## 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) : 2.340  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
P -3.60400 3.16100 2.07400  
C -5.05800 2.12200 2.31500  
H -5.81300 2.49600 1.81500  
H -4.86900 1.21600 1.99400  
H -5.28200 2.09000 3.26900  
C -4.18400 4.81500 2.49000  
H -4.48200 4.83200 3.42300  
H -3.45300 5.45700 2.36800  
H -4.93100 5.05600 1.90400  
C -3.31100 3.20700 0.27500  
C -2.05600 3.06700 -0.27000  
H -1.30900 2.92100 0.29800  
C -1.86900 3.13600 -1.65700  
H -1.00000 3.03900 -2.02900  
C -2.94300 3.34500 -2.46600  
H -2.81600 3.39500 -3.40600  
C -4.21800 3.48600 -1.94500  
H -4.95900 3.63400 -2.52200  
C -4.40400 3.40800 -0.55800  
H -5.27600 3.49300 -0.18900

### 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 -1.86491 0.70804 -1.22328  
C -3.31891 -0.33096 -0.98228  
H -4.07391 0.04304 -1.48228  
H -3.12991 -1.23696 -1.30328  
H -3.54291 -0.36296 -0.02828  
C -2.44491 2.36204 -0.80728  
H -2.74291 2.37904 0.12572  
H -1.71391 3.00404 -0.92928  
H -3.19191 2.60304 -1.39328  
C -1.57191 0.75404 -3.02228  
C -0.31691 0.61404 -3.56728  
H 0.43009 0.46804 -2.99928  
C -0.12991 0.68304 -4.95428  
H 0.73909 0.58604 -5.32628  
C -1.20391 0.89204 -5.76328  
H -1.07691 0.94204 -6.70328  
C -2.47891 1.03304 -5.24228  
H -3.21991 1.18104 -5.81928  
C -2.66491 0.95504 -3.85528  
H -3.53691 1.04004 -3.48628  
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  
 134.740 44.794 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 75.050 24.950 99.967

### The %V\_Bur of your molecule is: 25.0