## 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 : 35  
 Atom that is coordinated : 3  
 Atoms that define the axis : 2  
 ID of these atoms : 1 2  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.070  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
N -8.77200 1.06300 2.96600  
N -9.23100 2.51500 1.45600  
C -9.14100 2.34800 2.79700  
C -8.63300 0.42600 1.73500  
H -8.38600 -0.47900 1.58700  
C -8.91700 1.34600 0.80100  
H -8.90400 1.21400 -0.13900  
C -8.63600 0.40700 4.26900  
H -8.73100 1.08900 4.98000  
H -9.37600 -0.24200 4.37600  
C -7.33000 -0.31600 4.46500  
C -7.33700 -1.49400 5.18400  
H -8.16000 -1.84700 5.50000  
C -6.14800 -2.17200 5.45200  
H -6.16000 -2.97900 5.95400  
C -4.95600 -1.66300 4.98400  
H -4.14000 -2.11300 5.17000  
C -4.95000 -0.51000 4.25100  
H -4.12800 -0.17700 3.91100  
C -6.12600 0.18200 3.99600  
H -6.10400 0.99300 3.50100  
C -9.65800 3.75400 0.78200  
H -9.50200 3.66600 -0.19200  
H -10.62900 3.88500 0.92400  
C -8.91600 4.95900 1.29600  
C -7.52900 5.02900 1.19500  
H -7.05500 4.33800 0.74700  
C -6.83600 6.09000 1.73700  
H -5.88800 6.11100 1.68300  
C -7.50900 7.12600 2.36000  
H -7.03100 7.85700 2.73400  
C -8.88800 7.08200 2.43000  
H -9.35900 7.79700 2.84200  
C -9.59300 6.00900 1.91000  
H -10.54100 5.99100 1.97200

### 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 0.72039 -2.69306 -1.30707  
N 0.26139 -1.24106 -2.81707  
C 0.35139 -1.40806 -1.47607  
C 0.85939 -3.33006 -2.53807  
H 1.10639 -4.23506 -2.68607  
C 0.57539 -2.41006 -3.47207  
H 0.58839 -2.54206 -4.41207  
C 0.85639 -3.34906 -0.00407  
H 0.76139 -2.66706 0.70693  
H 0.11639 -3.99806 0.10293  
C 2.16239 -4.07206 0.19193  
C 2.15539 -5.25006 0.91093  
H 1.33239 -5.60306 1.22693  
C 3.34439 -5.92806 1.17893  
H 3.33239 -6.73506 1.68093  
C 4.53639 -5.41906 0.71093  
H 5.35239 -5.86906 0.89693  
C 4.54239 -4.26606 -0.02207  
H 5.36439 -3.93306 -0.36207  
C 3.36639 -3.57406 -0.27707  
H 3.38839 -2.76306 -0.77207  
C -0.16561 -0.00206 -3.49107  
H -0.00961 -0.09006 -4.46507  
H -1.13661 0.12894 -3.34907  
C 0.57639 1.20294 -2.97707  
C 1.96339 1.27294 -3.07807  
H 2.43739 0.58194 -3.52607  
C 2.65639 2.33394 -2.53607  
H 3.60439 2.35494 -2.59007  
C 1.98339 3.36994 -1.91307  
H 2.46139 4.10094 -1.53907  
C 0.60439 3.32594 -1.84307  
H 0.13339 4.04094 -1.43107  
C -0.10061 2.25294 -2.36307  
H -1.04861 2.23494 -2.30107  
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  
 114.826 64.708 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 63.958 36.042 99.967

### The %V\_Bur of your molecule is: 36.0