ForceField Manual

Amsterdam Modeling Suite 2021.1

www.scm.com

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CONTENTS

CHAPTER

ONE

INTRODUCTION

As per 2020 UFF force fields and simple classical force fields are unified in the ForceField engine. This replaces the old UFF engine and the NewMM functionality from ADF.

1.1 Available force fields

The default force field is UFF, it requires no configuration. UFF (Universal Force Field) is a full periodic table force field that can be used to calculate single point energies, do geometry optimizations, calculate frequencies, etc. It is also the default pre-optimizer in the Graphical User interface (GUI) to clean up manually drawn structures. For details on the inner workings of the force field, see the 1992 paper by Rappe et al. [*1* (page 55)]. By default UFF uses non-zero charges for water molecules only.

Other available force fields managed by this engine include Amber95, Tripos 5.2 and GAFF.

1.2 ForceField-GUI

Note that the graphical user interface UFF-GUI enables all users to set up force field calculations with a few mouse clicks. Most force fields require atom typing, and this needs to be done by hand. When using UFF, also for pre-optimizing, it is important to remember that any force field method relies on a set of parameters. This means that even though UFF supports all elements up to Z=103, it might not generate the desired structures for uncommon oxidation states in metallic structures. If this is the case, you could add new parameters to UFF or attach dummy hydrogen atoms to the metal atom.

1.3 What's new in ForceField 2021

- The engine has been parallelized with MPI using force decomposition.
- The particle mesh Ewald method (implemented through the helPME library (https://github.com/andysim/helpme)) is now used for electrostatic interactions in 3D systems.
- The default non-bonded cutoff has been reduced to 15 Angstrom, a value more typical in the force-field community.
- The engine has been optimized to be on par with the industry standards. The total speed-up compared to version 2020 can be up to factor 500.

1.4 What's new in ForceField 2020

1.4.1 New features

- Periodic support (chains,slabs, and crystals) for all force field types
- Import force field parameters from amber ".dat" files

shell script without atom typing:

```
#!/bin/sh

# This is a shell script for the ForceField engine

# You should use '$AMSBIN/ams' instead.

$AMSBIN/ams <<eor
   # Input options for the AMS driver:

   Task GeometryOptimization

   System
      Atoms
         H 0.0 0.0 0.0
         H 0.9 0.0 0.0
      End
   End

   # The input options for the ForceField, which are described in this manual,
   # should be specified in the 'Engine ForceField' block:

   Engine ForceField
      # the default one is UFF, requiring no options
   EndEngine
eor
```

1.5 Force field setup for AMS applications

When you do a geometry optimization of perform a MD calculation the details of the force field are determined only once and kept constant during the run. This applies to bond orders, partial charges, etc. In case of a polarizable force field (not currently supported) the charges are of course allowed to change.

1.6 Classical force fields

Most force fields require atom typing, as well as atomic charge specifications, see *Examples* (page 17).

CHAPTER

TWO

ATOM TYPING BEHAVIOR

To use a classical forcefield each atom should be given a type, and a partial charge. The power of the UFF forcefield is that this atomtyping is done automatically. For other force fields the atomtyping for most systems still has to be done by hand, possibly with the help of an external program. Unlike UFF parameters, the availabe parameters for the other available force fields typically cover only a fraction of all chemical elements. Nonetheless, experimental atomtyping options are available for small organic molecules (GAFF), and for biological systems (AMBER).

2.1 UFF

Atom typing is the process of matching MM atom types to elements. For example, a Carbon atom becomes a C_1, C_2, C_3 or C_R, depending on the number (and type) of bonds it has to neighboring atoms. UFF is capable of finding a matching MM atom type on its own, but might not always succeed in doing so. When doing calculations with UFF, it is important to check the beginning of the output file, as the program will print the detected MM atom types there. You can also take matters into your own hands, and tell UFF what MM atom types you want it to use (see the section on Input and examples).

The atom typing in UFF is mostly controlled by the elements and mmatomtypes parameter files, however, some part of it is hidden in the code itself and is (at the moment) not accessible to users. This is done by UFF to differentiate between:

- Carbon: double-bonded sp2 carbon (C_2) vs aromatic carbon (C_R), if any of the orders are close to 2, it's C_2.
- Oxygen: having a bond to silicon gives O_3_z; otherwise, having bond order of 1.44 or higher gives O_R, provided that the partner is not a hydrogen. Otherwise, it's just an O_3.
- Sulfur: having a bond order greater than 1.3 gives aromatic S_R.

By default, zero charges are used, unless a water molecule is detected.

2.2 Other forcefields

Automatic atomtyping via an experimental integration of the Antechamber toolkit is available for the Generalized AMBER Force Field (GAFF) for small organic molecules. This option was introduced in the 2020 release of AMS, and is still considered experimental and disabled by default.

See also:

Antechamber integration for GAFF forcefields (page 7)

Some atomtyping functionality for biological systems can be accessed via the GUI, using pdb files as input. A pdb file can be loaded into amsinput and then under the regions the residues can be found. Still, charges need to be set by hand.

Custom force field parameters can be provided as forcefield files. The two supported formats are “.ff” (originating from the ADF and QUILD programs) and the much more widely used amber “.dat” files.

CHAPTER

THREE

INPUT VIA THE AMS SYSTEM BLOCK

While usually options for an AMS engine are defined in its engine block, for the ForceField engine three ingredients are defined via the AMS system block: bonds, atom types and (partial) charges.

Here are some logical options

- 1) Specify Everything: elements, coordinates, MM atom types, charges, and bonds
- 2) Specify elements, coordinates, and bonds (UFF only)
- 3) Specify elements and coordinates (UFF only, most convenient)

Currently, for most force fields, everything needs to be specified (option 1). UFF and GAFF allow the automatic determination of bonds and atom types (option 2 and 3). For GAFF this option is considered experimental as of the 2020 release and is disabled by default, see *Antechamber integration* (page 7) below. See also the *BondsUsage* (page 10) key on how bond information can be tweaked.

3.1 ForceField input example

1) Specify Elements, coordinates, MM Atom Types, Charges, and bonds:

```
$AMSBIN/ams << eor

Task GeometryOptimization

System
    Atoms
        C   1.36012328  -0.14520095   0.60144543    ForceField.Type=C_3    ForceField.Charge=0.000000
        C   0.00000000   0.00000000   0.00000000    ForceField.Type=C_2    ForceField.Charge=0.000000
        H   2.09833847  -0.46327872  -0.16560721    ForceField.Type=H_     ForceField.Charge=0.000000
        H   1.32657807  -0.90546800   1.40917410    ForceField.Type=H_     ForceField.Charge=0.000000
        H   1.67935140   0.82750664   1.02977296    ForceField.Type=H_     ForceField.Charge=0.000000
        H  -0.83486863   0.30434056   0.62258487    ForceField.Type=H_     ForceField.Charge=0.000000
        O  -0.18030374  -0.22462371  -1.18585739    ForceField.Type=O_2    ForceField.Charge=0.000000
    End
    BondOrders
         1 5 1.0
```

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```
         1 4 1.0
         1 3 1.0
         1 2 1.0
         2 6 1.0
         2 7 2.0
    End
End

Engine ForceField
EndEngine

eor
```

The format in the bonds section is: atom A, atom B, bond order.

2) Specify Elements, coordinates, and bonds (UFF only):

If we leave out the MM atom types and charges, UFF will determine the MM atom types automatically from the bond information:

```
$AMSBIN/ams << eor

Task GeometryOptimization

System
    Atoms
        C  1.36012328 -0.14520095  0.60144543
        C  0.00000000  0.00000000  0.00000000
        H  2.09833847 -0.46327872 -0.16560721
        H  1.32657807 -0.90546800  1.40917410
        H  1.67935140  0.82750664  1.02977296
        H -0.83486863  0.30434056  0.62258487
        O -0.18030374 -0.22462371 -1.18585739
    End
    BondOrders
         1 5 1.0
         1 4 1.0
         1 3 1.0
         1 2 1.0
         2 6 1.0
         2 7 2.0
    End
End

Engine ForceField
EndEngine

eor
```

3) Specify Elements and coordinates (UFF only):

The third input format is similar to the second, but without a Bonds section in System:

```
$AMSBIN/ams << eor

Task GeometryOptimization

System
```

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```
    Atoms
        C  1.36012328 -0.14520095  0.60144543
        C  0.00000000  0.00000000  0.00000000
        H  2.09833847 -0.46327872 -0.16560721
        H  1.32657807 -0.90546800  1.40917410
        H  1.67935140  0.82750664  1.02977296
        H -0.83486863  0.30434056  0.62258487
        O -0.18030374 -0.22462371 -1.18585739
    End
End

Engine ForceField
EndEngine

eor
```

The GUI generates inputs of the second or third type, depending on the "Use existing bonds" setting in the ForceField main tab. Note that to specify the MM Atom Types, the charges also need to be set. UFF has automatic bond guessing and a very simple automatic charge guessing only assigning charges to atoms of water molecules.

