## 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 :  
  
  
  
  
 Number of atoms : 63  
 Atom that is coordinated : 4  
 Atoms that define the axis : 2  
 ID of these atoms : 5 6  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.080  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
C -4.58500 2.58500 13.30300  
C -6.27300 0.38200 15.56400  
C -5.41600 1.38000 15.34800  
C -6.34600 0.85600 13.36100  
N -6.85000 0.05000 14.33700  
N -5.46100 1.66200 13.98900  
C -5.08100 3.82500 12.90700  
C -4.21100 4.66400 12.20200  
C -2.91700 4.29000 11.91300  
C -2.45800 3.06200 12.35500  
C -3.26900 2.18200 13.06800  
C -6.48500 4.24400 13.21100  
C -1.99400 5.19700 11.12400  
C -2.74000 0.85300 13.55800  
C -7.81000 -0.99800 14.11600  
C -9.04400 -0.91400 14.74700  
C -9.99300 -1.89300 14.45500  
C -9.72600 -2.93100 13.57100  
C -8.46400 -3.00000 13.01200  
C -7.47700 -2.07100 13.27400  
C -9.38400 0.18100 15.74000  
C -10.77100 -3.97000 13.25900  
C -6.08600 -2.29100 12.72600  
H -6.06900 -3.20200 12.08700  
H -5.77400 -1.41400 12.11600  
H -5.36400 -2.42200 13.56300  
H -10.36700 -4.71100 12.53400  
H -11.07100 -4.50000 14.19100  
H -11.67100 -3.48500 12.81700  
H -8.05400 -4.02500 13.15100  
H -8.55400 -3.14400 11.91200  
H -10.49000 -2.93200 12.76100  
H -10.42400 0.04600 16.11400  
H -8.68100 0.14500 16.60200  
H -9.30200 1.17700 15.25100  
H -10.39800 -2.31000 15.40400  
H -10.95300 -1.40500 14.17400  
H -7.07700 -1.67600 12.31300  
H -9.48400 0.09200 14.56600  
H -1.67400 0.73600 13.26300  
H -2.81800 0.79800 14.66700  
H -3.33300 0.02100 13.11500  
H -1.00000 4.71300 11.00000  
H -2.42700 5.39900 10.11900  
H -1.86200 6.16400 11.65900  
H -1.97900 2.52000 11.50900  
H -1.49600 3.20000 12.89700  
H -2.74400 4.37700 10.81700  
H -6.67400 5.26400 12.80800  
H -7.20400 3.53200 12.74700  
H -6.65000 4.25400 14.31200  
H -4.71100 5.01700 11.27200  
H -4.20900 5.67300 12.67200  
H -2.78100 1.93200 14.03600  
H -5.47700 4.36600 13.79600  
H -7.33700 -1.97500 14.35900  
H -7.06600 0.72100 16.26800  
H -5.72300 -0.49800 15.96600  
H -3.66900 2.73300 13.91600  
H -4.39000 1.05200 15.62600  
H -5.73900 2.27600 15.92400  
H -7.16600 1.47100 12.92700  
H -5.81300 0.23600 12.60600

### 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 2.24169 1.72900 1.96569  
C 0.55369 -0.47400 4.22669  
C 1.41069 0.52400 4.01069  
C 0.48069 0.00000 2.02369  
N -0.02331 -0.80600 2.99969  
N 1.36569 0.80600 2.65169  
C 1.74569 2.96900 1.56969  
C 2.61569 3.80800 0.86469  
C 3.90969 3.43400 0.57569  
C 4.36869 2.20600 1.01769  
C 3.55769 1.32600 1.73069  
C 0.34169 3.38800 1.87369  
C 4.83269 4.34100 -0.21331  
C 4.08669 -0.00300 2.22069  
C -0.98331 -1.85400 2.77869  
C -2.21731 -1.77000 3.40969  
C -3.16631 -2.74900 3.11769  
C -2.89931 -3.78700 2.23369  
C -1.63731 -3.85600 1.67469  
C -0.65031 -2.92700 1.93669  
C -2.55731 -0.67500 4.40269  
C -3.94431 -4.82600 1.92169  
C 0.74069 -3.14700 1.38869  
H 0.75769 -4.05800 0.74969  
H 1.05269 -2.27000 0.77869  
H 1.46269 -3.27800 2.22569  
H -3.54031 -5.56700 1.19669  
H -4.24431 -5.35600 2.85369  
H -4.84431 -4.34100 1.47969  
H -1.22731 -4.88100 1.81369  
H -1.72731 -4.00000 0.57469  
H -3.66331 -3.78800 1.42369  
H -3.59731 -0.81000 4.77669  
H -1.85431 -0.71100 5.26469  
H -2.47531 0.32100 3.91369  
H -3.57131 -3.16600 4.06669  
H -4.12631 -2.26100 2.83669  
H -0.25031 -2.53200 0.97569  
H -2.65731 -0.76400 3.22869  
H 5.15269 -0.12000 1.92569  
H 4.00869 -0.05800 3.32969  
H 3.49369 -0.83500 1.77769  
H 5.82669 3.85700 -0.33731  
H 4.39969 4.54300 -1.21831  
H 4.96469 5.30800 0.32169  
H 4.84769 1.66400 0.17169  
H 5.33069 2.34400 1.55969  
H 4.08269 3.52100 -0.52031  
H 0.15269 4.40800 1.47069  
H -0.37731 2.67600 1.40969  
H 0.17669 3.39800 2.97469  
H 2.11569 4.16100 -0.06531  
H 2.61769 4.81700 1.33469  
H 4.04569 1.07600 2.69869  
H 1.34969 3.51000 2.45869  
H -0.51031 -2.83100 3.02169  
H -0.23931 -0.13500 4.93069  
H 1.10369 -1.35400 4.62869  
H 3.15769 1.87700 2.57869  
H 2.43669 0.19600 4.28869  
H 1.08769 1.42000 4.58669  
H -0.33931 0.61500 1.58969  
H 1.01369 -0.62000 1.26869  
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  
 115.560 63.974 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 64.367 35.633 99.967

### The %V\_Bur of your molecule is: 35.6