## 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 : 53  
 Atom that is coordinated : 23  
 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 1.40400 3.05100 -0.43800  
C 2.69500 2.64200 -0.35900  
N 0.61900 1.89600 -0.33800  
N 2.66300 1.25000 -0.21200  
C 3.83700 0.44400 -0.08200  
C 4.47800 -0.02100 -1.23300  
C 4.30800 0.15200 1.20600  
C 5.60300 -0.83300 -1.06900  
C 5.43700 -0.65300 1.31800  
C 6.09100 -1.16400 0.19200  
C -0.81100 1.90100 -0.32700  
C -1.50100 1.84000 -1.54400  
C -1.47100 2.00700 0.90300  
C -2.89300 1.87300 -1.50200  
C -2.86500 2.01100 0.89300  
C -3.59100 1.93500 -0.29600  
C -0.70600 2.10700 2.18800  
C -0.77900 1.69500 -2.85100  
C -5.08700 1.86100 -0.28100  
C 7.28600 -2.05500 0.35100  
C 3.60100 0.67000 2.42100  
C 4.00500 0.34900 -2.60700  
C 1.38200 0.77400 -0.19800  
C 0.80400 4.39800 -0.59300  
C 3.96900 3.39900 -0.39100  
H -1.37800 2.31500 3.02700  
H 6.11000 -1.21500 -1.95700  
H 5.81800 -0.89400 2.31200  
H -3.45000 1.82100 -2.44000  
H -3.39900 2.07900 1.84200  
H 0.05400 2.90100 2.15500  
H -0.17100 1.17100 2.40500  
H 7.79600 -2.21900 -0.60600  
H -0.44200 0.65700 -3.00000  
H 0.11500 2.32800 -2.91400  
H -1.43800 1.94800 -3.68900  
H -5.52900 2.38700 -1.13600  
H -5.50600 2.28300 0.64000  
H -5.41600 0.81300 -0.34100  
H 6.99500 -3.03900 0.74500  
H 8.01200 -1.63200 1.05700  
H 2.60800 0.20800 2.52600  
H 3.44000 1.75600 2.37400  
H 4.17300 0.45000 3.33000  
H 4.52100 1.24700 -2.97700  
H 2.92900 0.56500 -2.63200  
H 4.20800 -0.45700 -3.32200  
H 0.15500 4.65500 0.25500  
H 0.19000 4.47100 -1.50100  
H 1.58800 5.15900 -0.65800  
H 4.59900 3.10500 -1.24100  
H 4.55800 3.23300 0.52100  
H 3.77300 4.47300 -0.47600

### 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 0.63307 4.16212 -0.42167  
C 1.92407 3.75312 -0.34267  
N -0.15193 3.00712 -0.32167  
N 1.89207 2.36112 -0.19567  
C 3.06607 1.55512 -0.06567  
C 3.70707 1.09012 -1.21667  
C 3.53707 1.26312 1.22233  
C 4.83207 0.27812 -1.05267  
C 4.66607 0.45812 1.33433  
C 5.32007 -0.05288 0.20833  
C -1.58193 3.01212 -0.31067  
C -2.27193 2.95112 -1.52767  
C -2.24193 3.11812 0.91933  
C -3.66393 2.98412 -1.48567  
C -3.63593 3.12212 0.90933  
C -4.36193 3.04612 -0.27967  
C -1.47693 3.21812 2.20433  
C -1.54993 2.80612 -2.83467  
C -5.85793 2.97212 -0.26467  
C 6.51507 -0.94388 0.36733  
C 2.83007 1.78112 2.43733  
C 3.23407 1.46012 -2.59067  
C 0.61107 1.88512 -0.18167  
C 0.03307 5.50912 -0.57667  
C 3.19807 4.51012 -0.37467  
H -2.14893 3.42612 3.04333  
H 5.33907 -0.10388 -1.94067  
H 5.04707 0.21712 2.32833  
H -4.22093 2.93212 -2.42367  
H -4.16993 3.19012 1.85833  
H -0.71693 4.01212 2.17133  
H -0.94193 2.28212 2.42133  
H 7.02507 -1.10788 -0.58967  
H -1.21293 1.76812 -2.98367  
H -0.65593 3.43912 -2.89767  
H -2.20893 3.05912 -3.67267  
H -6.29993 3.49812 -1.11967  
H -6.27693 3.39412 0.65633  
H -6.18693 1.92412 -0.32467  
H 6.22407 -1.92788 0.76133  
H 7.24107 -0.52088 1.07333  
H 1.83707 1.31912 2.54233  
H 2.66907 2.86712 2.39033  
H 3.40207 1.56112 3.34633  
H 3.75007 2.35812 -2.96067  
H 2.15807 1.67612 -2.61567  
H 3.43707 0.65412 -3.30567  
H -0.61593 5.76612 0.27133  
H -0.58093 5.58212 -1.48467  
H 0.81707 6.27012 -0.64167  
H 3.82807 4.21612 -1.22467  
H 3.78707 4.34412 0.53733  
H 3.00207 5.58412 -0.45967  
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  
 117.770 61.764 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 65.598 34.402 99.967

### The %V\_Bur of your molecule is: 34.4