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# Comparative study of benznidazole encapsulation in boron nitride and carbon nanotubes: A quantum chemistry study

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**S1.** Script to generate cartesian coordinates for BNNT and CNT models.

```
#!/bin/bash
#UEG - UnUCET - Nanotubos das formas [(XY)n]m, com n e m PARES E IMPARES
#FORMA ZIG-ZAG ou BARCO  - v.08
#Dr. José Divino dos Santos e MsC.Jeziel Rodrigues
#como executar: ./shell-nano-otim-xy-par-impar.sh $1 $2 $3 $4 $5 $6 $7 $8 $9
$10 $11 $12 $13 $14

pi=` echo "scale=10;4*a(1)"|bc -l `
n0=$1         #Numero de atomos na base  GaAs, ZnO, C, BN ...
m=$2          #Numero de niveis do nanotubo
d=$3          #distancia X-X
tipo=$4       #tipo de crescimento - zig ou bar
atomo1=$5     #Simbolo atomico 1
atomo2=$6     #Simbolo atomico 2
metodo=$7     #Metodo semiempirico - MNDO, AM1, PM3
multi=$8      #Multiplicidades - SINGLET, DOUBLET, TRIPLET, QUARTET ...
carga=$9      #Cargas - +2, +1, 0, -1, -2 ...
shift;shift;shift;shift;shift;shift;shift;shift;shift;shift;
metodoAb=$1   #Metodo Ab-initio: HF, RHF, UHF, DFT, ...
baseAb=$2     #Base Ab-initio: 3-21G, 6-31G, lanl2dz, GEN, ...
multiAb=$3    #Multiplicidades  abinitio: 1, 2, 3, 4 ...
cargaAb=$4    #Cargas - +2, +1, 0, -1, -2 ...
grad=$5       #Gradiente procurado
fatd1=1.0  #fator de D1=fatd1*D1
fatd2=1.0  #fator de D2=fatd2*D2
fatd3=1.0  #fator de D3=fatd3*D3
```



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```
otimd=1.0  #otimizador de distancia
otima=1.0  #otimizador de angulo
otimt=1.0  #otimizador de torsao
#Exemplos:
if [ "${tipo}" = "zig" ]
then
   #Crescimento ZIG-ZAG
  n=` echo "${n0}"|bc -l ` #numero de atomos X na base
  nome=nano${tipo}-${atomo1}${atomo2}-n${n}-m${m}-${metodo}-${multi}-
c${carga}
  te=` echo "scale=10;(0.0000*2*${pi}/${n})"|bc -l `  #angulo inicial; zero
grau
  dte=` echo "scale=10;(2*${pi}/${n})"|bc -l ` #incremento do angulo
  D1=`echo "scale=10;${fatd1}*(2*${d}*c(${pi}/6))"|bc -l ` # distancia basica
X-X
  ra=`echo "scale=10;(${D1})/(sqrt(2 - 2*c(2*${pi}/${n})))"|bc -l ` #raio
ZIG-ZAG
  #curv=`echo "scale=10;1/${ra}"|bc -l ` # distancia basica do ZIG-ZAG
  inc1=0.00000
  inc2=` echo "scale=10;1.0000*(${pi}/${n})"|bc -l ` #angulo inicial de Y
  incte=` echo "scale=10;1.0000*(${pi}/${n})"|bc -l ` #incremento do angulo
no nivel
  D2=`echo "scale=10;${fatd2}*(${d}*s(${pi}/6))"|bc -l `  # incr D2*fat2
  D3=`echo "scale=10;${fatd3}*(${d} + ${d}*s(${pi}/6))"|bc -l `  # incr
D3*fat3
  tx=`echo "scale=10;-${ra}*c(${te} + ${inc1})"|bc -l ` #translacao em x
  ty=`echo "scale=10;-${ra}*s(${te} + ${inc1})"|bc -l ` #translacao em y
  z2=`echo "scale=10;0.0000*s(${pi}/6)"|bc -l `   #coord z2
#   echo "  ${metodo} PREC SHIFT1000 DEBUG LET T=1999999 + " > ${nome}.dat
#   echo "  DUMP=250000 XYZ PL GEO-OK ${multi} CHARGE=${carga}  " >>
${nome}.dat
   echo "  ${metodo} UHF CYCLES=30000 PREC SHIFT1000 DEBUG LET T=19999999 + "
> ${nome}.dat
   echo "  DUMP=250000 AUX GNORM=0.01 PL GEO-OK ${multi} CHARGE=${carga} " >>
${nome}.dat
   echo "  ${nome}" >> ${nome}.dat
   echo "         " >> ${nome}.dat
   j=1
   while [ ${j} -le ${m} ]
   do

