## 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 : 49  
 Atom that is coordinated : 21  
 Atoms that define the axis : 2  
 ID of these atoms : 1 2  
  
 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 :  
N 0.40200 1.70400 -1.06400  
N 2.47500 1.09600 -0.80900  
C 3.66300 0.35600 -0.53800  
C 4.19900 -0.48100 -1.52500  
C 4.32100 0.56900 0.68200  
C 5.38900 -1.15200 -1.24300  
C 5.51000 -0.11800 0.91700  
C 6.05100 -0.99200 -0.02800  
C -1.02100 1.76600 -1.05600  
C -1.69200 1.45300 -2.25000  
C -1.71200 2.21400 0.07500  
C -3.07800 1.55600 -2.27800  
C -3.10600 2.28100 0.00600  
C -3.80500 1.95100 -1.15200  
C -1.01900 2.64400 1.33400  
C -0.93200 0.99200 -3.45900  
C -5.30300 2.00900 -1.19100  
C 7.30200 -1.76300 0.27000  
C 3.76700 1.51700 1.70300  
C 3.55900 -0.63000 -2.87300  
C 1.19200 0.71100 -0.57500  
C 1.16800 2.88600 -1.47700  
C 2.56300 2.31300 -1.62300  
H 0.07300 2.57400 1.26000  
H 5.80900 -1.82000 -1.99800  
H 6.03000 0.03400 1.86500  
H -3.61100 1.30800 -3.19800  
H -3.65900 2.61500 0.88700  
H -1.27800 3.68300 1.58000  
H -5.70000 2.67800 -0.41800  
H -1.33100 2.02600 2.18700  
H -0.32100 0.10300 -3.24400  
H -0.23900 1.75900 -3.83400  
H -1.61700 0.73700 -4.27600  
H -5.66800 2.35600 -2.16600  
H -5.74200 1.01600 -1.01900  
H 7.86100 -1.99800 -0.64400  
H 7.06500 -2.72000 0.75800  
H 7.96600 -1.21200 0.94700  
H 2.82300 1.14700 2.12700  
H 3.54900 2.50300 1.26900  
H 4.47500 1.65900 2.52800  
H 3.98100 0.08900 -3.59100  
H 2.47500 -0.45800 -2.84500  
H 3.73500 -1.63100 -3.28300  
H 0.76600 3.30800 -2.40500  
H 1.10700 3.65800 -0.69300  
H 3.35100 2.97500 -1.24600  
H 2.79900 2.05300 -2.66800

### 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  
  
N -0.18899 2.67289 -1.37039  
N 1.88401 2.06489 -1.11539  
C 3.07201 1.32489 -0.84439  
C 3.60801 0.48789 -1.83139  
C 3.73001 1.53789 0.37561  
C 4.79801 -0.18311 -1.54939  
C 4.91901 0.85089 0.61061  
C 5.46001 -0.02311 -0.33439  
C -1.61199 2.73489 -1.36239  
C -2.28299 2.42189 -2.55639  
C -2.30299 3.18289 -0.23139  
C -3.66899 2.52489 -2.58439  
C -3.69699 3.24989 -0.30039  
C -4.39599 2.91989 -1.45839  
C -1.60999 3.61289 1.02761  
C -1.52299 1.96089 -3.76539  
C -5.89399 2.97789 -1.49739  
C 6.71101 -0.79411 -0.03639  
C 3.17601 2.48589 1.39661  
C 2.96801 0.33889 -3.17939  
C 0.60101 1.67989 -0.88139  
C 0.57701 3.85489 -1.78339  
C 1.97201 3.28189 -1.92939  
H -0.51799 3.54289 0.95361  
H 5.21801 -0.85111 -2.30439  
H 5.43901 1.00289 1.55861  
H -4.20199 2.27689 -3.50439  
H -4.24999 3.58389 0.58061  
H -1.86899 4.65189 1.27361  
H -6.29099 3.64689 -0.72439  
H -1.92199 2.99489 1.88061  
H -0.91199 1.07189 -3.55039  
H -0.82999 2.72789 -4.14039  
H -2.20799 1.70589 -4.58239  
H -6.25899 3.32489 -2.47239  
H -6.33299 1.98489 -1.32539  
H 7.27001 -1.02911 -0.95039  
H 6.47401 -1.75111 0.45161  
H 7.37501 -0.24311 0.64061  
H 2.23201 2.11589 1.82061  
H 2.95801 3.47189 0.96261  
H 3.88401 2.62789 2.22161  
H 3.39001 1.05789 -3.89739  
H 1.88401 0.51089 -3.15139  
H 3.14401 -0.66211 -3.58939  
H 0.17501 4.27689 -2.71139  
H 0.51601 4.62689 -0.99939  
H 2.76001 3.94389 -1.55239  
H 2.20801 3.02189 -2.97439  
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  
 119.558 59.977 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 66.593 33.407 99.967

### The %V\_Bur of your molecule is: 33.4