```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

## Results : Volumes in Angs^3

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
112.789 66.745 179.535 179.594
%V_Free %V_Bur % Tot/Ex
62.823 37.177 99.967
```

## The %V_Bur of your molecule is: 37.2

***$\%V_{bur}^{average}$ for AuCl(SIMes)***




## Molecule from input :

```
Molecule from input :
./temp/bf8bd1d07000506acaa6690ac92a3217.c3d1
Number of atoms : 49
Atom that is coordinated : 1
Atoms that define the axis : 2
ID of these atoms : 48 49
Radius of sphere (Angs) : 3.500
Distance from sphere (Angs) : 1.981
Mesh step (Angs) : 0.050
H atoms omitted in the V_bur calculation
```

## Cartesian coordinates from input :

```
C 21.16700 45.51000 12.90000
C 19.05000 46.25800 12.26700
C 19.11100 44.74800 12.08200
C 20.87200 47.96700 12.74500
C 20.72200 48.71400 13.90100
C 21.05300 50.07200 13.84500
C 21.50200 50.67200 12.68600
C 21.65100 49.88700 11.55700
C 21.38100 48.52700 11.56200
C 21.67600 47.67100 10.36000
C 21.84100 52.15000 12.64500
C 20.25300 48.09400 15.20500
C 20.95400 43.06800 12.63700
```

```
C 21.87000 42.67100 11.64700
C 22.37000 41.37100 11.71500
C 21.97100 40.47600 12.69800
C 21.01900 40.88900 13.61200
C 20.48600 42.18100 13.60900
C 19.43300 42.57000 14.61600
C 22.56400 39.09100 12.77300
C 22.28600 43.59600 10.53200
H 18.38900 46.50700 12.96000
H 18.81800 46.71400 11.41900
H 19.03900 44.50000 11.12600
H 18.39200 44.29400 12.59100
H 20.96600 50.59800 14.63100
H 21.94800 50.29300 10.75100
H 22.45100 47.10200 10.54600
H 20.89900 47.10800 10.16100
H 21.86900 48.24500 9.58900
H 22.47700 52.35900 13.36100
H 22.24200 52.36900 11.77800
H 21.02500 52.67500 12.76800
H 21.02900 47.78300 15.71500
H 19.76500 48.76400 15.72800
H 19.66300 47.33600 15.01200
H 23.00500 41.08800 11.06800
H 20.71500 40.27200 14.26700
H 18.54400 42.38900 14.24600
H 19.55800 42.05000 15.43700
H 19.51300 43.52600 14.81800
H 21.85200 38.43800 12.94000
H 23.00800 38.88000 11.92600
H 23.21700 39.05400 13.50300
H 22.75700 43.08400 9.84200
H 21.49100 44.01600 10.14200
H 22.88100 44.28900 10.88800
N 20.42200 46.59200 12.69300
N 20.44500 44.41600 12.62400
```

**Atoms and radius in the parameter file**

```
C2 1.99
C3 1.99
C 1.99
N2 1.81
N3 1.81
N 1.81
O 1.78
P 2.11
H 1.40
F 1.72
```

**Results : Volumes in Angs^3**

```
N of voxels examined : 1436277
Volume of voxel : 0.125E-03
V Free V Buried V Total V Exact
112.721 66.813 179.535 179.594
%V_Free %V_Bur % Tot/Ex
62.785 37.215 99.967
```

**The %V_Bur of your molecule is: 37.2**