## 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 : 34  
 Atom that is coordinated : 1  
 Atoms that define the axis : 3  
 ID of these atoms : 2 13 24  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.370  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
P -5.33700 1.31100 11.31200  
C -6.26000 1.31600 9.73700  
C -5.96000 2.27400 8.76500  
H -5.26700 2.90500 8.92000  
C -6.67000 2.30600 7.57900  
H -6.47300 2.97100 6.93100  
C -7.65900 1.38100 7.33100  
H -8.14000 1.40700 6.51200  
C -7.95100 0.41400 8.27300  
H -8.62700 -0.23000 8.09700  
C -7.26000 0.38100 9.47600  
H -7.47000 -0.28200 10.12400  
C -6.42500 0.38500 12.43900  
C -6.31000 -1.01200 12.49900  
H -5.60800 -1.45200 12.03500  
C -7.22500 -1.75300 13.23900  
H -7.14900 -2.69900 13.27800  
C -8.24500 -1.11400 13.91600  
H -8.87700 -1.62200 14.41000  
C -8.34700 0.26500 13.87400  
H -9.04000 0.70100 14.35600  
C -7.44600 1.01700 13.13700  
H -7.52700 1.96300 13.11000  
C -5.39600 3.03200 11.89600  
C -6.46500 3.86500 11.58600  
H -7.15000 3.55700 11.00500  
C -6.53800 5.14300 12.11900  
H -7.26300 5.71300 11.89400  
C -5.55000 5.58200 12.97700  
H -5.60200 6.45400 13.35200  
C -4.49000 4.76500 13.29400  
H -3.81700 5.07400 13.88900  
C -4.39700 3.48800 12.74800  
H -3.65500 2.93200 12.95600

### 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  
  
P -2.20651 0.85276 0.14497  
C -3.12951 0.85776 -1.43003  
C -2.82951 1.81576 -2.40203  
H -2.13651 2.44676 -2.24703  
C -3.53951 1.84776 -3.58803  
H -3.34251 2.51276 -4.23603  
C -4.52851 0.92276 -3.83603  
H -5.00951 0.94876 -4.65503  
C -4.82051 -0.04424 -2.89403  
H -5.49651 -0.68824 -3.07003  
C -4.12951 -0.07724 -1.69103  
H -4.33951 -0.74024 -1.04303  
C -3.29451 -0.07324 1.27197  
C -3.17951 -1.47024 1.33197  
H -2.47751 -1.91024 0.86797  
C -4.09451 -2.21124 2.07197  
H -4.01851 -3.15724 2.11097  
C -5.11451 -1.57224 2.74897  
H -5.74651 -2.08024 3.24297  
C -5.21651 -0.19324 2.70697  
H -5.90951 0.24276 3.18897  
C -4.31551 0.55876 1.96997  
H -4.39651 1.50476 1.94297  
C -2.26551 2.57376 0.72897  
C -3.33451 3.40676 0.41897  
H -4.01951 3.09876 -0.16203  
C -3.40751 4.68476 0.95197  
H -4.13251 5.25476 0.72697  
C -2.41951 5.12376 1.80997  
H -2.47151 5.99576 2.18497  
C -1.35951 4.30676 2.12697  
H -0.68651 4.61576 2.72197  
C -1.26651 3.02976 1.58097  
H -0.52451 2.47376 1.78897  
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  
 130.501 49.034 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 72.688 27.312 99.967

### The %V\_Bur of your molecule is: 27.3