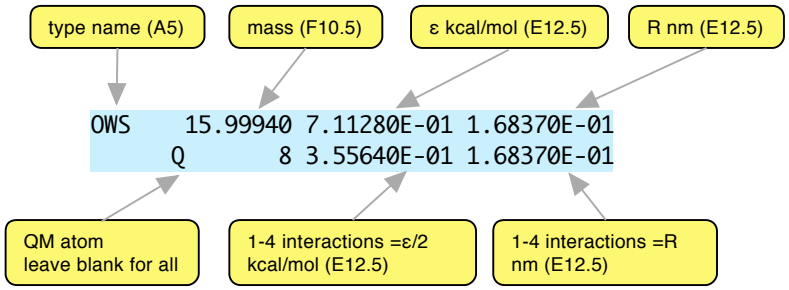
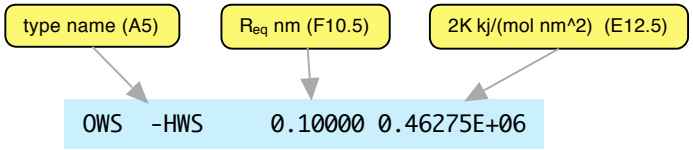
Parameter file format (amber.par) for NWChem

Created Marat Valiev October 6, 2010

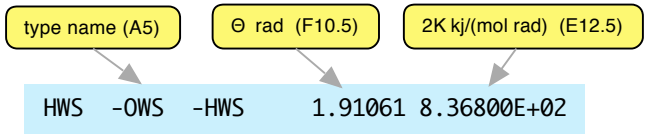
VDW Interactions format(a5,f10.5,2e12.5,24X,4x,"1",1x,"1111111111")
format(10x,i5,2e12.5)



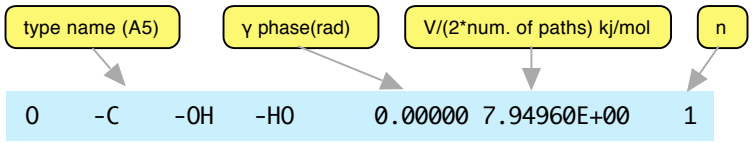
Bonds (format(a5,"-",a5,f10.5,e12.5))



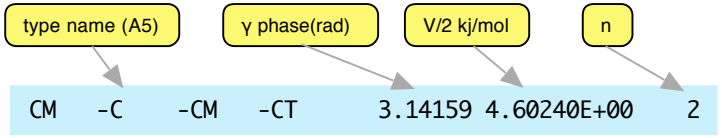
Angles (format(a5,"-",a5,"-",a5,f10.5,e12.5))



Proper dihedrals (format(a5,"-",a5,"-",a5,"-",a5,f10.5,e12.5,i5))



Improper dihedrals (format(a5,"-",a5,"-",a5,"-",a5,f10.5,e12.5,i5))




```
AMBER 99  custom parameters
Electrostatic 1-4 scaling factor     0.833333
Relative dielectric constant     1.000000
Parameters epsilon R*
Atoms
OWS    15.99940 7.11280E-01 1.68370E-01                              1 1111111111
      Q       8 3.55640E-01 1.68370E-01
CL     35.45300 0.41840E+00 2.47000E-01                              1 1111111111
             17 0.20920E+00 2.47000E-01
Bonds
OWS  -HWS     0.10000 0.46275E+06
Angles
HWS  -OWS  -HWS     1.91061 8.36800E+02
Proper dihedrals
O    -C    -OH   -HO      0.00000 7.94960E+00    1
Improper dihedrals
CM   -C    -CM   -CT      3.14159 4.60240E+00    2
End
```

1. NWChem amber.par file is **format sensitive**
2. Units are based on kj/mol, nm, and rad
3. Bond,angle constants are twice than those of AMBER
4. Dihedral constant has division by number of paths built in
5. Put your amber.par in the directory where you are running prepare
6. Use Q flag to restrict VDW parameters to QM atoms only