**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 : 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 :  
H -10.21300 4.96500 12.03700  
N -9.86000 2.55500 13.49100  
N -7.93000 1.71400 13.06900  
C -9.23400 1.66700 12.67800  
C -8.97700 3.13900 14.37500  
H -9.18700 3.77900 15.04500  
C -7.76800 2.63000 14.10700  
H -6.95300 2.85200 14.54200  
C -11.28300 2.82500 13.42200  
C -12.11700 2.22800 14.36200  
C -13.48500 2.43200 14.23100  
H -14.08200 2.01600 14.84100  
C -13.98700 3.22800 13.23000  
H -14.92500 3.34200 13.13800  
C -13.12300 3.86300 12.35700  
H -13.48000 4.43700 11.69000  
C -11.74900 3.68200 12.43000  
C -11.58000 1.37400 15.47400  
H -12.30900 1.13700 16.08500  
H -11.19000 0.55700 15.09900  
H -10.89200 1.87000 15.96400  
C -10.82000 4.40200 11.51200  
H -10.29900 3.75000 10.99900  
H -11.33700 4.96300 10.89800  
C -6.86000 0.93900 12.48300  
C -5.98800 1.57400 11.60800  
C -4.95300 0.81100 11.06600  
H -4.32700 1.21900 10.48000  
C -4.82900 -0.52900 11.37000  
H -4.13700 -1.04400 10.97200  
C -5.70200 -1.11600 12.24600  
H -5.59800 -2.03700 12.45400  
C -6.73900 -0.39900 12.84100  
C -6.14400 3.02700 11.24500  
H -5.94300 3.58200 12.02700  
H -5.52500 3.25000 10.51900  
H -7.06400 3.19300 10.95300  
C -7.65200 -1.05300 13.85100  
H -8.50200 -1.28500 13.42100  
H -7.22800 -1.86700 14.19600  
H -7.81900 -0.43300 14.59100

**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 -0.14592 4.44686 0.83839  
N 0.20708 2.03686 2.29239  
N 2.13708 1.19586 1.87039  
C 0.83308 1.14886 1.47939  
C 1.09008 2.62086 3.17639  
H 0.88008 3.26086 3.84639  
C 2.29908 2.11186 2.90839  
H 3.11408 2.33386 3.34339  
C -1.21592 2.30686 2.22339  
C -2.04992 1.70986 3.16339  
C -3.41792 1.91386 3.03239  
H -4.01492 1.49786 3.64239  
C -3.91992 2.70986 2.03139  
H -4.85792 2.82386 1.93939  
C -3.05592 3.34486 1.15839  
H -3.41292 3.91886 0.49139  
C -1.68192 3.16386 1.23139  
C -1.51292 0.85586 4.27539  
H -2.24192 0.61886 4.88639  
H -1.12292 0.03886 3.90039  
H -0.82492 1.35186 4.76539  
C -0.75292 3.88386 0.31339  
H -0.23192 3.23186 -0.19961  
H -1.26992 4.44486 -0.30061  
C 3.20708 0.42086 1.28439  
C 4.07908 1.05586 0.40939  
C 5.11408 0.29286 -0.13261  
H 5.74008 0.70086 -0.71861  
C 5.23808 -1.04714 0.17139  
H 5.93008 -1.56214 -0.22661  
C 4.36508 -1.63414 1.04739  
H 4.46908 -2.55514 1.25539  
C 3.32808 -0.91714 1.64239  
C 3.92308 2.50886 0.04639  
H 4.12408 3.06386 0.82839  
H 4.54208 2.73186 -0.67961  
H 3.00308 2.67486 -0.24561  
C 2.41508 -1.57114 2.65239  
H 1.56508 -1.80314 2.22239  
H 2.83908 -2.38514 2.99739  
H 2.24808 -0.95114 3.39239  
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  
 118.111 61.424 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 65.787 34.213 99.967

**The %V\_Bur of your molecule is: 34.2**