## Samb*V*ca @ MoLNaC Results page

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 | |  
 | 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 |  
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### Molecule from input :

Molecule from input :  
  
 00000001  
  
  
 Number of atoms : 65  
 Atom that is coordinated : 21  
 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 -0.16900 -1.79100 2.62800  
C -1.45200 -1.81400 2.21600  
N 0.53600 -1.02700 1.70900  
N -1.51200 -1.06000 1.05000  
C -2.71500 -0.98700 0.27200  
C -2.87700 -1.90300 -0.78100  
C -3.70100 -0.06200 0.64300  
C -4.09100 -1.87600 -1.46700  
C -4.90500 -0.09000 -0.06500  
C -5.09800 -0.98600 -1.10700  
C 1.97200 -0.99000 1.72000  
C 2.65100 -2.04900 1.09700  
C 2.63000 0.06300 2.36600  
C 4.04600 -2.02200 1.12500  
C 4.02600 0.04000 2.37100  
C 4.72700 -0.98800 1.75400  
C 1.87600 1.17000 3.06900  
C 1.92700 -3.19800 0.42800  
C -3.50400 0.92100 1.77800  
C -1.80500 -2.91700 -1.12700  
C -0.28600 -0.55100 0.71400  
C -3.83600 2.35400 1.36500  
C -4.33200 0.51400 2.99700  
C 2.44700 2.55100 2.76500  
C 1.84700 0.91400 4.57700  
C -1.63800 -3.12900 -2.62700  
C -2.08200 -4.24600 -0.42300  
C 2.29900 -3.32600 -1.04700  
C 2.17900 -4.50900 1.17200  
H -2.33400 -2.28900 2.62500  
H -4.25800 -2.57100 -2.28800  
H -5.70300 0.60300 0.20100  
H 4.60600 -2.82600 0.64700  
H 4.57400 0.84000 2.86800  
H 0.83400 1.15200 2.71000  
H 0.84600 -3.00200 0.47300  
H -2.44100 0.90200 2.07000  
H -0.84400 -2.53400 -0.75400  
H -4.08100 -0.49700 3.34300  
H 0.32600 -2.25200 3.47300  
H 5.81600 -0.98400 1.76600  
H -6.04200 -0.99200 -1.64900  
H -3.27300 2.66100 0.47300  
H -3.58400 3.04700 2.17900  
H -4.90700 2.47800 1.15000  
H -5.40600 0.52800 2.76000  
H -4.16300 1.21100 3.82900  
H 3.43500 2.69400 3.22600  
H 1.78600 3.33100 3.16600  
H 2.54900 2.71400 1.68400  
H 1.28500 1.70300 5.09400  
H 2.86700 0.90200 4.98700  
H 1.38000 -0.05100 4.81400  
H -2.52400 -3.59700 -3.08100  
H -0.78800 -3.79900 -2.81500  
H -1.44700 -2.18200 -3.14900  
H -1.28300 -4.97000 -0.64000  
H -3.03300 -4.67600 -0.76900  
H -2.14300 -4.12400 0.66800  
H 1.72900 -4.14300 -1.51100  
H 3.36700 -3.55500 -1.17700  
H 2.08200 -2.40000 -1.59600  
H 3.24200 -4.78700 1.14100  
H 1.60700 -5.32600 0.71200  
H 1.88200 -4.43600 2.22700

### 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 -0.35469 -2.39005 3.46802  
C -1.63769 -2.41305 3.05602  
N 0.35031 -1.62605 2.54902  
N -1.69769 -1.65905 1.89002  
C -2.90069 -1.58605 1.11202  
C -3.06269 -2.50205 0.05902  
C -3.88669 -0.66105 1.48302  
C -4.27669 -2.47505 -0.62698  
C -5.09069 -0.68905 0.77502  
C -5.28369 -1.58505 -0.26698  
C 1.78631 -1.58905 2.56002  
C 2.46531 -2.64805 1.93702  
C 2.44431 -0.53605 3.20602  
C 3.86031 -2.62105 1.96502  
C 3.84031 -0.55905 3.21102  
C 4.54131 -1.58705 2.59402  
C 1.69031 0.57095 3.90902  
C 1.74131 -3.79705 1.26802  
C -3.68969 0.32195 2.61802  
C -1.99069 -3.51605 -0.28698  
C -0.47169 -1.15005 1.55402  
C -4.02169 1.75495 2.20502  
C -4.51769 -0.08505 3.83702  
C 2.26131 1.95195 3.60502  
C 1.66131 0.31495 5.41702  
C -1.82369 -3.72805 -1.78698  
C -2.26769 -4.84505 0.41702  
C 2.11331 -3.92505 -0.20698  
C 1.99331 -5.10805 2.01202  
H -2.51969 -2.88805 3.46502  
H -4.44369 -3.17005 -1.44798  
H -5.88869 0.00395 1.04102  
H 4.42031 -3.42505 1.48702  
H 4.38831 0.24095 3.70802  
H 0.64831 0.55295 3.55002  
H 0.66031 -3.60105 1.31302  
H -2.62669 0.30295 2.91002  
H -1.02969 -3.13305 0.08602  
H -4.26669 -1.09605 4.18302  
H 0.14031 -2.85105 4.31302  
H 5.63031 -1.58305 2.60602  
H -6.22769 -1.59105 -0.80898  
H -3.45869 2.06195 1.31302  
H -3.76969 2.44795 3.01902  
H -5.09269 1.87895 1.99002  
H -5.59169 -0.07105 3.60002  
H -4.34869 0.61195 4.66902  
H 3.24931 2.09495 4.06602  
H 1.60031 2.73195 4.00602  
H 2.36331 2.11495 2.52402  
H 1.09931 1.10395 5.93402  
H 2.68131 0.30295 5.82702  
H 1.19431 -0.65005 5.65402  
H -2.70969 -4.19605 -2.24098  
H -0.97369 -4.39805 -1.97498  
H -1.63269 -2.78105 -2.30898  
H -1.46869 -5.56905 0.20002  
H -3.21869 -5.27505 0.07102  
H -2.32869 -4.72305 1.50802  
H 1.54331 -4.74205 -0.67098  
H 3.18131 -4.15405 -0.33698  
H 1.89631 -2.99905 -0.75598  
H 3.05631 -5.38605 1.98102  
H 1.42131 -5.92505 1.55202  
H 1.69631 -5.03505 3.06702  
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  
 115.994 63.540 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 64.608 35.392 99.967

### The %V\_Bur of your molecule is: 35.4