## 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 : 71  
 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 -0.13000 -1.97600 2.62000  
C -1.43100 -2.03200 2.25100  
N 0.51400 -1.15000 1.69300  
N -1.55000 -1.24200 1.10200  
C -2.79600 -1.09000 0.41200  
C -3.11500 -2.00600 -0.60200  
C -3.68100 -0.08800 0.84100  
C -4.36500 -1.88200 -1.20900  
C -4.93100 -0.02700 0.22200  
C -5.26800 -0.90900 -0.79600  
C 1.92600 -0.90600 1.75200  
C 2.79100 -1.84600 1.17400  
C 2.38800 0.23900 2.42500  
C 4.16400 -1.61000 1.27400  
C 3.76800 0.42100 2.50800  
C 4.64900 -0.49200 1.93700  
C 1.43100 1.23500 3.05400  
C 2.29500 -3.07800 0.44400  
C -3.32600 0.88400 1.94900  
C -2.17200 -3.11500 -1.01900  
C -0.35300 -0.69300 0.73200  
C -3.50100 2.33800 1.51300  
C -4.14500 0.60700 3.21000  
C 2.00400 2.64700 3.12700  
C 0.98900 0.79400 4.45100  
C -1.86900 -3.07800 -2.51400  
C -2.72900 -4.48000 -0.61300  
C 2.64700 -3.02400 -1.04200  
C 2.84700 -4.35900 1.06900  
C -2.55300 -2.79600 2.85700  
C 0.56900 -2.69000 3.71900  
H -6.24500 -0.83900 -1.27100  
H -4.64600 -2.56900 -2.00700  
H -5.64900 0.73100 0.53700  
H 4.86200 -2.31700 0.82800  
H 4.16800 1.29300 3.02200  
H 0.53100 1.27200 2.42000  
H 1.19700 -3.11000 0.52300  
H -2.26400 0.73900 2.20600  
H -1.21600 -2.97400 -0.49000  
H 5.72200 -0.32700 2.01100  
H 0.37400 1.57500 4.91800  
H -2.91700 2.56900 0.61200  
H -3.16700 3.01300 2.31300  
H -4.55400 2.57200 1.30300  
H -5.21900 0.73900 3.01900  
H -3.86100 1.30100 4.01100  
H -3.99400 -0.41600 3.57900  
H 2.78400 2.72700 3.89800  
H 1.21100 3.35500 3.39900  
H 2.43500 2.96800 2.17000  
H 1.86400 0.62300 5.09500  
H 0.39300 -0.12700 4.42800  
H -2.76600 -3.28700 -3.11500  
H -1.11900 -3.84100 -2.76600  
H -1.47800 -2.09800 -2.82100  
H -2.01700 -5.27700 -0.86700  
H -3.67100 -4.69500 -1.13800  
H -2.93000 -4.53300 0.46600  
H 2.21800 -3.89000 -1.56600  
H 3.73500 -3.05000 -1.19200  
H 2.25900 -2.11200 -1.51400  
H 3.93600 -4.42800 0.93800  
H 2.40200 -5.24100 0.59000  
H 2.64200 -4.41400 2.14600  
H -2.55700 -2.68500 3.94900  
H -2.47800 -3.87100 2.64100  
H -3.52400 -2.45200 2.48100  
H 0.91000 -3.68600 3.40300  
H -0.10800 -2.83500 4.57000  
H 1.44800 -2.13900 4.07400

### 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 -0.16507 -2.46602 3.45321  
C -1.46607 -2.52202 3.08421  
N 0.47893 -1.64002 2.52621  
N -1.58507 -1.73202 1.93521  
C -2.83107 -1.58002 1.24521  
C -3.15007 -2.49602 0.23121  
C -3.71607 -0.57802 1.67421  
C -4.40007 -2.37202 -0.37579  
C -4.96607 -0.51702 1.05521  
C -5.30307 -1.39902 0.03721  
C 1.89093 -1.39602 2.58521  
C 2.75593 -2.33602 2.00721  
C 2.35293 -0.25102 3.25821  
C 4.12893 -2.10002 2.10721  
C 3.73293 -0.06902 3.34121  
C 4.61393 -0.98202 2.77021  
C 1.39593 0.74498 3.88721  
C 2.25993 -3.56802 1.27721  
C -3.36107 0.39398 2.78221  
C -2.20707 -3.60502 -0.18579  
C -0.38807 -1.18302 1.56521  
C -3.53607 1.84798 2.34621  
C -4.18007 0.11698 4.04321  
C 1.96893 2.15698 3.96021  
C 0.95393 0.30398 5.28421  
C -1.90407 -3.56802 -1.68079  
C -2.76407 -4.97002 0.22021  
C 2.61193 -3.51402 -0.20879  
C 2.81193 -4.84902 1.90221  
C -2.58807 -3.28602 3.69021  
C 0.53393 -3.18002 4.55221  
H -6.28007 -1.32902 -0.43779  
H -4.68107 -3.05902 -1.17379  
H -5.68407 0.24098 1.37021  
H 4.82693 -2.80702 1.66121  
H 4.13293 0.80298 3.85521  
H 0.49593 0.78198 3.25321  
H 1.16193 -3.60002 1.35621  
H -2.29907 0.24898 3.03921  
H -1.25107 -3.46402 0.34321  
H 5.68693 -0.81702 2.84421  
H 0.33893 1.08498 5.75121  
H -2.95207 2.07898 1.44521  
H -3.20207 2.52298 3.14621  
H -4.58907 2.08198 2.13621  
H -5.25407 0.24898 3.85221  
H -3.89607 0.81098 4.84421  
H -4.02907 -0.90602 4.41221  
H 2.74893 2.23698 4.73121  
H 1.17593 2.86498 4.23221  
H 2.39993 2.47798 3.00321  
H 1.82893 0.13298 5.92821  
H 0.35793 -0.61702 5.26121  
H -2.80107 -3.77702 -2.28179  
H -1.15407 -4.33102 -1.93279  
H -1.51307 -2.58802 -1.98779  
H -2.05207 -5.76702 -0.03379  
H -3.70607 -5.18502 -0.30479  
H -2.96507 -5.02302 1.29921  
H 2.18293 -4.38002 -0.73279  
H 3.69993 -3.54002 -0.35879  
H 2.22393 -2.60202 -0.68079  
H 3.90093 -4.91802 1.77121  
H 2.36693 -5.73102 1.42321  
H 2.60693 -4.90402 2.97921  
H -2.59207 -3.17502 4.78221  
H -2.51307 -4.36102 3.47421  
H -3.55907 -2.94202 3.31421  
H 0.87493 -4.17602 4.23621  
H -0.14307 -3.32502 5.40321  
H 1.41293 -2.62902 4.90721  
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  
 114.439 65.096 179.535 179.594  
  
 %V\_Free %V\_Bur % Tot/Ex  
 63.742 36.258 99.967

### The %V\_Bur of your molecule is: 36.3