**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 : 41  
 Atom that is coordinated : 27  
 Atoms that define the axis : 2  
 ID of these atoms : 28 29  
  
 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 :  
H -6.14800 -0.94800 6.12300  
H -7.38500 -0.42300 6.99700  
C -6.65400 -1.08900 6.96200  
H -6.26900 -1.03000 8.98300  
C -5.73300 -0.89700 8.15000  
H -5.67800 4.44600 9.77000  
H -4.78100 4.92300 8.53100  
C -4.75600 4.67400 9.48900  
H -4.84000 6.64100 10.13700  
H -4.31100 5.63800 11.26800  
C -4.25800 5.85800 10.30500  
H -2.51800 6.95200 10.52200  
H -2.78700 6.50800 9.00600  
C -2.82900 6.20800 9.94800  
H -1.89900 4.75400 11.10100  
H -1.00000 5.23300 9.86500  
C -1.92100 4.99800 10.14100  
H -1.83000 3.01300 9.51500  
H -2.33300 4.00200 8.35800  
C -2.40400 3.79700 9.32400  
H -3.90100 3.18000 10.63000  
C -3.86000 3.46500 9.67200  
H -5.07600 0.97100 6.13400  
C -4.91800 1.23100 7.03400  
H -4.09000 3.10700 6.89300  
C -4.38400 2.39200 7.44500  
C -4.84900 1.17900 9.27200  
N -5.19300 0.48600 8.16400  
N -4.34300 2.34900 8.82700  
C -7.24400 -2.50000 6.97500  
H -7.81400 -2.62600 6.17600  
H -7.81200 -2.61200 7.77800  
C -6.14500 -3.54400 6.98300  
H -6.54900 -4.44500 7.04500  
H -5.63800 -3.49300 6.13400  
C -5.19700 -3.33500 8.14900  
H -5.68300 -3.48400 8.99800  
H -4.46200 -3.99600 8.09700  
C -4.61000 -1.92100 8.14300  
H -4.04900 -1.79600 7.33700  
H -4.03700 -1.79400 8.94000

**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 -1.09261 -1.51930 -5.12751  
H -2.32961 -0.99430 -4.25351  
C -1.59861 -1.66030 -4.28851  
H -1.21361 -1.60130 -2.26751  
C -0.67761 -1.46830 -3.10051  
H -0.62261 3.87470 -1.48051  
H 0.27439 4.35170 -2.71951  
C 0.29939 4.10270 -1.76151  
H 0.21539 6.06970 -1.11351  
H 0.74439 5.06670 0.01749  
C 0.79739 5.28670 -0.94551  
H 2.53739 6.38070 -0.72851  
H 2.26839 5.93670 -2.24451  
C 2.22639 5.63670 -1.30251  
H 3.15639 4.18270 -0.14951  
H 4.05539 4.66170 -1.38551  
C 3.13439 4.42670 -1.10951  
H 3.22539 2.44170 -1.73551  
H 2.72239 3.43070 -2.89251  
C 2.65139 3.22570 -1.92651  
H 1.15439 2.60870 -0.62051  
C 1.19539 2.89370 -1.57851  
H -0.02061 0.39970 -5.11651  
C 0.13739 0.65970 -4.21651  
H 0.96539 2.53570 -4.35751  
C 0.67139 1.82070 -3.80551  
C 0.20639 0.60770 -1.97851  
N -0.13761 -0.08530 -3.08651  
N 0.71239 1.77770 -2.42351  
C -2.18861 -3.07130 -4.27551  
H -2.75861 -3.19730 -5.07451  
H -2.75661 -3.18330 -3.47251  
C -1.08961 -4.11530 -4.26751  
H -1.49361 -5.01630 -4.20551  
H -0.58261 -4.06430 -5.11651  
C -0.14161 -3.90630 -3.10151  
H -0.62761 -4.05530 -2.25251  
H 0.59339 -4.56730 -3.15351  
C 0.44539 -2.49230 -3.10751  
H 1.00639 -2.36730 -3.91351  
H 1.01839 -2.36530 -2.31051  
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  
 131.718 47.817 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 73.366 26.634 99.967

**The %V\_Bur of your molecule is: 26.6**