Generation of a Glycam 2006 or OPLS type force field

Tutorial by:
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The quantum mechanics (QM) Gaussian, GAMESS or Firefly program is selected during the input submission procedure using the web interface: one can use the public account or a private account:
See http://q4md-forcefieldtools.org/REDServer-Development/faq.php#1

Input molecules of PyRED are provided in the PDB file format:
See http://q4md-forcefieldtools.org/REDServer-Development/Documentation/readme.txt

Please first read:
http://q4md-forcefieldtools.org/Tutorial/Tutorial-4-demo5.pdf

-I- APPROACH COMPATIBLE WITH THE GLYCAM 2006 FORCE FIELD

-II- APPROACH COMPATIBLE WITH OPLS

-I- APPROACH COMPATIBLE WITH THE GLYCAM 2006 FORCE FIELD [1]

Set to '`ON`' the '`OPT_Calc`', '`MEPCHR_Calc`' and '`Freq_Calc`' keywords in the *System.config* file as demonstrated in http://q4md-forcefieldtools.org/Tutorial/Tutorial-4-demo5.pdf.
Select the '`RESP-C2`' charge model in the *System.config* file.

Define the molecule total charge and spin multiplicity if different from zero and one by using the '`MOLECULE'$n'-TOTCHARGE`' and '`MOLECULE'$n'-SPINMULT`' keywords in the *Project.config* file, respectively.

Define the atom types using the MOLECULE'*$n*'-ATMTYPE in the *Project.config* file as demonstrated in http://q4md-forcefieldtools.org/Tutorial/Tutorial-4-demo5.pdf for GAFF.

In GLYCAM 2006, each hydrogen atom connected to a sp3 carbon atom has its partial charge equal to zero; this is achieved by using a constrained value = 0, the hydrogen atom index, and the '`Keep`' flag with the MOLECULE'*$n*'-INTRA-MCC1 keyword in the *Project.config* file. Such intra-molecular charge constraint is repeated for each hydrogen atom connected to a sp3 carbon atom.

$n represent the molecule(s) involved in force field generation

To create a new molecular fragment compatible with GLYCAM 2006, an intra-molecular charge constraint with the '`Remove`' flag can be applied to the hydroxyl group or to the methyl group of a monosaccharide unit. Inter-molecular charge constraint between the hydroxyl group and the methyl group belonging to two different monosaccharide units can also be used. The key point here is to use a correct constrained value for the charge constraint in agreement with GLYCAM 2006.
See examples at http://q4md-forcefieldtools.org/Tutorial/Tutorial-4.php#30

Provide the last version of Glycam_06j(*).dat force field parameter file from the AmberTools:
```
cp $AMBERHOME/dat/leap/parm/GLYCAM_06j(*).dat frcmod.user
```

(*) whatever version of the Glycam force field available in the AmberTools.

Create the archive file as described at:
See http://q4md-forcefieldtools.org/REDServer-Development/Documentation/Create-archive.php

```
tar -zcvf Archive.tgz Mol_red*.pdb Project.config System.config frcmod.user
```

→ Submit to https://upjv.q4md-forcefieldtools.org/REDServer-Development/

[1] https://doi.org/10.1002/jcc.20820; Kirschner et al. *J. Comput. Chem.* **2008**, 29, 622.

-II- APPROACH COMPATIBLE WITH OPLS [2]

Set to '`ON`' the '`OPT_Calc`', '`MEPCHR_Calc`' and '`Freq_Calc`' keywords in the *System.config* file as demonstrated in http://q4md-forcefieldtools.org/Tutorial/Tutorial-4-demo5.pdf.
Select the '`RESP-O1`' charge model in the *System.config* file.

Define the molecule total charge and spin multiplicity if different from zero and one by using the '`MOLECULE'$n'-TOTCHARGE`' and '`MOLECULE'$n'-SPINMULT`' keywords in the *Project.config* file, respectively.

Define also the OPLS atom types by using '`MOLECULE'$n'-ATMTYPE`' keyword in the *Project.config* file as demonstrated in http://q4md-forcefieldtools.org/Tutorial/Tutorial-4-demo5.pdf.

$n represent the molecule(s) involved in force field generation

Provide the OPLS force field parameters to the AMBER file format using the frcmod file format: such task may not be simple for novice users. Here the best bet may be to set '`FFPARM = OFF`' in the *Project.config* file and use a tool from another distribution to provide the OPLS atom types to the force field libraries generated by PyRED, and to generate the required force field parameters.

Create an archive file and submit to https://upjv.q4md-forcefieldtools.org/REDServer-Development/.

A key point to underline here is that atomic charges are empirical data. Thus, they have always to be validated: this is particularly true when using the '`RESP-O1`' charge model for OPLS.

[2] https://doi.org/10.1002/(SICI)1096-987X(19990415)20:5<483::AID-JCC2>3.0.CO;2-4; Henchman & Essex, *J. Comp. Chem.* **1999**, 20, 483.

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