## 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 : 52  
 Atom that is coordinated : 1  
 Atoms that define the axis : 3  
 ID of these atoms : 2 13 24  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.320  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
P -2.59300 1.35800 9.11100  
C -1.22800 2.30200 8.34500  
C -0.66000 3.34800 9.07500  
H -0.45900 3.04700 9.95400  
C 0.40800 4.05800 8.58000  
H 1.09100 4.10200 9.23900  
C 0.96800 3.70900 7.35700  
H 1.89900 3.55400 7.46900  
C 0.41400 2.67300 6.63400  
H 1.09600 2.05800 6.39000  
C -0.68800 1.97500 7.11000  
H -1.37400 1.98300 6.45300  
C -4.10300 2.35900 8.88600  
C -4.06700 3.73300 9.16700  
H -3.64100 3.87300 10.00600  
C -5.22100 4.48800 9.10700  
H -5.07400 5.24500 8.55300  
C -6.41600 3.90800 8.77700  
H -7.06200 4.11700 9.44100  
C -6.46600 2.55200 8.49600  
H -6.89000 2.41900 7.65700  
C -5.31700 1.77900 8.55900  
H -5.22400 1.28500 7.75300  
C -2.86300 -0.14800 8.12400  
C -3.37800 -0.11300 6.82900  
H -2.83000 0.44100 6.28600  
C -3.65100 -1.29600 6.15400  
H -3.21900 -1.28400 5.30800  
C -3.42100 -2.51900 6.77200  
H -4.21400 -3.04100 6.74400  
C -2.88700 -2.56700 8.03600  
H -2.11200 -3.11700 8.03100  
C -2.61000 -1.38600 8.71000  
H -3.00800 -1.41400 9.57300  
H -1.56200 -1.41100 9.08400  
H -3.51700 -3.22100 8.67900  
H -2.82500 -3.17000 6.09400  
H -4.69400 -1.26800 5.76600  
H -4.27800 0.54200 6.80600  
H -1.96600 -0.80600 8.14700  
H -5.49700 0.90100 9.21900  
H -7.26500 2.07700 9.10700  
H -6.88500 4.47600 7.94300  
H -5.33700 5.06200 10.05400  
H -3.27600 4.21600 8.55000  
H -4.54000 2.20000 7.87500  
H -0.47700 0.88300 7.07600  
H 0.21500 3.01300 5.59300  
H 1.04000 4.61300 6.71200  
H 0.16100 5.14300 8.57800  
H -1.45900 4.05500 9.39200  
H -1.51500 2.67000 7.33500

### 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 -0.46553 0.49245 -2.21882  
C 0.89947 1.43645 -2.98482  
C 1.46747 2.48245 -2.25482  
H 1.66847 2.18145 -1.37582  
C 2.53547 3.19245 -2.74982  
H 3.21847 3.23645 -2.09082  
C 3.09547 2.84345 -3.97282  
H 4.02647 2.68845 -3.86082  
C 2.54147 1.80745 -4.69582  
H 3.22347 1.19245 -4.93982  
C 1.43947 1.10945 -4.21982  
H 0.75347 1.11745 -4.87682  
C -1.97553 1.49345 -2.44382  
C -1.93953 2.86745 -2.16282  
H -1.51353 3.00745 -1.32382  
C -3.09353 3.62245 -2.22282  
H -2.94653 4.37945 -2.77682  
C -4.28853 3.04245 -2.55282  
H -4.93453 3.25145 -1.88882  
C -4.33853 1.68645 -2.83382  
H -4.76253 1.55345 -3.67282  
C -3.18953 0.91345 -2.77082  
H -3.09653 0.41945 -3.57682  
C -0.73553 -1.01355 -3.20582  
C -1.25053 -0.97855 -4.50082  
H -0.70253 -0.42455 -5.04382  
C -1.52353 -2.16155 -5.17582  
H -1.09153 -2.14955 -6.02182  
C -1.29353 -3.38455 -4.55782  
H -2.08653 -3.90655 -4.58582  
C -0.75953 -3.43255 -3.29382  
H 0.01547 -3.98255 -3.29882  
C -0.48253 -2.25155 -2.61982  
H -0.88053 -2.27955 -1.75682  
H 0.56547 -2.27655 -2.24582  
H -1.38953 -4.08655 -2.65082  
H -0.69753 -4.03555 -5.23582  
H -2.56653 -2.13355 -5.56382  
H -2.15053 -0.32355 -4.52382  
H 0.16147 -1.67155 -3.18282  
H -3.36953 0.03545 -2.11082  
H -5.13753 1.21145 -2.22282  
H -4.75753 3.61045 -3.38682  
H -3.20953 4.19645 -1.27582  
H -1.14853 3.35045 -2.77982  
H -2.41253 1.33445 -3.45482  
H 1.65047 0.01745 -4.25382  
H 2.34247 2.14745 -5.73682  
H 3.16747 3.74745 -4.61782  
H 2.28847 4.27745 -2.75182  
H 0.66847 3.18945 -1.93782  
H 0.61247 1.80445 -3.99482  
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  
 126.932 52.603 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 70.700 29.300 99.967

### The %V\_Bur of your molecule is: 29.3