    i=1
    while [ ${i} -le ${n} ]
    do
      x1=`echo "scale=10;${tx} + ${ra}*c(${te} + ${inc1})"|bc -l `   #coord
x1
      y1=`echo "scale=10;${ty} + ${ra}*s(${te} + ${inc1})"|bc -l `  #coord y1
      x2=`echo "scale=10;${tx} + ${ra}*c(${te} + ${inc2})"|bc -l `   #coord
x2
      y2=`echo "scale=10;${ty} + ${ra}*s(${te} + ${inc2})"|bc -l `  #coord y2
      echo "${atomo1} ${x1}  1  ${y1}  1  ${z2}  1 " >> ${nome}.dat
      echo "${atomo2} ${x2}  1  ${y2}  1  ${D2}  1 " >> ${nome}.dat
      te=` echo "scale=10;${te} + ${dte}"|bc -l `
```


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```
      i=` expr ${i} + 1 `
    done
      z2=` echo "scale=10;${z2} + ${D3}"|bc -l `
      D2=` echo "scale=10;${D2} + ${D3}"|bc -l `
      inc1=` echo "scale=10;${inc1} + ((-1)^(${j}-1))*${incte}"|bc -l `
      inc2=` echo "scale=10;${inc2} + ((-1)^(${j}-1))*${incte}"|bc -l `
      j=` expr ${j} + 1 `

   done
  #rodar-mopac2016.sh  ${nome}.dat
  #/opt/mopac/MOPAC2016.exe  ${nome}.dat
  conv-xyz-dat-gjf-supercomputador.sh  ${nome} ${metodoAb}  ${baseAb}
${cargaAb} ${multiAb}   14   24
#  conv-arc-dat-gjf.sh ${nome} ${metodoAb} ${baseAb} ${cargaAb} ${multiAb}
#  echo "batg03-vulc ${nome} " >> fila-abinitio-varredor.sh
#  batg03-vulc ${nome}
#  grep -H "SCF Done" ${nome}.log >> energias-abi-varredor.sh
else
   #Crescimento BARCO
   n=` echo "${n0}"|bc -l ` #numero de carbono vezes quatro
   nome=nano${tipo}-${atomo1}${atomo2}-n${n}-m${m}-${metodo}-${multi}-
c${carga}

   te=` echo "scale=10;0.0000*(2*${pi}/${n})"|bc -l ` # angulo
   te0=` echo "scale=10;2*${pi}/${n}"|bc -l ` # angulo
   incte=` echo "scale=10;${pi}/${n}"|bc -l ` #incremento do angulo de nivel
   dte=` echo "scale=10;(2*${pi}/${n})"|bc -l ` #incremento do angulo maior -
Zn-Zn
   D1=`echo "scale=10;${fatd1}*(2*(${d} + ${d}*c(2*${pi}/${n})))"|bc -l ` #
distancia basica do BARCO
   ra=`echo "scale=10;(${D1})/(sqrt(2 - 2*c(2*${pi}/${n})))"|bc -l ` #raio
BARCO
   #curv=`echo "scale=10;1/${ra}"|bc -l ` # curvatura BARCO
   #echo "curv=${curv}"
   inc=0.00000
   dte1=` echo "scale=10;${fatd2}*(${te0}/3)"|bc -l ` #incremento do angulo
menor - Zn-O
   D3=`echo "scale=10;${fatd3}*(${d}*s(${pi}/3))"|bc -l ` # incr em z2*fatdz2
   dz1=`echo "scale=10;${d}*s(${pi}/3)"|bc -l `  # incremento em z1
   #dz2=`echo "scale=10;${fatdz2}*(2*${d}*s(${pi}/3))"|bc -l ` # incr em
z2*fatdz2
   tx=`echo "scale=10;-${ra}*c(${te} + ${inc})"|bc -l `     #translacao em x
   ty=`echo "scale=10;-${ra}*s(${te} + ${inc})"|bc -l `     #translacao em y
   z1=`echo "scale=10;0.0000*s(${pi}/6)"|bc -l `            #coord z1
#  echo "  ${metodo}  PREC  SHIFT1000 DEBUG LET T=1999999 + " > ${nome}.dat
#  echo "  DUMP=250000 XYZ PL GEO-OK ${multi} CHARGE=${carga}  " >>
${nome}.dat
   echo "  ${metodo} UHF CYCLES=30000 PREC SHIFT1000 DEBUG LET T=19999999 + "
> ${nome}.dat
   echo "  DUMP=250000 AUX GNORM=0.01 PL GEO-OK ${multi} CHARGE=${carga} " >>
${nome}.dat
   echo "  ${nome}" >> ${nome}.dat
   echo "         " >> ${nome}.dat
```


