## 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 : 89  
 Atom that is coordinated : 21  
 Atoms that define the axis : 2  
 ID of these atoms : 3 4  
  
 Radius of sphere (Angs) : 3.500  
 Distance from sphere (Angs) : 2.000  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
C -0.63900 -1.05200 2.63100  
C -1.84200 -1.24800 2.05700  
N 0.21700 -0.60700 1.62900  
N -1.70500 -0.92300 0.71500  
C -2.82800 -0.96800 -0.17800  
C -3.06400 -2.14600 -0.90400  
C -3.65800 0.16300 -0.24500  
C -4.19700 -2.16800 -1.72000  
C -4.76200 0.09400 -1.09800  
C -5.03300 -1.06300 -1.81900  
C 1.62700 -0.49200 1.88300  
C 2.38000 -1.68200 1.89900  
C 2.17000 0.76600 2.18700  
C 3.73400 -1.57300 2.21800  
C 3.53500 0.81600 2.48800  
C 4.30500 -0.33800 2.50500  
C 1.30800 2.00900 2.20700  
C 1.75100 -3.01700 1.54500  
C -3.37000 1.40200 0.57800  
C -2.13500 -3.34500 -0.81100  
C -0.43500 -0.49100 0.42400  
C -3.44900 2.68400 -0.25800  
C -4.22400 1.44900 1.86000  
C 2.02200 3.22100 1.59800  
C 0.72200 2.26900 3.60800  
C -2.16100 -4.21300 -2.07700  
C -2.39700 -4.18500 0.45800  
C 1.74800 -3.24500 0.02100  
C 2.34500 -4.19300 2.32500  
C -3.02700 3.92100 0.51900  
C -5.71000 1.69900 1.66100  
C 1.09200 4.39600 1.34600  
C 1.72100 2.70200 4.66900  
C 3.10600 -3.50700 -0.60800  
C 1.57500 -5.48700 2.11000  
C -3.85100 -4.57100 0.68100  
C -0.96900 -5.15000 -2.19500  
H -3.80600 2.22800 2.51600  
H -4.42600 -3.06000 -2.30000  
H -5.42000 0.95500 -1.20000  
H 4.35700 -2.46600 2.24100  
H 3.99900 1.77400 2.71400  
H 0.44200 1.80900 1.55900  
H 0.68900 -2.97300 1.83700  
H -2.32400 1.33700 0.92200  
H -1.10800 -2.95400 -0.72100  
H 5.36500 -0.27800 2.74900  
H -5.90600 -1.10100 -2.47000  
H -2.79300 2.55800 -1.13300  
H -4.46400 2.83200 -0.65900  
H 2.34200 -3.93400 3.39500  
H -4.08500 0.50200 2.40300  
H 2.85900 3.54500 2.23600  
H 2.47600 2.90800 0.64400  
H -0.07000 3.02900 3.51300  
H 0.20900 1.35200 3.94100  
H -3.09200 -4.80300 -2.11500  
H -2.18500 -3.55700 -2.96200  
H -1.77700 -5.09300 0.40200  
H -2.02900 -3.63900 1.33900  
H 1.06600 -4.08100 -0.20300  
H 1.29800 -2.35700 -0.45000  
H 3.40000 -4.35200 2.05800  
H -3.74800 4.17900 1.30600  
H -2.93300 4.79200 -0.14000  
H -2.05100 3.76400 1.00600  
H -6.22900 1.73200 2.62700  
H -6.17900 0.90600 1.06300  
H -5.90100 2.65600 1.15500  
H 1.62000 5.21800 0.84900  
H 0.66400 4.79500 2.27600  
H 0.25800 4.09700 0.69300  
H 2.52200 1.96200 4.79500  
H 1.22800 2.82400 5.64100  
H 2.19100 3.66400 4.42000  
H 3.01000 -3.61000 -1.69800  
H 3.56200 -4.43500 -0.23400  
H 3.80500 -2.68300 -0.40700  
H 0.49900 -5.34200 2.28900  
H 1.92400 -6.27300 2.79100  
H 1.68900 -5.86800 1.08600  
H -4.47500 -3.68500 0.86800  
H -3.95000 -5.23800 1.54600  
H -4.27700 -5.09300 -0.18700  
H -0.89900 -5.85300 -1.35300  
H -0.02600 -4.58400 -2.23400  
H -1.03100 -5.75000 -3.11200  
H -0.28400 -1.21400 3.64000  
H -2.78300 -1.60200 2.45800

