

# AMBER8 Tutorial

## Nonstandard Residues - Water Molecule

### Example 1 - Using Gaussian to determine charges

Step 1: Generate a Gaussian input file for geometry optimization and charge calculations for Antechamber

[water\\_HF.com](#)

```
%Nproc=1
%chk=water_HF.chk
#HF/6-31G* opt

Water - with high symmetry

0 1
 H
 O 1 r2
 H 2 r3 1 a3
Variables:
r2= 0.9819
r3= 0.9819
a3= 109.50
```

→  
optimized  
geometry  
output  
[water\\_HF.log](#)

[water\\_HF\\_Charges.com](#)

```
%Nproc=1
%chk=water_HF_Charges.chk
#HF/6-31G* SCF=tight Test Pop=MK iop(6/33=2) iop(6/42=6)

Water - input from HF/6-31G* geom. opt.

0 1
 H
 O,1,r2
 H,2,r3,1,a3
Variables:
r2=0.94740748
r3=0.94740748
a3=105.41959655
```

↓  
[water\\_HF\\_Charges.log](#)

## Step 2: Run Antechamber

Antechamber: creates a prep file for AMBER calculations and suggest reasonable parameters for those that are missing using GAFF.

### Run.antechamber

```
#!/bin/csh -f
/share/apps/amber8/exe/antechamber -i water_HF_Charges.log \
  -fi pdb \
  -o water.prep \
  -fo prepi \
  -c bcc
```

notice that the Gaussian output for charge generation is the input for antechamber

### water.prep

```
0 0 2
This is a remark line
molecule.res
MOL INT 0
CORRECT OMIT DU BEG
0.0000
1 DUMM DU M 0 -1 -2 0.000 .0 .0 .00000
2 DUMM DU M 1 0 -1 1.449 .0 .0 .00000
3 DUMM DU M 2 1 0 1.522 111.1 .0 .00000
4 O1 oh M 3 2 1 1.540 111.208 180.000 -0.81497
5 H1 ho E 4 3 2 0.948 90.000 142.719 0.40748
6 H2 ho E 4 3 2 0.948 90.000 37.281 0.40748

LOOP

IMPROPER

DONE
STOP
```

## Second example - (easier) uses divcon within AMBER to assign AM1-BCC charges starting from a pdb file

Run.antechamber

```
#!/bin/csh -f
/share/apps/amber8/exe/antechamber -i water.pdb \
-fi pdb \
-o water.prep \
-fo prepi \
-c bcc
```

water.prep

```
0 0 2
This is a remark line
molecule.res
UNK INT 0
CORRECT OMIT DU BEG
0.0000
1 DUMM DU M 0 -1 -2 0.000 .0 .0 .00000
2 DUMM DU M 1 0 -1 1.449 .0 .0 .00000
3 DUMM DU M 2 1 0 1.522 111.1 .0 .00000
4 O oh M 3 2 1 1.540 111.208 180.000 -0.78473
5 H ho E 4 3 2 0.948 90.000 142.719 0.39235
6 H1 ho E 4 3 2 0.948 90.000 37.281 0.39238

LOOP

IMPROPER

DONE
STOP
```

To double check parameter run:  
parmchk -i water.prep -f prepi -o frcmod

← If there are missing parameters, they will appear in the frcmod file that parmchk generates

## Xleap Example

```
logFile leap_linear.log
source leaprc.gaff
x = loadAmberPrep water.prep
saveamberparm x water_no_TIP3P.top water_no_TIP3P.crd
savepdb x water_no_TIP3P.pdb
addions x Na+ 0
solvateBox x TIP3PBOX216 10
saveamberparm x water_TIP3P.top water_TIP3P.crd
savepdb x water_TIP3P.pdb
```