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```
  j=1
  while [ ${j} -le ${m} ]
  do

    i=1
    while [ ${i} -le ${n} ]
    do
     x1=`echo "scale=10;${tx} + ${ra}*c(${te} + ${inc})"|bc -l `      #coord
x1
     y1=`echo "scale=10;${ty} + ${ra}*s(${te} + ${inc})"|bc -l `      #coord
y1
     x2=`echo "scale=10;${tx} + ${ra}*c(${te} + ${dte1} + ${inc})"|bc -l `
#coord x2
     y2=`echo "scale=10;${ty} + ${ra}*s(${te} + ${dte1} + ${inc})"|bc -l `
#coord y2
    echo "${atomo1}   ${x1}  1  ${y1}   1   ${z1}  1 " >> ${nome}.dat
    echo "${atomo2}   ${x2}  1  ${y2}   1   ${z1}  1 " >> ${nome}.dat
     te=` echo "scale=10;${te} + ${dte}"|bc -l `
     #z1=` echo "scale=10;${z1} + ((-1)^${i})*${dz1}"|bc -l `
     i=` expr ${i} + 1 `
    done
    z1=` echo "scale=10;${z1} + ${D3}"|bc -l `
    inc=` echo "scale=10;${inc} + ((-1)^(${j}))*${incte}"|bc -l `