3.2 Antechamber integration

For the GAFF force field there is an experimental integration of the Antechamber toolkit (http://ambermd.org/antechamber/antechamber.html) for automatic atom typing. This allows the GAFF force field to be used with option 2 (only bonds and coordinates specified) and option 3 (coordinates only). As of the 2020 release of AMS, this option is still considered experimental and disabled by default. It can be enabled and configured from the input:

```
AntechamberIntegration Yes/No
```

AntechamberIntegration

Type Bool

Default value No

GUI name Automatic atom typing

Description EXPERIMENTAL: Use the Antechamber program to automatically determine atom types for the GAFF force field. This may run a geometry optimization with MOPAC under the hood in order to determine the charges (see keyword AntechamberTask), which might not work for very large systems.

```
AntechamberTask [GeometryOptimization | SinglePoint]
```

AntechamberTask

Type Multiple Choice

Default value GeometryOptimization

Options [GeometryOptimization, SinglePoint]

Description If antechamber is envoked to guess atomtypes and charges (GAFF force field), select the task for charge guessing with MOPAC

CHAPTER

FOUR

FORCEFIELD ENGINE OPTIONS

Details of the ForceField engine can be set via its input block. Some option are specific to UFF and others to other force fields.

4.1 Common options

These options apply to any force field.

4.1.1 Type

There are a few predefined force field types, that, if used, require no other input.

```
Type [UFF | Amber95 | GAFF | Tripos5.2 | UserDefined]
```

`Type`

Type Multiple Choice

Default value UFF

Options [UFF, Amber95, GAFF, Tripos5.2, UserDefined]

Description Type of force field to be used

4.1.2 Non bonded screening

The long range interaction (dispersion and Coulomb) are the most expensive to evaluate. This gives you the option to screen more aggressively the interaction.

```
NonBondedCutoff float
```

`NonBondedCutoff`

Type Float

Default value 15.0

Unit Angstrom

Description Distance beyond which the non-bonded pair interactions (Coulomb and Van der Waals) will be ignored. The interactions are smoothly damped starting from 0.9*NonBondedCutoff. Has no effect on the Coulomb term for periodic systems, as Ewald summation is used.

4.1.3 Feedback

If you want to know more about the details of the force field you should crank up the verbosity.

```
Verbosity [Silent | Normal | Verbose | VeryVerbose]
```

Verbosity

Type Multiple Choice

Default value Silent

Options [Silent, Normal, Verbose, VeryVerbose]

Description Controls the verbosity of the engine.

4.1.4 Bonds usage

Bonds can be specified in the input, still you may not want to use those. Here are some options to control this.

```
BondsUsage [Input | None | Guess | Auto]
```

BondsUsage

Type Multiple Choice

Default value Auto

Options [Input, None, Guess, Auto]

Description Controls what bonds are used by the engine. The choice auto means: guess in case there are no bonds. Guessing only happens at the first MD step, or first geometry optimization step.

4.1.5 Ewald summation

For periodic systems the Ewald summation is performed for the Coulomb interaction. It has a couple of options:

```
EwaldSummation
   Alpha float
   Enabled Yes/No
   GridSpacing float
   RealSpaceCutoff float
   Tolerance float
End
```

EwaldSummation

Type Block

Description Configures the details of the particle mesh Ewald (PME) summation of the Coulomb interaction.

Alpha

Type Float

Default value -1.0

Description This parameter shifts the workload from real space (smaller alpha) to reciprocal space (larger alpha). Using a larger [Alpha] without decreasing [GridSpacing] may increase the error in the reciprocal-space contribution. Set to zero to disable the reciprocal-space Ewald part. Negative value means the [Alpha] will be determined automatically from [Tolerance].

Enabled

Type Bool

Default value Yes

Description Set to false to use real-space pair summation instead of the Ewald, which is the default and the only option for molecules, 1D and 2D periodic systems.

GridSpacing

Type Float

Default value 0.5

Unit Angstrom

Description Grid spacing in the particle mesh Ewald method. Smaller grid spacing will make the reciprocal energy calculation more accurate but slower. Using a larger [Alpha] value may require a smaller GridSpacing to be accurate.

RealSpaceCutoff

Type Float

Default value 0.0

Unit Angstrom

Description Set the cutoff value for the real-space summation. Zero means the internal defaults will be used depending on the [Alpha] (if Alpha=0 then the cutoff will be set to 50 Bohr, otherwise to 20 Bohr).

Tolerance

Type Float

Default value 1e-10

Description Value of the error function that should be used to determine the cutoff radius for real-space Ewald summation. Larger values will make the real-space summation faster but less accurate.

4.1.6 Disabling energy terms

By default all force field energy terms are calculated, however, you can disable each one of them individually.

```
EnergyTerms
   Angle Yes/No
   Coulomb Yes/No
   Dispersion Yes/No
   Inversion Yes/No
   Stretch Yes/No
   Torsion Yes/No
End
```

EnergyTerms

Type Block

Description expert key, that allows you to disable specific energy terms.

`Angle`

Type Bool

Default value Yes

Description Whether to use angle (bend) energy.

`Coulomb`

Type Bool

Default value Yes

Description Whether to use coulomb energy.

`Dispersion`

Type Bool

Default value Yes

Description Whether to use dispersion energy.

`Inversion`

Type Bool

Default value Yes

Description Whether to use inversion energy.

`Stretch`

Type Bool

Default value Yes

Description Whether to use stretch energy.

`Torsion`

Type Bool

Default value Yes

Description Whether to use torsion energy.

4.1.7 Guessing or loading partial charges

The UFF forcefield has some very rudimentary partial charges guessing, only setting charges for atoms in water molecules. By default the partial charges in a force field calculation are zero. Essentially you will always need to specify atomic charges to make the results more realistic, either via the input or using one or the following options.

See also example *LoadCharges* (page 26), and *ChargedMolecules* (page 18).

GuessCharges

The simplest way is the use the GuessCharges key, that uses an engine that can calculate atomic charges. By default DFTB is used. DFTB is of course much more expensive than a forcefield, but if you run a MD calculation you can maybe afford a single DFTB calculation on the system.

```
GuessCharges Yes/No
```

GuessCharges

Type Bool

Default value No

Description Use another engine to calculate/guess the charges to be used by the force field.

If you want to control the engine use the GuessChargesConfig key.

```
GuessChargesConfig
   EngineType string
End
```

GuessChargesConfig

Type Block

Description Guess charges to be used by the forcefield

EngineType

Type String

Default value dftb

Description Engine that can calculate or guess charges

LoadCharges

You have more control over the charge guessing, by loading the charges of another calculation. This way you can set any engine specific detail, such as the basis set, or functional.

You can load charges form a previous calculation to be used as force field charges.

```
LoadCharges
   File string
   Section string
   Variable string
End
```

LoadCharges

Type Block

Description Load charges from a file to be used as forcefield charges

File

Type String

Description Name of the (kf) file

Section

Type String

Default value AMSResults

Description Section name of the kf file

Variable

Type String

Default value Charges

Description variable name of the kf file

4.2 Non UFF options

These options are relevant for non-UFF force fields:

```
AllowMissingParameters Yes/No
```

AllowMissingParameters

Type Bool

Default value No

Description When parameters are not found for bonds, angles, dihedrals, or inversions, the first entry in the database will be used.

```
CheckDuplicateRules Yes/No
```

CheckDuplicateRules

Type Bool

Default value Yes

Description The database could contain duplicate entries. For torsions this is a feature, and the potentials will be added. For all other terms this is no allowed, and if detected the program stops. One should fix the database or set the checking to false. As always the last entry will be used.

```
ForceFieldFile string
```

ForceFieldFile

Type String

Default value

GUI name Force field library

Description Path to the force field parameter file

4.3 UFF options

The following options are only relevant for the UFF force field:

```
UFF
   AtomTypesFile string
   Database string
   ElementsFile string
   Library [UFF | UFF4MOF | UFF4MOF-II]
End
```

UFF

Type Block

Description Option for the UFF force filed.

