## 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 : 43  
 Atom that is coordinated : 1  
 Atoms that define the axis : 3  
 ID of these atoms : 2 16 30  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.340  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
P -1.79900 18.34800 17.12800  
C -1.27800 18.43600 18.84900  
H -1.54700 17.59700 19.30100  
H -1.76600 19.17900 19.28600  
C 0.20500 18.64400 19.06900  
C 1.04700 17.55400 19.26900  
H 0.69000 16.67400 19.30900  
C 2.44200 17.76500 19.41200  
H 3.02600 17.02900 19.55300  
C 2.93500 19.02300 19.34600  
H 3.87200 19.16100 19.41800  
C 2.10400 20.10900 19.17600  
H 2.46300 20.98800 19.15700  
C 0.73800 19.91100 19.03300  
H 0.16500 20.65800 18.90900  
C -1.56600 20.07000 16.55900  
H -0.59600 20.26900 16.53100  
H -1.97900 20.68300 17.21700  
C -2.16200 20.34800 15.18900  
C -3.47100 20.84100 15.06300  
H -4.00400 20.96700 15.83900  
C -3.98600 21.14500 13.81800  
H -4.86200 21.50500 13.74100  
C -3.23100 20.92600 12.69300  
H -3.59600 21.11700 11.83700  
C -1.95000 20.43200 12.79600  
H -1.42800 20.29600 12.01400  
C -1.43000 20.13800 14.02900  
H -0.55100 19.78300 14.09100  
C -3.61600 18.14300 17.23700  
H -3.99600 18.21700 16.32600  
H -3.98400 18.88800 17.77500  
C -4.07300 16.85300 17.83800  
C -4.20300 16.74000 19.22400  
H -4.01200 17.49200 19.77300  
C -4.60000 15.56400 19.80700  
H -4.67700 15.50600 20.75200  
C -4.88500 14.47000 19.03100  
H -5.15000 13.65700 19.44500  
C -4.78700 14.54100 17.55500  
H -4.99900 13.80400 16.99400  
C -4.36600 15.74900 17.05700  
H -4.26900 15.83300 16.11600

### 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 -1.08086 1.63197 1.28219  
C -0.55986 1.71997 3.00319  
H -0.82886 0.88097 3.45519  
H -1.04786 2.46297 3.44019  
C 0.92314 1.92797 3.22319  
C 1.76514 0.83797 3.42319  
H 1.40814 -0.04203 3.46319  
C 3.16014 1.04897 3.56619  
H 3.74414 0.31297 3.70719  
C 3.65314 2.30697 3.50019  
H 4.59014 2.44497 3.57219  
C 2.82214 3.39297 3.33019  
H 3.18114 4.27197 3.31119  
C 1.45614 3.19497 3.18719  
H 0.88314 3.94197 3.06319  
C -0.84786 3.35397 0.71319  
H 0.12214 3.55297 0.68519  
H -1.26086 3.96697 1.37119  
C -1.44386 3.63197 -0.65681  
C -2.75286 4.12497 -0.78281  
H -3.28586 4.25097 -0.00681  
C -3.26786 4.42897 -2.02781  
H -4.14386 4.78897 -2.10481  
C -2.51286 4.20997 -3.15281  
H -2.87786 4.40097 -4.00881  
C -1.23186 3.71597 -3.04981  
H -0.70986 3.57997 -3.83181  
C -0.71186 3.42197 -1.81681  
H 0.16714 3.06697 -1.75481  
C -2.89786 1.42697 1.39119  
H -3.27786 1.50097 0.48019  
H -3.26586 2.17197 1.92919  
C -3.35486 0.13697 1.99219  
C -3.48486 0.02397 3.37819  
H -3.29386 0.77597 3.92719  
C -3.88186 -1.15203 3.96119  
H -3.95886 -1.21003 4.90619  
C -4.16686 -2.24603 3.18519  
H -4.43186 -3.05903 3.59919  
C -4.06886 -2.17503 1.70919  
H -4.28086 -2.91203 1.14819  
C -3.64786 -0.96703 1.21119  
H -3.55086 -0.88303 0.27019  
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  
 120.918 58.616 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 67.351 32.649 99.967

### The %V\_Bur of your molecule is: 32.6