## 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 : 41  
 Atom that is coordinated : 3  
 Atoms that define the axis : 2  
 ID of these atoms : 1 2  
  
 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 :  
N 4.22600 6.59300 17.09200  
N 5.28400 4.75600 17.50000  
C 4.63100 5.43900 16.52300  
C 4.61700 6.64200 18.42000  
H 4.45800 7.35200 19.03100  
C 5.26300 5.49700 18.67700  
H 5.63800 5.23800 19.51000  
C 3.55100 7.68100 16.35900  
H 3.18500 7.30100 15.50900  
C 4.55900 8.76700 15.99400  
H 4.95300 9.14600 16.81900  
H 5.29100 8.37400 15.45600  
C 3.87300 9.87600 15.19500  
H 3.58100 9.51600 14.32000  
H 4.52100 10.60400 15.02300  
C 2.66800 10.44200 15.93000  
H 2.97400 10.91900 16.74200  
H 2.20600 11.09600 15.34800  
C 1.68700 9.33900 16.33000  
H 0.95000 9.73000 16.86300  
H 1.29700 8.93300 15.51600  
C 2.39400 8.25700 17.15300  
H 1.75300 7.53700 17.37900  
H 2.73100 8.64700 17.99800  
C 5.93400 3.45300 17.30500  
H 5.99600 3.29700 16.32000  
C 7.35100 3.47000 17.85000  
H 7.86900 4.18500 17.40300  
H 7.33000 3.66600 18.82100  
C 8.02600 2.12800 17.61600  
H 8.91700 2.13400 18.04700  
H 8.16000 1.99800 16.64400  
C 7.21700 0.97000 18.16500  
H 7.65800 0.11700 17.92400  
H 7.18600 1.03000 19.15300  
C 5.80100 0.98000 17.61300  
H 5.82700 0.82200 16.63600  
H 5.28000 0.24900 18.02900  
C 5.11600 2.31400 17.89300  
H 5.02200 2.44200 18.87000  
H 4.21100 2.31400 17.49300

### 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  
  
N -0.08952 1.75317 2.53569  
N 0.96848 -0.08383 2.94369  
C 0.31548 0.59917 1.96669  
C 0.30148 1.80217 3.86369  
H 0.14248 2.51217 4.47469  
C 0.94748 0.65717 4.12069  
H 1.32248 0.39817 4.95369  
C -0.76452 2.84117 1.80269  
H -1.13052 2.46117 0.95269  
C 0.24348 3.92717 1.43769  
H 0.63748 4.30617 2.26269  
H 0.97548 3.53417 0.89969  
C -0.44252 5.03617 0.63869  
H -0.73452 4.67617 -0.23631  
H 0.20548 5.76417 0.46669  
C -1.64752 5.60217 1.37369  
H -1.34152 6.07917 2.18569  
H -2.10952 6.25617 0.79169  
C -2.62852 4.49917 1.77369  
H -3.36552 4.89017 2.30669  
H -3.01852 4.09317 0.95969  
C -1.92152 3.41717 2.59669  
H -2.56252 2.69717 2.82269  
H -1.58452 3.80717 3.44169  
C 1.61848 -1.38683 2.74869  
H 1.68048 -1.54283 1.76369  
C 3.03548 -1.36983 3.29369  
H 3.55348 -0.65483 2.84669  
H 3.01448 -1.17383 4.26469  
C 3.71048 -2.71183 3.05969  
H 4.60148 -2.70583 3.49069  
H 3.84448 -2.84183 2.08769  
C 2.90148 -3.86983 3.60869  
H 3.34248 -4.72283 3.36769  
H 2.87048 -3.80983 4.59669  
C 1.48548 -3.85983 3.05669  
H 1.51148 -4.01783 2.07969  
H 0.96448 -4.59083 3.47269  
C 0.80048 -2.52583 3.33669  
H 0.70648 -2.39783 4.31369  
H -0.10452 -2.52583 2.93669  
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  
 131.669 47.866 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 73.339 26.661 99.967

### The %V\_Bur of your molecule is: 26.7