`AtomTypesFile`

Type String

Default value mmatomtypes_db

Description Expert option: Select the file that defines how UFF determines the atom types

`Database`

Type String

Default value general_db

Description Expert option: Select the file that defines the UFF parameters per atom type

`ElementsFile`

Type String

Default value elements_db

Description Expert option: Select the file that defines the elements known to UFF

`Library`

Type Multiple Choice

Default value UFF

Options [UFF, UFF4MOF, UFF4MOF-II]

GUI name Force field library

Description Selects the used parameter library.

CHAPTER

FIVE

EXAMPLES

The *$AMSHOME/examples/forcefield* directory contains many different example files, covering various aspects. This is a selection of relevant examples showing what the engine input looks like.

We do not repeat here all functionality that is available from the AMS driver level, see the AMS Examples.

5.1 Example: single point for aspirin with UFF

Download SP_aspirin.run

```
#!/bin/sh

$AMSBIN/ams << eor

Task SinglePoint

Properties Gradients=yes

System
    Atoms
      C        0.000000  0.000000  0.000000
      C        1.402231  0.000000  0.000000
      C        2.091015  1.220378  0.000000
      C        1.373539  2.425321  0.004387
      C       -0.034554  2.451759  0.016301
      C       -0.711248  1.213529  0.005497
      O       -0.709522  3.637718  0.019949
      C       -2.141910  1.166077 -0.004384
      O       -2.727881  2.161939 -0.690916
      C       -0.730162  4.530447  1.037168
      C       -0.066705  4.031914  2.307663
      H       -0.531323 -0.967191 -0.007490
      H        1.959047 -0.952181 -0.004252
      H        3.194073  1.231720 -0.005862
      H        1.933090  3.376356 -0.002746
      O       -2.795018  0.309504  0.548870
      H       -2.174822  2.832497 -1.125018
      O       -1.263773  5.613383  0.944221
      H       -0.337334  4.693941  3.161150
      H        1.041646  4.053111  2.214199
      H       -0.405932  3.005321  2.572927
    End
End
```

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```

Engine ForceField
EndEngine

eor
```

5.2 Example: partial charges and total charge

This example shows you some ways to use partial atomic charges for ions. The atomic charges should add up to the total charge.

Download ChargedMolecules.run

```
#!/bin/sh

# Here we consider a Butane molecule with the C in the end groups changed to N
# The ion has a charge of plus two.
# The (partial) atomic charges used in the forcefield need to add up to the total␣
↪charge


# There is explicit specification via the inut, Loading charges, and guessing charges


# Charges taken "manually" from a DFTB calc., specified via the System%Atoms block

export AMS_JOBNAME=C2H10N2++

rm -rf $AMS_JOBNAME.results

"$AMSBIN/ams" << eor

Task GeometryOptimization

Properties Charges=yes

GeometryOptimization
  Convergence Gradients=1.0e-6
End

System
    Atoms
        N -0.005073166519502884 0.008770355996886468   1.060120635725228   ForceField.
↪Charge=-0.224106970135964811E+000
              C -0.003379615065181385 0.005774705419397744 -0.4323726711546611  ␣
↪ForceField.Charge=0.481803346892513140E-001
              C 0.7147029862216027 -1.238161594687982      -0.9787933548287219  ␣
↪ForceField.Charge=0.481357488383262755E-001
              N 0.7166487936613554 -1.241183181538415       -2.471469363728673  ␣
↪ForceField.Charge=-0.224111043229265006E+000
              H -0.489254727061788 0.8470579056083724        1.393322418122902  ␣
↪ForceField.Charge=0.327048167700910608E+000
              H 0.9419603270459358 0.02859511576851682       1.443864570589139  ␣
↪ForceField.Charge=0.312019677649949589E+000
```

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```
              H -0.4954439060007188 -0.801643243084588       1.443905390218997  ␣
↪ForceField.Charge=0.312016700963803795E+000
              H 0.497012567535054 0.9247340386709353       -0.7538297483507286  ␣
↪ForceField.Charge=0.112420754799849087E+000
              H -1.049427360359161 0.0320094307806696      -0.7537906795101232  ␣
↪ForceField.Charge=0.112425859786873958E+000
              H 1.760678843023289 -1.264262738726653       -0.6572703272452628  ␣
↪ForceField.Charge=0.112415997624231642E+000
              H 0.2140471968077103 -2.156981931600252      -0.6574882069415752  ␣
↪ForceField.Charge=0.112419970108937881E+000
              H 1.207324110469442 -0.4308282262683778       -2.854859298860555  ␣
↪ForceField.Charge=0.312043881750391661E+000
              H -0.2304034502578771 -1.260970512043685      -2.855040966499596  ␣
↪ForceField.Charge=0.312048243703216099E+000
              H 1.200917269444972 -2.079821003490794        -2.803581935602674  ␣
↪ForceField.Charge=0.327042675749500744E+000
    End

    GuessBonds True
    Charge 2.0
End


Engine ForceField
EndEngine

eor


# Now the neutral molecule, to show it behaves differently

export AMS_JOBNAME=C2H10N2

rm -rf $AMS_JOBNAME.results

"$AMSBIN/ams" << eor

Task GeometryOptimization

Properties Charges=yes

GeometryOptimization
  Convergence Gradients=1.0e-6
End

System
    Atoms
        N -0.005073166519502884 0.008770355996886468   1.060120635725228   ForceField.
↪Charge=-0.571011278205044492E+000
               C -0.003379615065181385 0.005774705419397744 -0.4323726711546611  ␣
↪ForceField.Charge=-0.628203646719944775E-001
               C 0.7147029862216027 -1.238161594687982      -0.9787933548287219  ␣
↪ForceField.Charge=-0.628837746183146251E-001
               N 0.7166487936613554 -1.241183181538415       -2.471469363728673  ␣
↪ForceField.Charge=-0.571125568500377101E+000
               H -0.489254727061788 0.8470579056083724        1.393322418122902  ␣
↪ForceField.Charge=0.194366247283714433E+000
```

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```
               H 0.9419603270459358 0.02859511576851682       1.443864570589139  ␣
↪ForceField.Charge=0.194416030458134853E+000
               H -0.4954439060007188 -0.801643243084588       1.443905390218997  ␣
↪ForceField.Charge=0.194415295916033237E+000
               H 0.497012567535054 0.9247340386709353       -0.7538297483507286  ␣
↪ForceField.Charge=0.253223131130085044E-001
               H -1.049427360359161 0.0320094307806696      -0.7537906795101232  ␣
↪ForceField.Charge=0.253801306729796901E-001
               H 1.760678843023289 -1.264262738726653       -0.6572703272452628  ␣
↪ForceField.Charge=0.253595653793994673E-001
               H 0.2140471968077103 -2.156981931600252      -0.6574882069415752  ␣
↪ForceField.Charge=0.254060553518517668E-001
               H 1.207324110469442 -0.4308282262683778       -2.854859298860555  ␣
↪ForceField.Charge=0.194371032691725371E+000
               H -0.2304034502578771 -1.260970512043685      -2.855040966499596  ␣
↪ForceField.Charge=0.194368207022870332E+000
               H 1.200917269444972 -2.079821003490794        -2.803581935602674  ␣
↪ForceField.Charge=0.194436108106012751E+000
    End