### 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 -0.92728 -1.20236 3.95786  
C -2.13028 -1.39836 3.38386  
N -0.07128 -0.75736 2.95586  
N -1.99328 -1.07336 2.04186  
C -3.11628 -1.11836 1.14886  
C -3.35228 -2.29636 0.42286  
C -3.94628 0.01264 1.08186  
C -4.48528 -2.31836 -0.39314  
C -5.05028 -0.05636 0.22886  
C -5.32128 -1.21336 -0.49214  
C 1.33872 -0.64236 3.20986  
C 2.09172 -1.83236 3.22586  
C 1.88172 0.61564 3.51386  
C 3.44572 -1.72336 3.54486  
C 3.24672 0.66564 3.81486  
C 4.01672 -0.48836 3.83186  
C 1.01972 1.85864 3.53386  
C 1.46272 -3.16736 2.87186  
C -3.65828 1.25164 1.90486  
C -2.42328 -3.49536 0.51586  
C -0.72328 -0.64136 1.75086  
C -3.73728 2.53364 1.06886  
C -4.51228 1.29864 3.18686  
C 1.73372 3.07064 2.92486  
C 0.43372 2.11864 4.93486  
C -2.44928 -4.36336 -0.75014  
C -2.68528 -4.33536 1.78486  
C 1.45972 -3.39536 1.34786  
C 2.05672 -4.34336 3.65186  
C -3.31528 3.77064 1.84586  
C -5.99828 1.54864 2.98786  
C 0.80372 4.24564 2.67286  
C 1.43272 2.55164 5.99586  
C 2.81772 -3.65736 0.71886  
C 1.28672 -5.63736 3.43686  
C -4.13928 -4.72136 2.00786  
C -1.25728 -5.30036 -0.86814  
H -4.09428 2.07764 3.84286  
H -4.71428 -3.21036 -0.97314  
H -5.70828 0.80464 0.12686  
H 4.06872 -2.61636 3.56786  
H 3.71072 1.62364 4.04086  
H 0.15372 1.65864 2.88586  
H 0.40072 -3.12336 3.16386  
H -2.61228 1.18664 2.24886  
H -1.39628 -3.10436 0.60586  
H 5.07672 -0.42836 4.07586  
H -6.19428 -1.25136 -1.14314  
H -3.08128 2.40764 0.19386  
H -4.75228 2.68164 0.66786  
H 2.05372 -4.08436 4.72186  
H -4.37328 0.35164 3.72986  
H 2.57072 3.39464 3.56286  
H 2.18772 2.75764 1.97086  
H -0.35828 2.87864 4.83986  
H -0.07928 1.20164 5.26786  
H -3.38028 -4.95336 -0.78814  
H -2.47328 -3.70736 -1.63514  
H -2.06528 -5.24336 1.72886  
H -2.31728 -3.78936 2.66586  
H 0.77772 -4.23136 1.12386  
H 1.00972 -2.50736 0.87686  
H 3.11172 -4.50236 3.38486  
H -4.03628 4.02864 2.63286  
H -3.22128 4.64164 1.18686  
H -2.33928 3.61364 2.33286  
H -6.51728 1.58164 3.95386  
H -6.46728 0.75564 2.38986  
H -6.18928 2.50564 2.48186  
H 1.33172 5.06764 2.17586  
H 0.37572 4.64464 3.60286  
H -0.03028 3.94664 2.01986  
H 2.23372 1.81164 6.12186  
H 0.93972 2.67364 6.96786  
H 1.90272 3.51364 5.74686  
H 2.72172 -3.76036 -0.37114  
H 3.27372 -4.58536 1.09286  
H 3.51672 -2.83336 0.91986  
H 0.21072 -5.49236 3.61586  
H 1.63572 -6.42336 4.11786  
H 1.40072 -6.01836 2.41286  
H -4.76328 -3.83536 2.19486  
H -4.23828 -5.38836 2.87286  
H -4.56528 -5.24336 1.13986  
H -1.18728 -6.00336 -0.02614  
H -0.31428 -4.73436 -0.90714  
H -1.31928 -5.90036 -1.78514  
H -0.57228 -1.36436 4.96686  
H -3.07128 -1.75236 3.78486  
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  
 112.901 66.633 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 62.886 37.114 99.967

### The %V\_Bur of your molecule is: 37.1