## 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 : 47  
 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) : 2.100  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
N -4.44700 15.65300 13.39800  
N -5.21100 14.05900 14.59400  
C -5.16400 15.40500 14.51700  
C -4.09700 14.46000 12.75400  
H -3.62000 14.36800 11.93800  
C -4.57200 13.48300 13.52300  
H -4.48500 12.55200 13.36000  
C -3.94300 16.92500 12.92200  
C -4.63100 17.60700 11.94300  
C -4.09800 18.78200 11.45300  
H -4.58100 19.27800 10.80300  
C -2.85900 19.25500 11.89500  
C -2.15900 18.50800 12.84800  
H -1.31000 18.80900 13.15000  
C -2.69200 17.33200 13.35600  
C -5.95800 17.11500 11.37000  
H -6.09200 17.50300 10.48000  
H -5.94200 16.13800 11.30100  
H -6.69000 17.39000 11.96000  
C -2.28600 20.54000 11.34400  
H -1.54800 20.33300 10.73300  
H -2.98400 21.02800 10.86000  
H -1.95300 21.09200 12.08200  
C -1.89600 16.50900 14.37200  
H -1.82000 15.58500 14.05600  
H -1.00000 16.89400 14.47300  
H -2.35600 16.52300 15.23600  
C -5.80700 13.26200 15.66000  
C -5.01600 12.91000 16.72300  
C -5.64800 12.14900 17.71400  
H -5.14500 11.87600 18.47200  
C -6.97900 11.78200 17.62700  
C -7.69900 12.15900 16.54200  
H -8.60500 11.88200 16.47300  
C -7.17200 12.91100 15.56000  
C -3.60700 13.38500 16.82600  
H -3.59900 14.35500 16.96600  
H -3.16700 12.94200 17.58000  
H -3.13000 13.17200 15.99700  
C -7.60100 11.00900 18.77100  
H -8.28900 10.40600 18.42100  
H -6.90900 10.48600 19.22700  
H -8.00800 11.63600 19.40600  
C -7.97700 13.34700 14.35000  
H -8.27700 14.27100 14.47300  
H -7.41700 13.28900 13.54700  
H -8.75600 12.76100 14.24800

### 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 1.56696 -1.14492 -2.44088  
N 0.80296 -2.73892 -1.24488  
C 0.84996 -1.39292 -1.32188  
C 1.91696 -2.33792 -3.08488  
H 2.39396 -2.42992 -3.90088  
C 1.44196 -3.31492 -2.31588  
H 1.52896 -4.24592 -2.47888  
C 2.07096 0.12708 -2.91688  
C 1.38296 0.80908 -3.89588  
C 1.91596 1.98408 -4.38588  
H 1.43296 2.48008 -5.03588  
C 3.15496 2.45708 -3.94388  
C 3.85496 1.71008 -2.99088  
H 4.70396 2.01108 -2.68888  
C 3.32196 0.53408 -2.48288  
C 0.05596 0.31708 -4.46888  
H -0.07804 0.70508 -5.35888  
H 0.07196 -0.65992 -4.53788  
H -0.67604 0.59208 -3.87888  
C 3.72796 3.74208 -4.49488  
H 4.46596 3.53508 -5.10588  
H 3.02996 4.23008 -4.97888  
H 4.06096 4.29408 -3.75688  
C 4.11796 -0.28892 -1.46688  
H 4.19396 -1.21292 -1.78288  
H 5.01396 0.09608 -1.36588  
H 3.65796 -0.27492 -0.60288  
C 0.20696 -3.53592 -0.17888  
C 0.99796 -3.88792 0.88412  
C 0.36596 -4.64892 1.87512  
H 0.86896 -4.92192 2.63312  
C -0.96504 -5.01592 1.78812  
C -1.68504 -4.63892 0.70312  
H -2.59104 -4.91592 0.63412  
C -1.15804 -3.88692 -0.27888  
C 2.40696 -3.41292 0.98712  
H 2.41496 -2.44292 1.12712  
H 2.84696 -3.85592 1.74112  
H 2.88396 -3.62592 0.15812  
C -1.58704 -5.78892 2.93212  
H -2.27504 -6.39192 2.58212  
H -0.89504 -6.31192 3.38812  
H -1.99404 -5.16192 3.56712  
C -1.96304 -3.45092 -1.48888  
H -2.26304 -2.52692 -1.36588  
H -1.40304 -3.50892 -2.29188  
H -2.74204 -4.03692 -1.59088  
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  
 123.503 56.031 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 68.791 31.209 99.967

### The %V\_Bur of your molecule is: 31.2