    GuessBonds True
End


Engine ForceField
EndEngine

eor

# The remaining calculations are again on the +2 ion

# Charges obtained with GuessCharges, using by default dftb.

export AMS_JOBNAME=C2H10N2++.guessed

rm -rf $AMS_JOBNAME.results

"$AMSBIN/ams" << eor

Task GeometryOptimization

Properties Charges=yes

GeometryOptimization
  Convergence Gradients=1.0e-6
End

System
    Atoms
        N -0.005073166519502884 0.008770355996886468   1.060120635725228
               C -0.003379615065181385 0.005774705419397744 -0.4323726711546611
               C 0.7147029862216027 -1.238161594687982      -0.9787933548287219
               N 0.7166487936613554 -1.241183181538415       -2.471469363728673
               H -0.489254727061788 0.8470579056083724        1.393322418122902
               H 0.9419603270459358 0.02859511576851682       1.443864570589139
               H -0.4954439060007188 -0.801643243084588       1.443905390218997
               H 0.497012567535054 0.9247340386709353       -0.7538297483507286
```

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```
               H -1.049427360359161 0.0320094307806696      -0.7537906795101232
               H 1.760678843023289 -1.264262738726653       -0.6572703272452628
               H 0.2140471968077103 -2.156981931600252      -0.6574882069415752
               H 1.207324110469442 -0.4308282262683778       -2.854859298860555
               H -0.2304034502578771 -1.260970512043685      -2.855040966499596
               H 1.200917269444972 -2.079821003490794        -2.803581935602674
    End

    GuessBonds True
    Charge 2.0
End


Engine ForceField
   GuessCharges True
EndEngine

eor


# Charges are now both specified on input and also Guessed
# The values on the input (ForceField.Charge) are on purpose unreasonable
# The Guessed charges have a higher priority and the input values are ignored
# The output is a bit confusing as unused ForceField.Charge is printed

export AMS_JOBNAME=C2H10N2++.inputandguessed

rm -rf $AMS_JOBNAME.results

"$AMSBIN/ams" << eor

Task GeometryOptimization

Properties Charges=yes

GeometryOptimization
  Convergence Gradients=1.0e-6
End

System
    Atoms
        N -0.005073166519502884 0.008770355996886468   1.060120635725228   ForceField.
↪Charge=-1.224106970135964811E+000
               C -0.003379615065181385 0.005774705419397744 -0.4323726711546611  ␣
↪ForceField.Charge=0.481803346892513140E-001
               C 0.7147029862216027 -1.238161594687982      -0.9787933548287219  ␣
↪ForceField.Charge=0.481357488383262755E-001
               N 0.7166487936613554 -1.241183181538415       -2.471469363728673  ␣
↪ForceField.Charge=-0.224111043229265006E+000
               H -0.489254727061788 0.8470579056083724        1.393322418122902  ␣
↪ForceField.Charge=1.327048167700910608E+000
               H 0.9419603270459358 0.02859511576851682       1.443864570589139  ␣
↪ForceField.Charge=0.312019677649949589E+000
               H -0.4954439060007188 -0.801643243084588       1.443905390218997  ␣
↪ForceField.Charge=0.312016700963803795E+000
               H 0.497012567535054 0.9247340386709353       -0.7538297483507286  ␣
↪ForceField.Charge=0.112420754799849087E+000
```

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```
               H -1.049427360359161 0.0320094307806696      -0.7537906795101232  ␣
↪ForceField.Charge=0.112425859786873958E+000
               H 1.760678843023289 -1.264262738726653       -0.6572703272452628  ␣
↪ForceField.Charge=0.112415997624231642E+000
               H 0.2140471968077103 -2.156981931600252      -0.6574882069415752  ␣
↪ForceField.Charge=0.112419970108937881E+000
               H 1.207324110469442 -0.4308282262683778       -2.854859298860555  ␣
↪ForceField.Charge=0.312043881750391661E+000
               H -0.2304034502578771 -1.260970512043685      -2.855040966499596  ␣
↪ForceField.Charge=0.312048243703216099E+000
               H 1.200917269444972 -2.079821003490794        -2.803581935602674  ␣
↪ForceField.Charge=0.327042675749500744E+000
    End

    GuessBonds True
    Charge 2.0
End


Engine ForceField
   GuessCharges True
EndEngine

eor






# Charges obtained with Load Charges from a DFTB calc.

export AMS_JOBNAME=C2H10N2++.dftb

rm -rf $AMS_JOBNAME.results

"$AMSBIN/ams" << eor

Task SinglePoint

Properties Charges=yes

GeometryOptimization
  Convergence Gradients=1.0e-6
End

System
    Atoms
        N -0.005073166519502884 0.008770355996886468   1.060120635725228
               C -0.003379615065181385 0.005774705419397744 -0.4323726711546611
               C 0.7147029862216027 -1.238161594687982      -0.9787933548287219
               N 0.7166487936613554 -1.241183181538415       -2.471469363728673
               H -0.489254727061788 0.8470579056083724        1.393322418122902
               H 0.9419603270459358 0.02859511576851682       1.443864570589139
               H -0.4954439060007188 -0.801643243084588       1.443905390218997
               H 0.497012567535054 0.9247340386709353       -0.7538297483507286
               H -1.049427360359161 0.0320094307806696      -0.7537906795101232
```

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```
               H 1.760678843023289 -1.264262738726653        -0.6572703272452628
               H 0.2140471968077103 -2.156981931600252       -0.6574882069415752
               H 1.207324110469442 -0.4308282262683778        -2.854859298860555
               H -0.2304034502578771 -1.260970512043685       -2.855040966499596
               H 1.200917269444972 -2.079821003490794         -2.803581935602674
    End

    Charge 2.0
End


Engine DFTB
EndEngine

eor

loadChargeFile='C2H10N2++.dftb.results/dftb.rkf'

export AMS_JOBNAME=C2H10N2++.loaded

rm -rf $AMS_JOBNAME.results

"$AMSBIN/ams" << eor

Task GeometryOptimization

Properties Charges=yes

GeometryOptimization
  Convergence Gradients=1.0e-6
End

System
    Atoms
        N -0.005073166519502884 0.008770355996886468   1.060120635725228
               C -0.003379615065181385 0.005774705419397744 -0.4323726711546611
               C 0.7147029862216027 -1.238161594687982       -0.9787933548287219
               N 0.7166487936613554 -1.241183181538415        -2.471469363728673
               H -0.489254727061788 0.8470579056083724         1.393322418122902
               H 0.9419603270459358 0.02859511576851682        1.443864570589139
               H -0.4954439060007188 -0.801643243084588        1.443905390218997
               H 0.497012567535054 0.9247340386709353        -0.7538297483507286
               H -1.049427360359161 0.0320094307806696       -0.7537906795101232
               H 1.760678843023289 -1.264262738726653        -0.6572703272452628
               H 0.2140471968077103 -2.156981931600252       -0.6574882069415752
               H 1.207324110469442 -0.4308282262683778        -2.854859298860555
               H -0.2304034502578771 -1.260970512043685       -2.855040966499596
               H 1.200917269444972 -2.079821003490794         -2.803581935602674
    End

    GuessBonds True
    Charge 2.0
End


Engine ForceField
   LoadCharges
```

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```
      File $loadChargeFile
   End
EndEngine

eor


# Charges are now both specified on input and also Guessed
# The values on the input (ForceField.Charge) are on purpose unreasonable
# The Guessed charges have a higher priority and the input values are ignored
# The output is a bit confusing as unused ForceField.Charge is printed

export AMS_JOBNAME=C2H10N2++.inputandloaded

rm -rf $AMS_JOBNAME.results

"$AMSBIN/ams" << eor

Task GeometryOptimization

Properties Charges=yes

GeometryOptimization
  Convergence Gradients=1.0e-6
End

System
    Atoms
        N -0.005073166519502884 0.008770355996886468   1.060120635725228   ForceField.
↪Charge=-1.224106970135964811E+000
               C -0.003379615065181385 0.005774705419397744 -0.4323726711546611  ␣
↪ForceField.Charge=0.481803346892513140E-001
               C 0.7147029862216027 -1.238161594687982      -0.9787933548287219  ␣
↪ForceField.Charge=0.481357488383262755E-001
               N 0.7166487936613554 -1.241183181538415       -2.471469363728673  ␣
↪ForceField.Charge=-0.224111043229265006E+000
               H -0.489254727061788 0.8470579056083724        1.393322418122902  ␣
↪ForceField.Charge=1.327048167700910608E+000
               H 0.9419603270459358 0.02859511576851682       1.443864570589139  ␣
↪ForceField.Charge=0.312019677649949589E+000
               H -0.4954439060007188 -0.801643243084588       1.443905390218997  ␣
↪ForceField.Charge=0.312016700963803795E+000
               H 0.497012567535054 0.9247340386709353      -0.7538297483507286  ␣
↪ForceField.Charge=0.112420754799849087E+000
               H -1.049427360359161 0.0320094307806696      -0.7537906795101232  ␣
↪ForceField.Charge=0.112425859786873958E+000
               H 1.760678843023289 -1.264262738726653       -0.6572703272452628  ␣
↪ForceField.Charge=0.112415997624231642E+000
               H 0.2140471968077103 -2.156981931600252      -0.6574882069415752  ␣
↪ForceField.Charge=0.112419970108937881E+000
               H 1.207324110469442 -0.4308282262683778       -2.854859298860555  ␣
↪ForceField.Charge=0.312043881750391661E+000
               H -0.2304034502578771 -1.260970512043685      -2.855040966499596  ␣
↪ForceField.Charge=0.312048243703216099E+000
               H 1.200917269444972 -2.079821003490794        -2.803581935602674  ␣
↪ForceField.Charge=0.327042675749500744E+000
    End
```

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```
    GuessBonds True
    Charge 2.0
End


Engine ForceField
   LoadCharges
      File $loadChargeFile
   End
EndEngine

eor



# finally let us make on purpose an error (total charge incorrect), this calculation␣
↪is supposed to fail, and not print an energy

echo "The following error is intended"

export AMS_JOBNAME=C2H10N2++.inputerror

rm -rf $AMS_JOBNAME.results

"$AMSBIN/ams" << eor

Task GeometryOptimization

Properties Charges=yes

GeometryOptimization
  Convergence Gradients=1.0e-6
End

System
    Atoms
        N -0.005073166519502884 0.008770355996886468   1.060120635725228   ForceField.
↪Charge=-0.224106970135964811E+000
               C -0.003379615065181385 0.005774705419397744 -0.4323726711546611  ␣
↪ForceField.Charge=0.481803346892513140E-001
               C 0.7147029862216027 -1.238161594687982      -0.9787933548287219  ␣
↪ForceField.Charge=0.481357488383262755E-001
               N 0.7166487936613554 -1.241183181538415       -2.471469363728673  ␣
↪ForceField.Charge=-0.224111043229265006E+000
               H -0.489254727061788 0.8470579056083724        1.393322418122902  ␣
↪ForceField.Charge=0.327048167700910608E+000
               H 0.9419603270459358 0.02859511576851682       1.443864570589139  ␣
↪ForceField.Charge=0.312019677649949589E+000
               H -0.4954439060007188 -0.801643243084588       1.443905390218997  ␣
↪ForceField.Charge=0.312016700963803795E+000
               H 0.497012567535054 0.9247340386709353       -0.7538297483507286  ␣
↪ForceField.Charge=0.112420754799849087E+000
               H -1.049427360359161 0.0320094307806696      -0.7537906795101232  ␣
↪ForceField.Charge=0.112425859786873958E+000
               H 1.760678843023289 -1.264262738726653       -0.6572703272452628  ␣
↪ForceField.Charge=0.112415997624231642E+000
```

