## 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 : 47  
 Atom that is coordinated : 4  
 Atoms that define the axis : 2  
 ID of these atoms : 2 3  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.050  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
C -8.22000 1.26300 8.94000  
N -12.83200 -2.05800 9.44600  
N -14.54300 -3.09500 10.20500  
C -13.63900 -2.15400 10.54200  
C -13.21900 -2.96500 8.47200  
H -12.79900 -3.10800 7.63200  
C -14.29400 -3.59800 8.94100  
H -14.79500 -4.26800 8.49100  
C -11.66100 -1.21400 9.34500  
C -11.85300 0.11700 8.95500  
C -10.69100 0.88600 8.86100  
H -10.78100 1.80000 8.61800  
C -9.43400 0.40700 9.09600  
C -9.31500 -0.92300 9.45100  
H -8.44900 -1.28100 9.60600  
C -10.42400 -1.76100 9.59000  
C -13.20800 0.69000 8.63200  
H -13.71100 0.05200 8.08400  
H -13.69700 0.86300 9.46400  
H -13.09800 1.53000 8.13800  
H -18.89700 -4.50100 14.25500  
H -8.06800 1.44500 7.98900  
H -8.35300 2.10800 9.41700  
H -7.44200 0.79700 9.31100  
C -10.25900 -3.20600 9.94700  
H -10.37400 -3.75600 9.14400  
H -9.36300 -3.35100 10.31700  
H -10.93200 -3.45700 10.61400  
C -15.58800 -3.60600 11.06200  
C -15.25200 -4.44900 12.09500  
C -16.24800 -4.93900 12.91800  
H -16.01900 -5.48700 13.65900  
C -17.58500 -4.63500 12.67200  
C -17.88900 -3.84800 11.59000  
H -18.80100 -3.66400 11.39800  
C -16.91600 -3.31600 10.77100  
C -13.83200 -4.84100 12.34600  
H -13.80500 -5.57700 12.99200  
H -13.41900 -5.12900 11.50500  
H -13.33900 -4.07300 12.70400  
C -18.67200 -5.17400 13.58000  
H -19.46800 -5.38200 13.04800  
H -18.35300 -5.98800 14.02300  
C -17.29000 -2.44800 9.59100  
H -18.24900 -2.25000 9.62200  
H -16.78200 -1.61100 9.62700  
H -17.08100 -2.92100 8.75900

### 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 5.29967 2.37749 -3.36486  
N 0.68767 -0.94351 -2.85886  
N -1.02333 -1.98051 -2.09986  
C -0.11933 -1.03951 -1.76286  
C 0.30067 -1.85051 -3.83286  
H 0.72067 -1.99351 -4.67286  
C -0.77433 -2.48351 -3.36386  
H -1.27533 -3.15351 -3.81386  
C 1.85867 -0.09951 -2.95986  
C 1.66667 1.23149 -3.34986  
C 2.82867 2.00049 -3.44386  
H 2.73867 2.91449 -3.68686  
C 4.08567 1.52149 -3.20886  
C 4.20467 0.19149 -2.85386  
H 5.07067 -0.16651 -2.69886  
C 3.09567 -0.64651 -2.71486  
C 0.31167 1.80449 -3.67286  
H -0.19133 1.16649 -4.22086  
H -0.17733 1.97749 -2.84086  
H 0.42167 2.64449 -4.16686  
H -5.37733 -3.38651 1.95014  
H 5.45167 2.55949 -4.31586  
H 5.16667 3.22249 -2.88786  
H 6.07767 1.91149 -2.99386  
C 3.26067 -2.09151 -2.35786  
H 3.14567 -2.64151 -3.16086  
H 4.15667 -2.23651 -1.98786  
H 2.58767 -2.34251 -1.69086  
C -2.06833 -2.49151 -1.24286  
C -1.73233 -3.33451 -0.20986  
C -2.72833 -3.82451 0.61314  
H -2.49933 -4.37251 1.35414  
C -4.06533 -3.52051 0.36714  
C -4.36933 -2.73351 -0.71486  
H -5.28133 -2.54951 -0.90686  
C -3.39633 -2.20151 -1.53386  
C -0.31233 -3.72651 0.04114  
H -0.28533 -4.46251 0.68714  
H 0.10067 -4.01451 -0.79986  
H 0.18067 -2.95851 0.39914  
C -5.15233 -4.05951 1.27514  
H -5.94833 -4.26751 0.74314  
H -4.83333 -4.87351 1.71814  
C -3.77033 -1.33351 -2.71386  
H -4.72933 -1.13551 -2.68286  
H -3.26233 -0.49651 -2.67786  
H -3.56133 -1.80651 -3.54586  
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  
 119.063 60.471 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 66.318 33.682 99.967

### The %V\_Bur of your molecule is: 33.7