## 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 : 53  
 Atom that is coordinated : 4  
 Atoms that define the axis : 2  
 ID of these atoms : 2 3  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.050  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
C -2.62800 -0.08100 8.05400  
N -5.97900 0.98900 6.89200  
N -7.34500 2.41800 6.07100  
C -6.39400 2.27200 7.03000  
C -6.65900 0.33200 5.85500  
C -7.51700 1.22400 5.34500  
C -6.41300 -1.10200 5.53700  
H -6.81100 -1.31600 4.66700  
H -5.44800 -1.26800 5.50400  
H -6.81800 -1.66400 6.22900  
C -8.51100 1.09500 4.23800  
H -8.48200 0.18400 3.87700  
H -9.40900 1.28100 4.58200  
H -8.29400 1.73400 3.52800  
C -4.93900 0.36400 7.67500  
C -5.29200 -0.47600 8.73300  
C -4.26400 -1.09800 9.44100  
H -4.48300 -1.66800 10.16800  
C -2.94500 -0.90700 9.11600  
C -9.66200 2.59400 7.75800  
H -1.71500 0.05300 7.83000  
C -3.61200 0.56200 7.30200  
C -6.74600 -0.73200 9.09400  
H -7.31800 -0.09400 8.61800  
H -6.99000 -1.64600 8.83600  
H -6.86700 -0.62300 10.06000  
C -1.83300 -1.60500 9.89100  
H -1.70700 -2.51000 9.53700  
H -1.00000 -1.09800 9.79400  
H -2.07700 -1.65500 10.83800  
C -3.25400 1.42600 6.12700  
H -3.34400 2.37000 6.37600  
H -2.32800 1.24700 5.85900  
H -3.85500 1.22700 5.37900  
C -8.20600 3.56600 5.91700  
C -9.35400 3.64000 6.71800  
C -10.21300 4.71200 6.53000  
H -10.99900 4.77300 7.06100  
C -9.95900 5.70300 5.58600  
C -8.81400 5.59100 4.80700  
H -8.62300 6.26700 4.16800  
C -7.93800 4.51500 4.93800  
H -10.61500 2.62800 7.98200  
H -9.44000 1.70700 7.40400  
H -9.13000 2.76700 8.56200  
C -10.93500 6.83600 5.39200  
H -11.64900 6.77000 6.06000  
H -10.46800 7.69100 5.49700  
H -11.32300 6.78300 4.49400  
C -6.75100 4.39100 4.01000  
H -6.82500 3.56100 3.49500  
H -6.73500 5.15500 3.39700  
H -5.92500 4.37600 4.53700

### 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 3.10739 -3.75008 -0.32393  
N -0.24361 -2.68008 -1.48593  
N -1.60961 -1.25108 -2.30693  
C -0.65861 -1.39708 -1.34793  
C -0.92361 -3.33708 -2.52293  
C -1.78161 -2.44508 -3.03293  
C -0.67761 -4.77108 -2.84093  
H -1.07561 -4.98508 -3.71093  
H 0.28739 -4.93708 -2.87393  
H -1.08261 -5.33308 -2.14893  
C -2.77561 -2.57408 -4.13993  
H -2.74661 -3.48508 -4.50093  
H -3.67361 -2.38808 -3.79593  
H -2.55861 -1.93508 -4.84993  
C 0.79639 -3.30508 -0.70293  
C 0.44339 -4.14508 0.35507  
C 1.47139 -4.76708 1.06307  
H 1.25239 -5.33708 1.79007  
C 2.79039 -4.57608 0.73807  
C -3.92661 -1.07508 -0.61993  
H 4.02039 -3.61608 -0.54793  
C 2.12339 -3.10708 -1.07593  
C -1.01061 -4.40108 0.71607  
H -1.58261 -3.76308 0.24007  
H -1.25461 -5.31508 0.45807  
H -1.13161 -4.29208 1.68207  
C 3.90239 -5.27408 1.51307  
H 4.02839 -6.17908 1.15907  
H 4.73539 -4.76708 1.41607  
H 3.65839 -5.32408 2.46007  
C 2.48139 -2.24308 -2.25093  
H 2.39139 -1.29908 -2.00193  
H 3.40739 -2.42208 -2.51893  
H 1.88039 -2.44208 -2.99893  
C -2.47061 -0.10308 -2.46093  
C -3.61861 -0.02908 -1.65993  
C -4.47761 1.04292 -1.84793  
H -5.26361 1.10392 -1.31693  
C -4.22361 2.03392 -2.79193  
C -3.07861 1.92192 -3.57093  
H -2.88761 2.59792 -4.20993  
C -2.20261 0.84592 -3.43993  
H -4.87961 -1.04108 -0.39593  
H -3.70461 -1.96208 -0.97393  
H -3.39461 -0.90208 0.18407  
C -5.19961 3.16692 -2.98593  
H -5.91361 3.10092 -2.31793  
H -4.73261 4.02192 -2.88093  
H -5.58761 3.11392 -3.88393  
C -1.01561 0.72192 -4.36793  
H -1.08961 -0.10808 -4.88293  
H -0.99961 1.48592 -4.98093  
H -0.18961 0.70692 -3.84093  
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  
 120.469 59.065 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 67.101 32.899 99.967

### The %V\_Bur of your molecule is: 32.9