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```
               H 0.2140471968077103 -2.156981931600252      -0.6574882069415752  ␣
↪ForceField.Charge=0.112419970108937881E+000
               H 1.207324110469442 -0.4308282262683778       -2.854859298860555  ␣
↪ForceField.Charge=0.312043881750391661E+000
               H -0.2304034502578771 -1.260970512043685      -2.855040966499596  ␣
↪ForceField.Charge=0.312048243703216099E+000
               H 1.200917269444972 -2.079821003490794        -2.803581935602674  ␣
↪ForceField.Charge=0.327042675749500744E+000
    End

    GuessBonds True
End


Engine ForceField
EndEngine

eor
```

5.3 Example: load partial charges from another engine

You can use *LoadCharges* (page 13) to load charges from another calculation. The key *GuessCharges* (page 13) is a simplified version of this, being more convenient, but less flexible.

Download LoadCharges.run

```
#!/bin/sh

# First we calculate the charges for a system

# Here we use the dftb engine, but any engine can be used for this purpose


export AMS_JOBNAME=CalculateCharges

rm -rf $AMS_JOBNAME.results

$AMSBIN/ams << eor
Task SinglePoint

Properties Charges=yes

System
   Atoms
      C 0.0 0.0 0.0
      O 1.13 0.0 0.0
      C 0.0 0.0 2.0
      O 1.13 0.0 2.0
   End
End

Engine DFTB
EndEngine

```

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```
eor

# let us first optimize without charges

export AMS_JOBNAME=DoNotUseCharges

rm -rf $AMS_JOBNAME.results

$AMSBIN/ams << eor
Task GeometryOptimization

GeometryOptimization
   Convergence Step=1.0e-3
End

System
   Atoms
      C 0.0 0.0 0.0
      O 1.13 0.0 0.0
      C 0.0 0.0 2.1
      O 1.13 0.0 1.9
   End
End

Engine ForceField
EndEngine

eor


# Now that we have charges from our previous fancy calculation, let us use them for a␣
↪UFF geometry optimization
# * The name of the file depends on the engine used (in this case dftb.rkf)
# * The geometry does not need to be the same

export AMS_JOBNAME=LoadCharges

rm -rf $AMS_JOBNAME.results

$AMSBIN/ams << eor
Task GeometryOptimization

GeometryOptimization
   Convergence Step=1.0e-3
End

System
   Atoms
      C 0.0 0.0 0.0
      O 1.13 0.0 0.0
      C 0.0 0.0 2.1
      O 1.13 0.0 1.9
   End
End

Engine ForceField
   Verbosity Verbose
```

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```
   LoadCharges File=CalculateCharges.results/dftb.rkf
EndEngine

eor

# Finally let us use the charge guessing, by default dftb is used for charge guessing

export AMS_JOBNAME=GuessCharges

rm -rf $AMS_JOBNAME.results

$AMSBIN/ams << eor
Task GeometryOptimization

GeometryOptimization
   Convergence Step=1.0e-3
End

System
   Atoms
      C 0.0 0.0 0.0
      O 1.13 0.0 0.0
      C 0.0 0.0 2.1
      O 1.13 0.0 1.9
   End
End

Engine ForceField
   Verbosity Verbose
   GuessCharges True
EndEngine

eor
```

5.4 Example: load atom types from a previous run

You can load the atom types from another force field calculation.

Observe that this is done with the `LoadForceFieldAtomTypes` inside the `System` block, see the System definition section of the AMS manual.

`Download LoadTypes.run`

```
#!/bin/sh

# In this example we use the amber forcefield that cannot guess atom types

# First we "calculate" the types

# We do this by specifying them as atom attributes (ForceField.Type)

export AMS_JOBNAME=CalculateTypes

rm -rf $AMS_JOBNAME.results
```

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```
$AMSBIN/ams << eor
Task GeometryOptimization

Properties Charges=yes

System
   Atoms
     C       1.94807   3.58290  -0.58162       ForceField.Charge=0.0       ForceField.
↪Type=CT
     H       1.69949   4.49893  -1.05273       ForceField.Charge=0.0       ForceField.
↪Type=HC
     H       2.99455   3.17964  -0.86304       ForceField.Charge=0.0       ForceField.
↪Type=HC
     C       0.94659   2.40054  -0.92364       ForceField.Charge=0.0       ForceField.
↪Type=CT
     C       1.94191   3.61595   1.09448       ForceField.Charge=0.0       ForceField.
↪Type=CT
     N      -1.74397  -3.46417   0.31178       ForceField.Charge=-0.9530    ForceField.
↪Type=N2
     C      -1.00720  -2.20758   0.33536       ForceField.Charge=0.8185     ForceField.
↪Type=CA
     C      -1.66928  -1.00652   0.31001       ForceField.Charge=-0.5215    ForceField.
↪Type=CM
     C      -0.92847   0.25653   0.34895       ForceField.Charge=0.0053     ForceField.
↪Type=CM
     N       0.43971   0.26735   0.38232       ForceField.Charge=-0.0484    ForceField.
↪Type=N*
     N       0.36409  -2.20477   0.28992       ForceField.Charge=-0.7584    ForceField.
↪Type=NC
     C       1.09714  -0.95413   0.22469       ForceField.Charge=0.7538     ForceField.
↪Type=C
     H      -2.89781  -3.50815   0.31746       ForceField.Charge=0.4234     ForceField.
↪Type=H
     H      -1.21484  -4.49217   0.31721       ForceField.Charge=0.4234     ForceField.
↪Type=H
     H      -2.80940  -0.93497   0.30550       ForceField.Charge=0.1928     ForceField.
↪Type=HA
     H      -1.55324   1.21497   0.33885       ForceField.Charge=0.1958     ForceField.
↪Type=H4
     C       1.23309   1.44017   0.30994       ForceField.Charge=0.0066     ForceField.
↪Type=CT
     O       2.58277  -1.01636   0.23914       ForceField.Charge=-0.6252    ForceField.
↪Type=O
     H       2.37276   1.25557   0.29984       ForceField.Charge=0.2902     ForceField.
↪Type=H2
     O       1.02358   2.43085   1.50880       ForceField.Charge=-0.2033    ForceField.
↪Type=OS
     H       1.17136   1.95097  -1.87367       ForceField.Charge=0.0       ForceField.
↪Type=HC
     H      -0.10600   2.77333  -0.80348       ForceField.Charge=0.0       ForceField.
↪Type=HC
     H       1.62170   4.54039   1.51392       ForceField.Charge=0.0       ForceField.
↪Type=H1
     H       2.99608   3.28749   1.41345       ForceField.Charge=0.0       ForceField.
↪Type=H1
   End
End
```

