## 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 : 47  
 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) : 2.110  
 Mesh step (Angs) : 0.050  
 H atoms omitted in the V\_bur calculation

### Cartesian coordinates from input :

Cartesian coordinates from input :  
N 1.47200 0.99300 5.34000  
N 2.59400 1.78400 3.66800  
C 1.35000 1.76100 4.23300  
C 2.79900 0.56600 5.45600  
H 3.15200 0.02400 6.15100  
C 3.47300 1.04400 4.43800  
H 4.39600 0.90600 4.26100  
C 0.49300 0.67000 6.33200  
C 0.36200 1.51300 7.43200  
C -0.52400 1.12800 8.41000  
H -0.64300 1.69400 9.16300  
C -1.25400 -0.05200 8.34400  
C -1.06500 -0.85600 7.22600  
H -1.54000 -1.67600 7.16700  
C -0.21100 -0.50700 6.19900  
C 1.14400 2.80500 7.55900  
H 2.09400 2.62800 7.39800  
H 0.81500 3.45200 6.90100  
H 1.02800 3.16900 8.46200  
C -2.16500 -0.48600 9.46200  
H -2.57700 0.30200 9.87200  
H -2.86500 -1.07200 9.10400  
H -1.64600 -0.97200 10.13600  
C -0.04700 -1.41200 5.01100  
H 0.88900 -1.40300 4.72000  
H -0.30300 -2.32500 5.25800  
H -0.61900 -1.09900 4.28000  
C 3.03300 2.60800 2.57400  
C 3.08000 2.09600 1.27800  
C 3.43200 2.96300 0.26200  
H 3.43200 2.65100 -0.63500  
C 3.78700 4.28300 0.52000  
C 3.82900 4.72200 1.83600  
H 4.12700 5.60500 2.02000  
C 3.44500 3.90200 2.89200  
C 2.79900 0.64600 0.97300  
H 2.27900 0.25300 1.70500  
H 2.29100 0.57900 0.13800  
H 3.64600 0.16200 0.87900  
C 4.10700 5.24800 -0.60700  
H 3.34000 5.83800 -0.76000  
H 4.89000 5.78600 -0.36400  
H 4.29900 4.74300 -1.42500  
C 3.47700 4.40000 4.31100  
H 4.05200 3.81700 4.85000  
H 3.83100 5.31400 4.32900  
H 2.56900 4.39400 4.68000

### 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 1.87132 -1.72206 1.80109  
N 2.99332 -0.93106 0.12909  
C 1.74932 -0.95406 0.69409  
C 3.19832 -2.14906 1.91709  
H 3.55132 -2.69106 2.61209  
C 3.87232 -1.67106 0.89909  
H 4.79532 -1.80906 0.72209  
C 0.89232 -2.04506 2.79309  
C 0.76132 -1.20206 3.89309  
C -0.12468 -1.58706 4.87109  
H -0.24368 -1.02106 5.62409  
C -0.85468 -2.76706 4.80509  
C -0.66568 -3.57106 3.68709  
H -1.14068 -4.39106 3.62809  
C 0.18832 -3.22206 2.66009  
C 1.54332 0.08994 4.02009  
H 2.49332 -0.08706 3.85909  
H 1.21432 0.73694 3.36209  
H 1.42732 0.45394 4.92309  
C -1.76568 -3.20106 5.92309  
H -2.17768 -2.41306 6.33309  
H -2.46568 -3.78706 5.56509  
H -1.24668 -3.68706 6.59709  
C 0.35232 -4.12706 1.47209  
H 1.28832 -4.11806 1.18109  
H 0.09632 -5.04006 1.71909  
H -0.21968 -3.81406 0.74109  
C 3.43232 -0.10706 -0.96491  
C 3.47932 -0.61906 -2.26091  
C 3.83132 0.24794 -3.27691  
H 3.83132 -0.06406 -4.17391  
C 4.18632 1.56794 -3.01891  
C 4.22832 2.00694 -1.70291  
H 4.52632 2.88994 -1.51891  
C 3.84432 1.18694 -0.64691  
C 3.19832 -2.06906 -2.56591  
H 2.67832 -2.46206 -1.83391  
H 2.69032 -2.13606 -3.40091  
H 4.04532 -2.55306 -2.65991  
C 4.50632 2.53294 -4.14591  
H 3.73932 3.12294 -4.29891  
H 5.28932 3.07094 -3.90291  
H 4.69832 2.02794 -4.96391  
C 3.87632 1.68494 0.77209  
H 4.45132 1.10194 1.31109  
H 4.23032 2.59894 0.79009  
H 2.96832 1.67894 1.14109  
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  
 124.552 54.983 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 69.375 30.625 99.967

### The %V\_Bur of your molecule is: 30.6