## Samb*V*ca @ MoLNaC Results page

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

### Molecule from input :

Molecule from input :  
  
 00000001  
  
  
 Number of atoms : 35  
 Atom that is coordinated : 19  
 Atoms that define the axis : 2  
 ID of these atoms : 3 4  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 1.990  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
C -1.91900 3.32600 -0.68800  
C -0.80000 3.23600 -1.43800  
N -2.03600 2.13100 0.00300  
N -0.25200 1.98600 -1.19100  
C -4.20700 0.93900 0.23200  
C -4.59200 1.11800 -1.09700  
C -4.80500 -0.07200 0.98400  
C -5.54700 0.28300 -1.66900  
C -5.76600 -0.90300 0.41600  
C -6.13500 -0.73100 -0.91500  
C 2.22200 2.09900 -0.96500  
C 2.14800 3.20100 -0.11300  
C 3.45300 1.45800 -1.13500  
C 3.28500 3.65800 0.55100  
C 4.58600 1.90900 -0.46800  
C 4.50600 3.01500 0.37700  
C 1.03200 1.57500 -1.73300  
C -3.16400 1.81700 0.87200  
C -1.01400 1.27200 -0.30500  
H -3.59300 2.78000 1.18000  
H -4.13000 1.90300 -1.69700  
H -4.49500 -0.22400 2.02000  
H -5.83100 0.42300 -2.71100  
H -6.21700 -1.69500 1.01100  
H -6.87700 -1.38700 -1.36600  
H 1.19600 3.70900 0.04400  
H 3.51600 0.58600 -1.78700  
H 3.21100 4.52000 1.21300  
H 5.53500 1.39300 -0.60400  
H 5.39200 3.36900 0.90100  
H -0.33200 3.93700 -2.11600  
H -2.64400 4.12200 -0.57700  
H 1.07200 1.91600 -2.77700  
H 1.04900 0.47900 -1.75600  
H -2.77800 1.34000 1.78300

### 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  
  
C -1.21009 3.89981 -1.06124  
C -0.09109 3.80981 -1.81124  
N -1.32709 2.70481 -0.37024  
N 0.45691 2.55981 -1.56424  
C -3.49809 1.51281 -0.14124  
C -3.88309 1.69181 -1.47024  
C -4.09609 0.50181 0.61076  
C -4.83809 0.85681 -2.04224  
C -5.05709 -0.32919 0.04276  
C -5.42609 -0.15719 -1.28824  
C 2.93091 2.67281 -1.33824  
C 2.85691 3.77481 -0.48624  
C 4.16191 2.03181 -1.50824  
C 3.99391 4.23181 0.17776  
C 5.29491 2.48281 -0.84124  
C 5.21491 3.58881 0.00376  
C 1.74091 2.14881 -2.10624  
C -2.45509 2.39081 0.49876  
C -0.30509 1.84581 -0.67824  
H -2.88409 3.35381 0.80676  
H -3.42109 2.47681 -2.07024  
H -3.78609 0.34981 1.64676  
H -5.12209 0.99681 -3.08424  
H -5.50809 -1.12119 0.63776  
H -6.16809 -0.81319 -1.73924  
H 1.90491 4.28281 -0.32924  
H 4.22491 1.15981 -2.16024  
H 3.91991 5.09381 0.83976  
H 6.24391 1.96681 -0.97724  
H 6.10091 3.94281 0.52776  
H 0.37691 4.51081 -2.48924  
H -1.93509 4.69581 -0.95024  
H 1.78091 2.48981 -3.15024  
H 1.75791 1.05281 -2.12924  
H -2.06909 1.91381 1.40976  
XX 0.00000 0.00000 0.00000

### Results : Volumes in Angs^3

Results : Volumes in Angs^3  
  
 N of voxels examined : 1436277  
 Volume of voxel : 0.125E-03  
  
 V Free V Buried V Total V Exact  
 125.690 53.844 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 70.009 29.991 99.967

### The %V\_Bur of your molecule is: 30.0