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```
Engine ForceField
   Type Amber95
EndEngine

eor


# Now we load the types from the previous result

# The result should be identical to the first calculation

export AMS_JOBNAME=LoadTypes

rm -rf $AMS_JOBNAME.results

$AMSBIN/ams << eor
Task GeometryOptimization

System
   Atoms
     C       1.94807   3.58290  -0.58162
     H       1.69949   4.49893  -1.05273
     H       2.99455   3.17964  -0.86304
     C       0.94659   2.40054  -0.92364
     C       1.94191   3.61595   1.09448
     N      -1.74397  -3.46417   0.31178
     C      -1.00720  -2.20758   0.33536
     C      -1.66928  -1.00652   0.31001
     C      -0.92847   0.25653   0.34895
     N       0.43971   0.26735   0.38232
     N       0.36409  -2.20477   0.28992
     C       1.09714  -0.95413   0.22469
     H      -2.89781  -3.50815   0.31746
     H      -1.21484  -4.49217   0.31721
     H      -2.80940  -0.93497   0.30550
     H      -1.55324   1.21497   0.33885
     C       1.23309   1.44017   0.30994
     O       2.58277  -1.01636   0.23914
     H       2.37276   1.25557   0.29984
     O       1.02358   2.43085   1.50880
     H       1.17136   1.95097  -1.87367
     H      -0.10600   2.77333  -0.80348
     H       1.62170   4.54039   1.51392
     H       2.99608   3.28749   1.41345
   End
   LoadForceFieldCharges    file=CalculateTypes.results
   LoadForceFieldAtomTypes  file=CalculateTypes.results
End

Engine ForceField
   Type Amber95
   Verbosity Verbose

EndEngine

eor
```

5.5 Example: using amber or tripos

Download 2h2o.run

```
#! /bin/sh

AMS_JOBNAME=amber95 $AMSBIN/ams << eor

Task SinglePoint

System
  Atoms
       O      0.0000      0.0000      0.0000      ForceField.Type=OW         ForceField.
↪Charge=-0.8340
       H     -0.5220      0.2660     -0.7570      ForceField.Type=HW         ForceField.
↪Charge=0.4170
       H     -0.5220      0.2660      0.7570      ForceField.Type=HW         ForceField.
↪Charge=0.4170
       O      0.0000     -3.2000      0.0000      ForceField.Type=OW         ForceField.
↪Charge=-0.8340
       H      0.0570     -2.2440      0.0000      ForceField.Type=HW         ForceField.
↪Charge=0.4170
       H      0.9110     -3.4950      0.0000      ForceField.Type=HW         ForceField.
↪Charge=0.4170
  End
  BondOrders
        1   2   1.0
        1   3   1.0
        4   5   1.0
        4   6   1.0
  End
End

Engine ForceField
  Type Amber95
EndEngine
eor


AMS_JOBNAME=tripos5.2 $AMSBIN/ams << eor

Task SinglePoint

System
  Atoms
       O      0.0000      0.0000      0.0000      ForceField.Type=O.3       ForceField.
↪Charge=-0.8340
       H     -0.5220      0.2660     -0.7570      ForceField.Type=H         ForceField.
↪Charge=0.4170
       H     -0.5220      0.2660      0.7570      ForceField.Type=H         ForceField.
↪Charge=0.4170
       O      0.0000     -3.2000      0.0000      ForceField.Type=O.3       ForceField.
↪Charge=-0.8340
       H      0.0570     -2.2440      0.0000      ForceField.Type=H         ForceField.
↪Charge=0.4170
       H      0.9110     -3.4950      0.0000      ForceField.Type=H         ForceField.
↪Charge=0.4170
```

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```
  End
  BondOrders
        1  2  1.0
        1  3  1.0
        4  5  1.0
        4  6  1.0
  End
End

Engine ForceField
  Type Tripos5.2
EndEngine
eor
```

5.6 Example: calculate some simple properties for water

Download water_properties.run

```
#! /bin/sh

$AMSBIN/ams << eor

Task GeometryOptimization

Properties
  BondOrders Yes
  Charges Yes
  DipoleMoment Yes
  NormalModes Yes
End

System
  Atoms
       O  0.0000  0.0000   0.0000  ForceField.Type=OW  ForceField.Charge=-0.8340
       H -0.5220  0.2660  -0.7570  ForceField.Type=HW  ForceField.Charge=0.4170
       H -0.5220  0.2660   0.7570  ForceField.Type=HW  ForceField.Charge=0.4170
  End
  BondOrders
        1  2  1.0
        1  3  1.0
  End
End

Engine ForceField
  Type Amber95
  ForceFieldFile $AMSRESOURCES/ForceFields/amber95.ff
EndEngine

eor

echo "MM Charges:"
$AMSBIN/amsreport ams.results/forcefield.rkf -r "AMSResults%Charges"
```

5.7 Example: single point for ammonia with TRIPOS

Download Ammonia_Tripos.run

```
#!/bin/sh

#
# This is a technical example comparing analytical and numerical gradients for the␣
↪Tripos forcefield
#
# The allowMissingParameters is a trick to run this molecule even though it is not␣
↪fully supported by the definition file
#

for num in no yes
do

export AMS_JOBNAME=tripos3.num=$num

rm -rf $AMS_JOBNAME.results

$AMSBIN/ams << eor

Task SinglePoint
Properties Gradients=yes

EngineDebugging IgnoreGradientsRequest=$num IgnorePreviousResults=true

NumericalDifferentiation NuclearStepSize=1.0e-4


System
  Atoms
    N       0.00000000       0.00000000       0.26448000   ForceField.Charge=0.0 ␣
↪ForceField.Type=N.2
    H      -0.48379000       0.83795000      -0.08816000   ForceField.Charge=0.0 ␣
↪ForceField.Type=H
    H      -0.48379000      -0.83795000      -0.08816000   ForceField.Charge=0.0 ␣
↪ForceField.Type=H
    H       0.96758000      -0.00000000      -0.08816000   ForceField.Charge=0.0 ␣
↪ForceField.Type=H
  End

  BondOrders
         1 2 1.0
         1 3 1.0
         1 4 1.0
  End
End


Engine ForceField
  Type Tripos5.2
  AllowMissingParameters yes
EndEngine
eor

done
```

CHAPTER

SIX

REQUIRED CITATIONS

When you publish results in the scientific literature that were obtained with programs of the AMS package, you are required to include references to the program package with the appropriate release number, and a few key publications.

For calculations with the UFF4MOF parameters: M.A. Addicoat, N. Vankova, I.F. Akter, and T. Heine, *An extension of the Universal Force Field to Metal-Organic Frameworks*, J. Chem. Theory Comput. 10, 880-891 (2013) (https://doi.org/10.1021/ct400952t)

For calculations with the UFF4MOFII parameters: D.E. Coupry, M.A. Addicoat, and T. Heine, *An Extension of the Universal Force Field for Metal-Organic Frameworks*, J. Chem. Theory Comput. 12, 5215-5225 (2016) (https://doi.org/10.1021/acs.jctc.6b00664)

6.1 External programs and libraries

Click here for the list of programs and/or libraries used in the AMS package. On some platforms optimized libraries have been used and/or vendor specific MPI implementations.

CHAPTER

SEVEN

PARAMETER FILES

The parameters of a forcefield are defined via one or more files, automatically set when using a standard *type* (page 9) . One way to change it is to use a parametrization made by someone else, that works better for systems of your interest.

A far more advanced use is to tweak an existing file, or create a new one, possibly to improve the results for specific systems of interest. For such a project the PARAMS tool might be helpful.

Here we distinguish the UFF and the AMBER case.

7.1 UFF parameters

The parameter set used by UFF can be changed via the *UFF* (page 14) key block. Aside from the standard UFF forcefield, we ship two parameter sets for Metal-Organic Frameworks:

UFF4MOF parameters

We ship the extended parameter set for Metal-Organic Frameworks created by M.A. Addicoat et al. (2013). Select the UFF4MOF_general_db, UFF4MOF_elements_db and UFF4MOF_mmatomtypes_db files to use these parameters, and check that the proper atom types are detected for your system or set them manually. Please see [*7* (page 55)] for details on the parameters.

UFF4MOFII parameters

We ship a second extended parameter set for Metal-Organic Frameworks created by D.E. Coupry et al. (2016). Select the UFF4MOFII_general_db, UFF4MOFII_elements_db and UFF4MOFII_mmatomtypes_db files to use these parameters, and check that the proper atom types are detected for your system or set them manually. Please see [*8* (page 55)] for details on the parameters.

7.1.1 User-modified force fields (expert option)

Finding good UFF parameters can be a challenging task, and any results with modified parameters should be checked very carefully. SCM has no experience with this, and the parameters supplied for UFF have not been generated by us. Feel free to test new parameters, and feel free to let us know if you have a good working set for a specialized situation.

General parameters file

The general_db file ($AMSHOME/atomicdata/UFF/general_db) contains all the parameters used to calculate the forces and energies. The format is:

MMAtomType, ri, phi, xi, di, psi, zmm, vsp3, vsp2, chi, nc.

