## Samb*V*ca @ MoLNaC Results page

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

Molecule from input :  
  
 00000001  
  
  
 Number of atoms : 20  
 Atom that is coordinated : 1  
 Atoms that define the axis : 3  
 ID of these atoms : 2 6 10  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.350  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
P -12.64900 3.18100 4.46800  
C -13.72500 4.44300 5.18500  
H -14.65600 4.13700 5.15100  
H -13.46700 4.60100 6.11700  
H -13.63700 5.27600 4.67600  
C -12.87500 1.76500 5.57400  
H -12.38300 0.99400 5.22100  
H -12.53500 1.98900 6.46500  
H -13.82800 1.54500 5.63300  
C -13.44800 2.67500 2.91600  
C -14.22800 3.58000 2.20500  
H -14.36600 4.45800 2.54000  
C -14.80700 3.19400 0.99700  
H -15.33300 3.81400 0.50600  
C -14.62000 1.92000 0.51200  
H -15.02700 1.66100 -0.30700  
C -13.84200 1.01400 1.21200  
H -13.71400 0.13500 0.87600  
C -13.25100 1.39600 2.40700  
H -12.70600 0.77900 2.88100

### Atoms and radius in the parameter file

Atoms and radius in the parameter file  
H 1.29  
C2 1.99  
C3 1.99  
C 1.99  
N2 1.81  
N3 1.81  
N 1.81  
O 1.78  
F 1.72  
Si 2.45  
P 2.11  
S 2.10  
Cl 2.05  
As 2.17  
Br 2.16  
I 2.31

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

Coordinates scaled to put the metal at the origin  
  
P -2.22520 -0.69901 0.28702  
C -3.30120 0.56299 1.00402  
H -4.23220 0.25699 0.97002  
H -3.04320 0.72099 1.93602  
H -3.21320 1.39599 0.49502  
C -2.45120 -2.11501 1.39302  
H -1.95920 -2.88601 1.04002  
H -2.11120 -1.89101 2.28402  
H -3.40420 -2.33501 1.45202  
C -3.02420 -1.20501 -1.26498  
C -3.80420 -0.30001 -1.97598  
H -3.94220 0.57799 -1.64098  
C -4.38320 -0.68601 -3.18398  
H -4.90920 -0.06601 -3.67498  
C -4.19620 -1.96001 -3.66898  
H -4.60320 -2.21901 -4.48798  
C -3.41820 -2.86601 -2.96898  
H -3.29020 -3.74501 -3.30498  
C -2.82720 -2.48401 -1.77398  
H -2.28220 -3.10101 -1.29998  
XX 0.00000 0.00000 0.00000

### Results : Volumes in Angs^3

Results : Volumes in Angs^3  
  
 N of voxels examined : 1436277  
 Volume of voxel : 0.125E-03  
  
 V Free V Buried V Total V Exact  
 137.764 41.770 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 76.734 23.266 99.967

### The %V\_Bur of your molecule is: 23.3