## 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 : 23  
 Atoms that define the axis : 2  
 ID of these atoms : 3 4  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.000  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
C -0.02300 -2.95200 1.84800  
C -1.35500 -2.90500 1.65300  
N 0.52300 -1.89100 1.14000  
N -1.60100 -1.81300 0.82800  
C -2.94000 -1.46800 0.45200  
C -3.46700 -1.98200 -0.73800  
C -3.70600 -0.71600 1.34900  
C -4.79800 -1.69300 -1.03200  
C -5.03500 -0.46000 1.01300  
C -5.59600 -0.93800 -0.17000  
C 1.92900 -1.61400 1.16100  
C 2.74300 -2.15300 0.15800  
C 2.44400 -0.86000 2.21900  
C 4.10500 -1.86700 0.20800  
C 3.81400 -0.59600 2.22200  
C 4.65600 -1.08000 1.22100  
C 1.57000 -0.39500 3.34500  
C 2.17200 -3.01700 -0.92500  
C 6.12000 -0.75700 1.22800  
C -7.03500 -0.67400 -0.50000  
C -3.11700 -0.19700 2.62600  
C -2.63600 -2.82900 -1.65200  
C -0.44500 -1.15800 0.49700  
H 0.57400 -0.08300 3.00200  
H -5.22800 -2.08000 -1.95800  
H -5.64600 0.13300 1.69500  
H 4.75800 -2.27500 -0.56500  
H 4.23400 -0.00300 3.03700  
H 1.41200 -1.19800 4.07900  
H 6.50100 -0.62900 2.24900  
H 2.02900 0.44900 3.87400  
H 1.43700 -2.47000 -1.53300  
H 1.65300 -3.89400 -0.51200  
H 2.96200 -3.37700 -1.59300  
H 6.70700 -1.54400 0.73900  
H 6.32000 0.17900 0.68900  
H -7.66500 -1.53600 -0.23800  
H -7.17500 -0.49100 -1.57300  
H -7.42200 0.19200 0.04900  
H -2.23200 0.42900 2.44300  
H -2.79000 -1.01200 3.28700  
H -3.84800 0.40700 3.17500  
H -2.16600 -3.66400 -1.11300  
H -1.82000 -2.24800 -2.10600  
H -3.24600 -3.24600 -2.46200  
H -2.16300 -3.53100 2.00900  
H 0.60100 -3.62700 2.41900

### 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 0.20161 -3.42116 2.49283  
C -1.13039 -3.37416 2.29783  
N 0.74761 -2.36016 1.78483  
N -1.37639 -2.28216 1.47283  
C -2.71539 -1.93716 1.09683  
C -3.24239 -2.45116 -0.09317  
C -3.48139 -1.18516 1.99383  
C -4.57339 -2.16216 -0.38717  
C -4.81039 -0.92916 1.65783  
C -5.37139 -1.40716 0.47483  
C 2.15361 -2.08316 1.80583  
C 2.96761 -2.62216 0.80283  
C 2.66861 -1.32916 2.86383  
C 4.32961 -2.33616 0.85283  
C 4.03861 -1.06516 2.86683  
C 4.88061 -1.54916 1.86583  
C 1.79461 -0.86416 3.98983  
C 2.39661 -3.48616 -0.28017  
C 6.34461 -1.22616 1.87283  
C -6.81039 -1.14316 0.14483  
C -2.89239 -0.66616 3.27083  
C -2.41139 -3.29816 -1.00717  
C -0.22039 -1.62716 1.14183  
H 0.79861 -0.55216 3.64683  
H -5.00339 -2.54916 -1.31317  
H -5.42139 -0.33616 2.33983  
H 4.98261 -2.74416 0.07983  
H 4.45861 -0.47216 3.68183  
H 1.63661 -1.66716 4.72383  
H 6.72561 -1.09816 2.89383  
H 2.25361 -0.02016 4.51883  
H 1.66161 -2.93916 -0.88817  
H 1.87761 -4.36316 0.13283  
H 3.18661 -3.84616 -0.94817  
H 6.93161 -2.01316 1.38383  
H 6.54461 -0.29016 1.33383  
H -7.44039 -2.00516 0.40683  
H -6.95039 -0.96016 -0.92817  
H -7.19739 -0.27716 0.69383  
H -2.00739 -0.04016 3.08783  
H -2.56539 -1.48116 3.93183  
H -3.62339 -0.06216 3.81983  
H -1.94139 -4.13316 -0.46817  
H -1.59539 -2.71716 -1.46117  
H -3.02139 -3.71516 -1.81717  
H -1.93839 -4.00016 2.65383  
H 0.82561 -4.09616 3.06383  
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  
 121.282 58.253 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 67.553 32.447 99.967

### The %V\_Bur of your molecule is: 32.4