    j=` expr ${j} + 1 `

  done


#!/bin/bash
#adiçao de hidrogenio nas pontas de nanobar
#Msc.Jeziel e Dr.José Divino dos Santos          v.01         23/08/2018
nome=$1         #nomes dos arquivos bar.mol (sem .mol)
tipo=$2         #tipo de nanotubos: 1-armchair 2-zigzag
if [ ${tipo}  -eq 1 ]
then
    ###Armchair
   echo > temp1; rm temp1; echo > temp2; rm temp2; n=` echo ${nome}.mol|cut -
d- -f3|cut -dn -f2 `;  m=` echo ${nome}.mol|cut -d- -f4|cut -dm -f2 `; nat=`
echo "2*${n}*${m}"|bc `; nf=` echo "2*${n}*(${m} - 1) + 2"|bc ` ;nu=` echo
"2*${n} + 2"|bc `;nl=` expr ${nat} + 2 `; i=3; while [ ${i} -le ${nl} ];do
v=(` head -${i} ${nome}.mol|tail -1|awk '{printf("%s   %6.6f   %6.6f   %6.6f
\n",  $1, $2, $3, $4 )}'`); if [ ${i} -le ${nu} ]; then  echo "${v[0]}
${v[1]}   ${v[2]}   ${v[3]}" >> temp1 ; awk -v vx="${v[1]}" -v  vy="${v[2]}"
-v  vz="${v[3]}" 'BEGIN{printf("%s   %6.6f   %6.6f   %6.6f   \n", "H", vx,
vy, vz - 1.0)}' >> temp2 ;  fi ; if [ ${i} -gt ${nu} ] && [ ${i} -le ${nf} ];
then  echo "${v[0]}  ${v[1]}   ${v[2]}   ${v[3]}" >> temp1  ;  fi;  if [ ${i}
-gt ${nf} ]; then  echo "${v[0]}  ${v[1]}   ${v[2]}   ${v[3]}" >> temp1 ; awk
-v vx="${v[1]}" -v  vy="${v[2]}" -v  vz="${v[3]}" 'BEGIN{printf("%s   %6.6f
%6.6f   %6.6f   \n", "H", vx, vy, vz + 1.0)}' >> temp2 ;  fi ; i=` expr ${i}
+ 1 ` ; done ; natH=` echo "4*${n}"|bc ` ; natotal=` echo "2*${n}*${m} +
${natH}"|bc `; echo "   ${natotal}  " > ${nome}-${natH}H.mol ; echo "
```


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```
">> ${nome}-${natH}H.mol;  cat temp1 temp2 >> ${nome}-${natH}H.mol;  molden
${nome}-${natH}H.mol
else
    ###Zigzag
    #rm temp1; echo > temp2; rm temp2; n=` echo ${nome}.mol|cut -d- -f3|cut -
dn -f2 `;  m=` echo ${nome}.mol|cut -d- -f4|cut -dm -f2 `; nat=` echo
"2*${n}*${m}"|bc `; nf=` echo "2*${n}*(${m} - 1) + 2"|bc ` ;nu=` echo "2*${n}
+ 2"|bc `;nl=` expr ${nat} + 2 `; i=3; while [ ${i} -le ${nl} ];do v=(` head
-${i} ${nome}.mol|tail -1|awk '{printf("%s   %6.6f   %6.6f   %6.6f   \n",
$1, $2, $3, $4 )}'`); if [ ${i} -le ${nu} ]; then  echo "${v[0]}  ${v[1]}
${v[2]}   ${v[3]}" >> temp1 ; awk -v vx="${v[1]}" -v  vy="${v[2]}" -v
vz="${v[3]}"  -v i0="${i}"  'BEGIN{ip=(-1)^(i0);  if(ip==-1){  printf("%s
%6.6f   %6.6f   %6.6f   \n", "H", vx, vy, vz - 1.0); }; }' >> temp2 ;  fi ;
if [ ${i} -gt ${nu} ] && [ ${i} -le ${nf} ]; then  echo "${v[0]}  ${v[1]}
${v[2]}   ${v[3]}" >> temp1  ;  fi;  if [ ${i} -gt ${nf} ]; then  echo
"${v[0]}  ${v[1]}   ${v[2]}   ${v[3]}" >> temp1 ; awk -v vx="${v[1]}" -v
vy="${v[2]}" -v  vz="${v[3]}"   -v i0="${i}"  'BEGIN{ ip=(-1)^(i0);
if(ip==1){  printf("%s   %6.6f   %6.6f   %6.6f   \n", "H", vx, vy, vz + 1.0);
}; }' >> temp2 ;  fi ; i=` expr ${i} + 1 ` ; done ; natH=` echo "2*${n}"|bc `
; natotal=` echo "2*${n}*${m} + ${natH}"|bc `; echo "   ${natotal}  " >
${nome}-${natH}H.mol ; echo "       ">> ${nome}-${natH}H.mol;  cat temp1
temp2 >> ${nome}-${natH}H.mol;  molden ${nome}-${natH}H.mol
    echo > temp1; rm temp1; echo > temp2; rm temp2;  echo > temp3; rm temp3;
n=` echo ${nome}.mol|cut -d- -f3|cut -dn -f2 `;  m=` echo ${nome}.mol|cut -d-
-f4|cut -dm -f2 `; nat=` echo "2*${n}*${m}"|bc `; meio=` echo "${n}*${m}"|bc
`; nf=` echo "2*${n}*(${m} - 1) + 2"|bc ` ;nu=` echo "2*${n} + 2"|bc `;nl=`
expr ${nat} + 2 `; i=3; while [ ${i} -le ${nl} ];do v=(` head -${i}
${nome}.mol|tail -1|awk '{printf("%s   %6.6f   %6.6f   %6.6f   \n",  $1, $2,
$3, $4 )}'`); if [ ${i} -le ${nu} ]; then  echo "${v[0]}  ${v[1]}   ${v[2]}
${v[3]}" >> temp1 ; awk -v vx="${v[1]}" -v  vy="${v[2]}" -v  vz="${v[3]}"  -v
i0="${i}"  'BEGIN{ip=(-1)^(i0);  if(ip==-1){  printf("%s   %6.6f   %6.6f
%6.6f   \n", "H", vx, vy, vz - 1.0); }; }' >> temp2 ;  fi ; if [ ${i} -gt
${nu} ] && [ ${i} -le ${nf} ]; then  echo "${v[0]}  ${v[1]}   ${v[2]}
${v[3]}" >> temp1  ;  fi;  if [ ${i} -gt ${nf} ]; then  echo "${v[0]}
${v[1]}   ${v[2]}   ${v[3]}" >> temp1 ; awk -v vx="${v[1]}" -v  vy="${v[2]}"
-v  vz="${v[3]}"   -v i0="${i}"  'BEGIN{ ip=(-1)^(i0); if(ip==1){  printf("%s
%6.6f   %6.6f   %6.6f   \n", "H", vx, vy, vz + 1.0); }; }' >> temp2 ;  fi ;
if [ ${i} -eq ${meio} ]; then  awk -v vx="${v[1]}" -v  vy="${v[2]}" -v
vz="${v[3]}"   'BEGIN{  printf("%s   %6.6f   %6.6f   %6.6f   \n", "C", vx +
1.70 , vy , vz  ); }' >> temp3 ;  fi ;  i=` expr ${i} + 1 ` ; done ; natH=`
echo "2*${n}"|bc ` ; natotal=` echo "2*${n}*${m} + ${natH} + 1"|bc `; echo "
${natotal}  " > ${nome}-${natH}H.mol ; echo "       ">> ${nome}-${natH}H.mol;
cat temp1 temp2 temp3 >> ${nome}-${natH}H.mol;  molden ${nome}-${natH}H.mol
fi
```