The items in the list are:

- MMAtomType: name, max 5 characters

- ri: Valence Bond [Å]
- phi: Valence Angle [Degree]
- xi: Nonbond Distance [Å]
- di: Nonbond Energy [kcal/mol]
- psi: Nonbond scale [Number]
- zmm: Effective Charge [Charge]
- vsp3: sp3 Torsional Barrier [kcal/mol]
- vsp2: sp2 Torsional Barrier [kcal/mol]
- chi: Electronegativity
- nc: Number of directly attached atoms, aka coordination number. This is required for counting the number of possible dihedrals, and is defined only for the sp2 and sp3 centers (types 2, R, and 3)

The current set of parameters comes from the deMonNano program, and is a combination of published parameters and fitted data to fill in the gaps. The deMonNano documentation says the following about the parameters:

```
Implementation of the Universal Force Field (UFF) in deMonNano
--------------------------------------------------------------

As far as possible, UFF molecular mechanics forcefield in deMon
follows the published forcefield definition in [1]. In several
cases, the definitions and expressions in [1] are not consistent
with the published applications of the forcefield [1,5,6].
In those cases, an attempt was made to correct the errors and omissions,
using information from [2].

The following changed were made, compared to the published UFF
forcefield description (all equation and page numbers refer to [1]).

1. Sign error in Eq. 2 (equilibrium bond length) was corrected
   - electronegativity correction must be negative!

2. Equilibrium valence angle for O_3_z was corrected from 146.0
   degree to 145.45 degree.

3. Bending periodicity (Eq. 10) for linear coordination was
   corrected from 1 to 2.

4. Sign errors were corrected in eqs. 13 and and unnumbered equation
   for the beta parameter (between eqs. 13 and 14).

5. The reference value of the UFF amide force constant, of 105.5
   kcal/mol/rad**2 (p. 10028) is wrong. The results are consistent
   with the force constant of 211.0 kcal/mol/rad**2.

6. Equilibrium torsional angle for a bond between a group-6A atom
   (oxygen ...) and an sp2 atom (90 degree) is wrong (p. 10028).
   It should be 0 degree.

7. The conditional for the special-case sp2-sp3 torsion (p. 10029)
   is wrong, and should be inverted - see [4].

8. The overall shape of the UFF torsional potential degenerates to
```

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```
   a Heavyside function when one of the bond angles becomes linear,
   leading to failures in geometry optimization and force constant
   evaluation. The UFF torsional term was augmented with a smooth
   masking function, to avoid this.

9. UFF inversion potential is not defined in [1] for group 5A
   elements (from phosphorus down). Taking the equilibrium inversion
   coordinate of 87 degree, and the suitable expressions for the
   cosine weights (see uff_get_inversion_shape in "uff_database.f90")
   appears to reproduce published UFF structures and energetics.

The following atom types have been fully tested, and are believed
to reproduce published UFF forcefield results exactly. The examples
refer to the $deMon/examples/test.mm directory.

  Atom type  Example     Description
  ---------  -------     -----------

    Al3      alme3tma    Trivalent aluminum
    As3+3    asf3        Trivalent arsenic
    B_2      bcl3        Planar (sp2) boron
    B_3      b2h5nme2    Tetrahedral (sp2) boron, including
                         charge transfer adducts and borohydrates
    Br       bbr3        Univalent bromine
    C_1      c2h2, co    Linear (sp) carbon
    C_2      acetone     Planar tricoordinated (sp2) carbon
    C_3      c2h6        Tetrahedral (sp3) carbon
    C_R      c4h6        Resonant, variable bond order (sp2) carbon.
    Cl       socl2       Univalent chlorine
    F_       sof2ncl     Univalent fluorine
    Ge3      geh3ogeh3   Tetrahedral (sp3) germanium
    H_       h2o         Normal, non-bridging hydrogen
    H_b      b2h5nme2    Bridging hydrogen, for use in boranes
                         (NOT SUITABLE FOR H-BONDS!)
    I_       bi3         Univalent iodine
    N_1      ch3cn       Monocoordinated (sp) nitrogen, triple bond
    N_2      ch3n2ch3    Dicoordinated (sp2) nitrogen, single-double bond
    N_3      ch3nh2      Amine (sp3) nitrogen, three single bonds
    N_3+4    b2h5nme2    Charged amine (sp3) nitrogen, four single bonds
                         (THIS IS NOT A STANDARD UFF TYPE!)
    N_R      c5h5n       Resonant planar (sp2) nitrogen, for use in
                         aromatics and amides. For amides, use 1.41 bond
                         order!
    O_1      co          Special "co" type, one triple bond.
    O_2      acetone     One-coordinated (sp2) oxygen, one double bond.
    O_3      h2o         Two-coordinated (sp3) oxygen, two single bonds
    O_3_z    sih3osih3   Special two-coordinated oxygen, for use in
                         Si-O bonds
    O_R      c4h4o       Resonant planar (sp2) oxygen, also for use in
                         nitro groups and such.
    P_3+3    ph3         Pyramidal (sp3) phosphorus, three single bonds
    P_3+5    p4o7        Tetrahedral hypervalent phosphorus
    P_3+q    bh3ph3      Dative tetrahedral (sp3) phosphorus, watch for
                         the bond order!
    S_3+2    ch3sch3     Bent two-coordinated sulfur (sp3), two single bonds
    S_3+4    socl2       Pyramidal three-coordinated hypervalent sulfur
    S_3+6    so2cl2      Tetrahedral four-coordinated hypervalent sulfur
```

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```
    Se3+2     h2se        Bent two-coordinated (sp3) selenium
    Si3       si4o4h8     Tetrahedral silicon

Additionally, parameter sets for the following atom types are believed
be complete, and may be expected produce results identical to the published
UFF data: Li, Na, K_, Rb, Cs (Note that UFF does not specify atomic charges
- it is your responsibility to assign those, if charges are needed!)

For the remaining atom types, UFF definition [1] relies on an unpublished
set of electronegativities [2]. In deMon, these values were replaced by
Pauling electronegativities, scaled to fit published UFF electronegativities.
This can be expected to produce small deviations in bond lengths and bond
angles, compared to published UFF results.
```

If you wish to use other parameters, you should copy the general_db file, and rename it. This new file can also be placed outside of $AMSHOME/atomicdata/UFF.

Elements file

The elements_db file holds all the elements known to UFF. Keep in mind that these are not the MMAtomTypes, but pure chemical elements. The table contains for every element: atomic number, symbol, minimal valence number, maximum valence number, minimal bond order, maximal bond order. The data in the elements_db is mainly used for cleaning up the Pauling bond orders guessed by UFF, and will probably not need to be modified.

MM Atom Types file

The mmatomtypes_db file contains the matching rules for assigning MM atom types to chemical elements, based on their valence number, and the number of neighbor (bonded) atoms. The current implementation of UFF is limited to 6 MM atom types per element. The table contains for every MM atom type: Number of the element it belongs to, the i-th type of this element, the valence number corresponding to this MM atom type, number of neighbors this MM atom type has, the name of this MM atom type. The naming convention follows the original UFF paper [1]:

A five-character mnemonic label is used to describe the atom types. The first two characters correspond to the chemical symbol; an underscore appears in the second column if the symbol has one letter (e.g., `N_` is nitrogen, `Rh` is rhodium). The third column describes the hybridization or geometry: 1 = linear, 2 = trigonal, R = resonant, 3 = tetrahedral, 4 = square planar, 5 = trigonal bipyramidal, 6 = octahedral. Thus N_3 is tetrahedral nitrogen, while Rh6 is octahedral rhodium. The forth and fifth columns are used as indicators of alternate parameters such as formal oxidation state: Rh6+3 indicates an octahedral rhodium formally in the +3 oxidation state, e.g., Rh(NH3)_6^3+. H_b indicates a bridging hydrogen as in B2Hs O_3_z is an oxygen suited for framework oxygens of a zeolite lattice. P_3_q is a tetrahedral four-coordinate phosphorus used to describe organo-metallic coordinated phosphines.

You can copy the mmatomtypes_db and change it if you need to modify the atom typing behavior of UFF.

7.2 AMBER parameters

If you want to use a non-standard forcefield you can specify the *ForceFieldFile* (page 14).

Currently two formats are supported for non-uff forcefields. The first is the ADF/SCM related ".ff" format. The other is the much more widely used AMBER ".dat" format.

