## 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 : 29  
 Atoms that define the axis : 3  
 ID of these atoms : 14 28 30  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.360  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
H -6.53200 2.07900 16.69900  
C -6.03700 2.46400 17.41300  
H -6.21900 0.87100 18.66300  
C -5.86500 1.74900 18.58300  
H -5.04100 1.82800 20.44500  
C -5.17100 2.31900 19.64200  
H -4.22100 3.98800 20.26200  
C -4.67500 3.59000 19.52800  
H -4.48300 5.18600 18.26900  
C -4.83200 4.30500 18.34200  
C -5.49800 3.73200 17.26400  
H -5.57600 5.45700 16.15600  
H -6.60000 4.34600 15.64500  
C -5.67400 4.49100 15.96400  
H -5.53500 1.43000 12.16300  
C -4.61100 1.21900 12.23400  
H -4.44100 0.35800 10.39500  
C -3.96200 0.57600 11.18600  
H -2.18700 -0.19100 10.57300  
C -2.62500 0.25300 11.29000  
H -1.00000 0.35300 12.50800  
C -1.92100 0.57500 12.43500  
H -2.08300 1.44200 14.26600  
C -2.56700 1.22200 13.47900  
C -3.90900 1.55300 13.38500  
H -4.24900 1.87500 15.38300  
H -5.57700 1.97300 14.50400  
C -4.62100 2.22900 14.53700  
P -4.51800 4.05900 14.58500  
C -5.48000 4.57300 13.09900  
H -6.30800 4.03300 13.05600  
H -4.94600 4.36800 12.29100  
C -5.85500 6.03100 13.07000  
C -4.97300 6.99900 12.59500  
H -4.11200 6.74100 12.28700  
C -5.33800 8.33600 12.56800  
H -4.72800 8.98800 12.24400  
C -6.59300 8.72500 13.01400  
H -6.84200 9.64100 13.00400  
C -7.47400 7.77000 13.47000  
H -8.33800 8.03000 13.76900  
C -7.11300 6.42800 13.49700  
H -7.73100 5.77800 13.81000

### 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  
  
H -4.20210 -2.85091 1.96130  
C -3.70710 -2.46591 2.67530  
H -3.88910 -4.05891 3.92530  
C -3.53510 -3.18091 3.84530  
H -2.71110 -3.10191 5.70730  
C -2.84110 -2.61091 4.90430  
H -1.89110 -0.94191 5.52430  
C -2.34510 -1.33991 4.79030  
H -2.15310 0.25609 3.53130  
C -2.50210 -0.62491 3.60430  
C -3.16810 -1.19791 2.52630  
H -3.24610 0.52709 1.41830  
H -4.27010 -0.58391 0.90730  
C -3.34410 -0.43891 1.22630  
H -3.20510 -3.49991 -2.57470  
C -2.28110 -3.71091 -2.50370  
H -2.11110 -4.57191 -4.34270  
C -1.63210 -4.35391 -3.55170  
H 0.14290 -5.12091 -4.16470  
C -0.29510 -4.67691 -3.44770  
H 1.32990 -4.57691 -2.22970  
C 0.40890 -4.35491 -2.30270  
H 0.24690 -3.48791 -0.47170  
C -0.23710 -3.70791 -1.25870  
C -1.57910 -3.37691 -1.35270  
H -1.91910 -3.05491 0.64530  
H -3.24710 -2.95691 -0.23370  
C -2.29110 -2.70091 -0.20070  
P -2.18810 -0.87091 -0.15270  
C -3.15010 -0.35691 -1.63870  
H -3.97810 -0.89691 -1.68170  
H -2.61610 -0.56191 -2.44670  
C -3.52510 1.10109 -1.66770  
C -2.64310 2.06909 -2.14270  
H -1.78210 1.81109 -2.45070  
C -3.00810 3.40609 -2.16970  
H -2.39810 4.05809 -2.49370  
C -4.26310 3.79509 -1.72370  
H -4.51210 4.71109 -1.73370  
C -5.14410 2.84009 -1.26770  
H -6.00810 3.10009 -0.96870  
C -4.78310 1.49809 -1.24070  
H -5.40110 0.84809 -0.92770  
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  
 125.700 53.834 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 70.015 29.985 99.967

### The %V\_Bur of your molecule is: 30.0