

Generation of a force field with lone-pairs and/or extra-points

Tutorial by:

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Three different types of lone-pairs and extra-points are implemented in PyRED. The user has to provide the right keyword(s) in the *Project.config* file in agreement with the lone-pairs/extra-points she/he wishes to add to the input molecule(s). [1,2] Lone-pairs and/or extra-points are added to each optimized geometry after molecular electrostatic computation and before charge fitting.

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#3>

Input molecules of PyRED are provided in the PDB file format:

See <http://q4md-forcefieldtools.org/REDServer-Development/Documentation/readme.txt>

– Lone pairs on heteroatoms [1]

Lone-pairs can be added to heteroatoms (nitrogen, oxygen and sulfur atoms).

```
# Provide the index of each heteroatom (HA_index) to add lone-pair(s) (LP)
#   to be repeated for each heteroatom
MOLECULE1-LONEPAIR   = HA_index
# Modification of the default algorithm (provide on a single line)
MOLECULE1-LONEPAIR   = HA_index Distance_HA-LP Atom1_index Angle_value1_Atom1-HA-LP
  Atom2_index Angle_value2_Atom2-HA-LP | Number_of_LP

MOLECULE1-TITLE      = CH3OCH3
MOLECULE1-LONEPAIR   = 5
# or
MOLECULE1-LONEPAIR   = 5 0.35 1 109.5 6 109.5 | 2
```



– Extra-point for alkanes [2]

Extra-points can be added to alkane.

```
# The methyl and methylene groups of alkanes:
MOLECULE1-EXTRAPOINT1 = ICMMG | 0 or 1
# ICMMG: List of carbon atom indexes (methylene and methyl groups)
# 1: add three extra-points for the methyl group (default)
# 0: add one extra-point for the methyl group

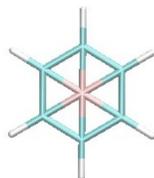
MOLECULE1-TITLE      = Propane_CH3-CH2-CH3
MOLECULE1-EXTRAPOINT1 = 1 5 8 | 1
# or
MOLECULE1-EXTRAPOINT1 = 1 5 8 | 0
```



– *Extra-point for a set of atoms*

Extra-points can be added for a set of atoms such as an aromatic cycle.

```
# The barycenter of different atoms:  
MOLECULE1-EXTRAPOINT2 = atom indexes  
  
MOLECULE1-TITLE      = Benzene_(CH)6  
MOLECULE1-EXTRAPOINT2 = 1 3 5 7 9 11  
# or  
MOLECULE1-EXTRAPOINT2 = 1 5 9
```



[1] R. W. Dixon, P. A. Kollman, *J. Comput. Chem.* 1997, 18, 1632.

[2] D. E. Williams, *J. Comput. Chem.* 1994, 15, 719.

Last update of this tutorial: November 30th, 2014.