## 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 : 41  
 Atom that is coordinated : 5  
 Atoms that define the axis : 2  
 ID of these atoms : 3 4  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.100  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
C 1.39500 3.08300 0.61800  
C 2.65100 2.59000 0.61700  
N 0.53800 2.00900 0.44700  
N 2.54700 1.22000 0.44500  
C 1.23800 0.83900 0.33600  
C -0.91500 2.16100 0.31400  
C -1.27700 2.89700 -0.97100  
C -1.52100 2.83800 1.53700  
C -2.79300 2.98900 -1.11500  
C -3.03700 2.91200 1.38900  
C -3.42600 3.64400 0.10900  
C 3.71300 0.34000 0.32000  
C 4.61200 0.42800 1.54700  
C 4.48300 0.62500 -0.96500  
C 5.79000 -0.53100 1.40800  
C 5.66700 -0.32800 -1.09500  
C 6.57200 -0.25400 0.12900  
H -1.11300 3.85800 1.63800  
H 3.60400 3.08900 0.72900  
H 1.03500 4.09700 0.73200  
H -1.31100 1.13900 0.24800  
H -0.84600 3.91200 -0.94700  
H -0.82800 2.37600 -1.83000  
H -4.51900 3.67700 0.00200  
H -1.23500 2.28800 2.44600  
H -3.05000 3.54300 -2.02800  
H -3.20600 1.97400 -1.24000  
H -3.47700 3.40500 2.26700  
H -3.44700 1.88700 1.36400  
H -3.08500 4.69200 0.17500  
H 3.30400 -0.67900 0.25300  
H 4.99600 1.45700 1.65200  
H 4.02700 0.21300 2.45400  
H 4.84600 1.66700 -0.94900  
H 3.80300 0.53600 -1.82500  
H 6.44200 -0.45400 2.28800  
H 5.41300 -1.56800 1.38700  
H 6.23000 -0.10300 -2.01100  
H 5.28800 -1.35900 -1.20600  
H 7.40700 -0.96100 0.03000  
H 7.01800 0.75400 0.18900

### 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 0.91792 4.18190 0.55688  
C 2.17392 3.68890 0.55588  
N 0.06092 3.10790 0.38588  
N 2.06992 2.31890 0.38388  
C 0.76092 1.93790 0.27488  
C -1.39208 3.25990 0.25288  
C -1.75408 3.99590 -1.03212  
C -1.99808 3.93690 1.47588  
C -3.27008 4.08790 -1.17612  
C -3.51408 4.01090 1.32788  
C -3.90308 4.74290 0.04788  
C 3.23592 1.43890 0.25888  
C 4.13492 1.52690 1.48588  
C 4.00592 1.72390 -1.02612  
C 5.31292 0.56790 1.34688  
C 5.18992 0.77090 -1.15612  
C 6.09492 0.84490 0.06788  
H -1.59008 4.95690 1.57688  
H 3.12692 4.18790 0.66788  
H 0.55792 5.19590 0.67088  
H -1.78808 2.23790 0.18688  
H -1.32308 5.01090 -1.00812  
H -1.30508 3.47490 -1.89112  
H -4.99608 4.77590 -0.05912  
H -1.71208 3.38690 2.38488  
H -3.52708 4.64190 -2.08912  
H -3.68308 3.07290 -1.30112  
H -3.95408 4.50390 2.20588  
H -3.92408 2.98590 1.30288  
H -3.56208 5.79090 0.11388  
H 2.82692 0.41990 0.19188  
H 4.51892 2.55590 1.59088  
H 3.54992 1.31190 2.39288  
H 4.36892 2.76590 -1.01012  
H 3.32592 1.63490 -1.88612  
H 5.96492 0.64490 2.22688  
H 4.93592 -0.46910 1.32588  
H 5.75292 0.99590 -2.07212  
H 4.81092 -0.26010 -1.26712  
H 6.92992 0.13790 -0.03112  
H 6.54092 1.85290 0.12788  
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  
 134.654 44.881 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 75.001 24.999 99.967

### The %V\_Bur of your molecule is: 25.0