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**S2.** script to encapsulate the BNZ in the geometric center of the BNNT and CNT models.

```
#!/bin/bash
#Ponto geométrico
#MsC. Jeziel Rodrigues dos Santos      28/03/2019       v.01
nome=$1             #nome do arquivo.mol (sem .mol)
nl=` wc -l ${nome}.mol|awk '{print $1}' `
nat=` wc -l ${nome}.mol|awk '{print $1 - 2}' `
#######ponto médio coordenada x
i=3; sx=0.000000;  while [ ${i} -le ${nat} ]
do
at=` head -${i} ${nome}.mol|tail -1|awk '{print $1}' `
x=` head -${i} ${nome}.mol|tail -1|awk '{print $2}' `
sx=` echo "scale=6;${sx} + ${x}"|bc -l `
#echo "${at}   ${x}   ${sx}"
i=` expr ${i} + 1 `
done
mx=` echo "scale=6;${sx}/${nat}"|bc -l `
#echo [ mediax=${mx} ]
#######ponto médio coordenada y
i=3; sy=0.000000;  while [ ${i} -le ${nat} ]
do
at=` head -${i} ${nome}.mol|tail -1|awk '{print $1}' `
y=` head -${i} ${nome}.mol|tail -1|awk '{print $3}' `
sy=` echo "scale=6;${sy} + ${y}"|bc -l `
#echo "${at}   ${y}   ${sy}"
i=` expr ${i} + 1 `
done
my=` echo "scale=6;${sy}/${nat}"|bc -l `
#echo [ mediax=${my} ]
#######ponto médio coordenada z
i=3; sz=0.000000;  while [ ${i} -le ${nat} ]
do
at=` head -${i} ${nome}.mol|tail -1|awk '{print $1}' `
z=` head -${i} ${nome}.mol|tail -1|awk '{print $3}' `
sz=` echo "scale=6;${sz} + ${z}"|bc -l `
#echo "${at}   ${z}   ${sz}"
i=` expr ${i} + 1 `
done
mz=` echo "scale=6;${sz}/${nat}"|bc -l `
echo [${mx}    ${my}    ${mz} ] > ponto-medio-${nome}.mol
```


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