7.2.1 AMBER forcefield file

The format of the AMBER ".dat" files is described here http://ambermd.org/FileFormats.php#parm.dat. Currently the following features are not supported

- Parameter modification files
- The torsions have extra info about 1-4 scaling for nonbonded terms, ignored
- AMBER term 8: INPUT FOR H-BOND 10-12 POTENTIAL PARAMETERS
- AMBER term 9: INPUT FOR EQUIVALENCING ATOM SYMBOLS FOR THE NON-BONDED 6-12 POTENTIAL PARAMETERS

7.2.2 SCM forcefield file

An example of this is `$AFDHOME/atomicdata/ForceField/amber95.ff`. It has a flexible format and is fully self documented. It is not used outside of the ADF/SCM context.

The file must contain the force field parameters and the MM potential for each kind of MM interaction. Although predefined force field files (AMBER and SYBYL) are provided, these force field files can be customized. For example, one may want to change a particular force constant, or one may need to introduce a new atom type, for instance a transition metal. This section provides a detailed description of the force field file.

Format

The force field file is keyword driven with each key block defining parameters for each molecular mechanics interaction type such as bond types, angle types, torsion types, . . . etc. The key block begins with the keyword, such as "BONDS".

The lines that actually contain the parameters are sandwiched between two lines that contain "========". The lines between the keyword and the first line containing "========" are not read by the program. These lines are intended for the user to define the columns as shown below. There can be as many lines between the keyword and the first '=====' as needed.

Example:

```
BONDS
Atoms  pot  K              ro    Notes
i - j  type (kcal/molA^2) (Ang)
================================
...
CA  CA 1    938.0          1.400 amber95
CT  CT 1    620.0          1.526 amber95
...
===============================
```

Force Field Atom types

The force field atom types are the labels given to each atom in the real system, which determine all interaction parameters involving that atom.

There are some limitations to the force field label types that the user can specify:

- Labels can be a maximum of four characters long, with no spaces.
- The atom types are case sensitive.
- They can contain letters, numbers and other characters except ',' '.' or '=' and tabs.

Example of atom types that are not compatible with the program: C.3, C 3, C=3, C_sp3, *

Examples of atom types that are correct: C_3, C3, Csp3, and C*

Wild Cards

Wild cards can be specified with the asterisk, '*'. Wild cards can be specified for angles, torsions and out-of-plane bends. Please refer to the specific sections for the limitations.

CAUTION: When using wild cards, place the wild cards at the beginning of the data section, beginning with the parameters with the most wild cards and ending with those that posses the least wild cards.

Example:

•	C_3	•	100.310	111.000	*two wild cards*
•	C_3	C_3	100.310	111.000	*one wild card*
C_2	C_3	C_3	100.310	111.000	*no wild cards*

If this ordering is not followed, then the wild card parameters will over-ride the specific parameters.

Miscellaneous Notes

- Do not remove the '======' separator lines.
- Units are in kcal/mol, Angstroms, degrees, amu unless otherwise specified
- Sections can be in any order; i.e. BENDS can come before BONDS.
- All keywords are case sensitive and most are in ALL-CAPS
- Input is all free format
- Blank lines will be ignored
- Comment lines can be added to parameter data sections by beginning the line with the '#' symbol.

Example:

```
H H 1.0080
HC H 1.0080
   # example of comment line denoted with # mark.
H1 H 1.0080
H2 H 1.0080
```

A (partial) Example File

Here we provide an example force field file to illustrate the format of the file. Only a limited number of parameters are included. A detailed description of each section of the force field file is provided in the next section.

```
FORCE_FIELD_SETTINGS
================================
ELSTAT_1-4_SCALE          1.0000
VDW_1-4_SCALE             1.0000
VDW_DEFAULT_POTENTIAL     1      (1:6-12 2:exp-6 3:exp purely repulsive)
DIELECTRIC_CONSTANT       1.000
================================


MASSES & ATOM LABELS
-----------------------------------
force_field atomic
atom_type   symbol mass    NOTES
==========================
C_3         C      12.0110 sp3 hybridized carbon
C_2         C      12.0110 sp2 hybridized carbon
C_1         C      12.0110 sp1 hybridized carbon
C_ar        C      12.0110 aromatic
N_3         N      14.0070
```

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```
N_2         N      14.0070
O_3         O      15.9990
==========================

BONDS Ebond = 0.5*K(r-ro)**2
--------------------------------------
Atoms   pot
i - j   type K        R      NOTES
==========================
C_2 C_2 1    1340.00 1.335 WHITE_77
C_2 C_3 1     639.00 1.501 WHITE_75
C_3 C_3 1     633.60 1.540 *
C_3 N_2 1     760.20 1.440 *
==========================
BENDS Ebend = 0.5*k(a-ao)^2
------------------------------------
Atoms           pot
i - j - k       type   K      theta  NOTES
===================================
*    C_2  *     1      78.79 120.00 WHITE_77
*    C_3  *     1      65.66 109.50 WHITE_77
*    C_ar *     1      78.79 120.00 *
C_ar C_2  N_2   1     131.31 120.00 *
C_3  C_3  C_ar  1      78.79 109.50 *
===================================

TORSIONS
--------------------------------------------
Atoms               pot
i - j - k - l       type  k       per          NOTES
============================================
*    C_2  C_2  *    2     12.5000 -2.0
*    C_1  C_3  *    2      0.0000  1.0
C_2  C_2  C_3  *    2      0.1260 -3.0
C_3  C_2  C_3  *    2      0.1260  3.0
H    C_2  C_3  *    2      0.2740  3.0
*    C_ar C_ar C_ar 2      2.3500 -2.0
*    C_2  C_3  C_2  2      0.1260  3.0
*    C_2  C_3  C_3  2      0.1260  3.0
C_3  C_3  C_3  C_3  0      0.5000  3.0       no torsion potential
C_2  C_2  C_3  C_2  2      0.1260 -3.0
C_3  C_3  N_2  C_2  1      0.5000  4   180.0 This and the next 3 lines
&                          0.1500  3   180.0 are part of a multi-component
&                          0.5300  1     0.0 Fourier potential
C_3  C_3  C_2  N_2  1      0.1000  4     0.0
&                          0.0700  2     0.0 '&' is a continuation marker
============================================

OUT-OF-PLANE
-------------------------
Atoms           pot
i - j - k - l   type  K   NOTES
=========================
*   *   C_2 *   2     480 TRIPOS_85
*   *   N_2 *   2     120 TRIPOS_85
H   H   N_2 C_3 2     120 TRIPOS_85
C_3 H   N_2 *   2     120 TRIPOS_85
```

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```
=========================

VAN DER WAALS
atom(s)      Emin    Rmin    gamma NOTES
==================================
C_3          0.1070  3.4000  12.00
C_2          0.1070  3.4000  12.00
C_ca         0.1070  3.4000  12.00
C_ar         0.1070  3.4000  12.00
C_1          0.1070  3.4000  12.00
N_3          0.0950  3.1000  12.00
N_2          0.0950  3.1000  12.00
N_2 - N_2 2 0.0950  3.1000  12.00 purely repulsive potential for this pair
==================================

type  charge(e)  NOTES
================
OW    -0.82      TIP3P water model
HW     0.41      TIP3P water model
================
```

Section by Section Description

FORCE_FIELD_SETTINGS Key block (required) This key block specifies various global options for the force field file, mostly concerned with the treatment of the non-bonded potentials.

```
FORCE_FIELD_SETTINGS
================================
ELSTAT_1-4_SCALE           0.5
VDW_1-4_SCALE              0.5
VDW_DEFAULT_POTENTIAL      1      (1:6-12)
DIELECTRIC_CONSTANT        1.000
================================
```

ELSTAT_1-4_SCALE & VDW_1-4_SCALE Most force fields scale the non-bonded interactions by a factor of 0.5 if the atoms are the terminal atoms of a defined torsion. This scaling factor, which is termed the 1-4 scaling factor, can also be different for the electrostatic potential and for the Van der Waals potentials and thus they are separately defined in the input.

VDW_DEFAULT_POTENTIAL Only the Lennard Jones potential (option 1) is implemented. The Lennard Jones interaction energy between atoms A and B is defined as a function of the distance between atoms A and B (R^{AB}). The two parameters are D_0 and R_0.

$$E_{VDW}(R^{AB}) = D_0\left[\left(\frac{R_0}{R^{AB}}\right)^{12} - 2\left(\frac{R_0}{R^{AB}}\right)^{6}\right]$$

DIELECTRIC_CONSTANT This option is ignored.

BONDS Key block (required) This key block specifies the potential type and parameters for each kind of MM bond stretching interaction. An example is given below.

```
BONDS
Atoms pot   K             ro    NOTES
i - j type  (kcal/molA^2) (Ang)
===============================
CA CA 1     938.0         1.400 amber95
CT CT 1     620.0         1.526 amber95
```

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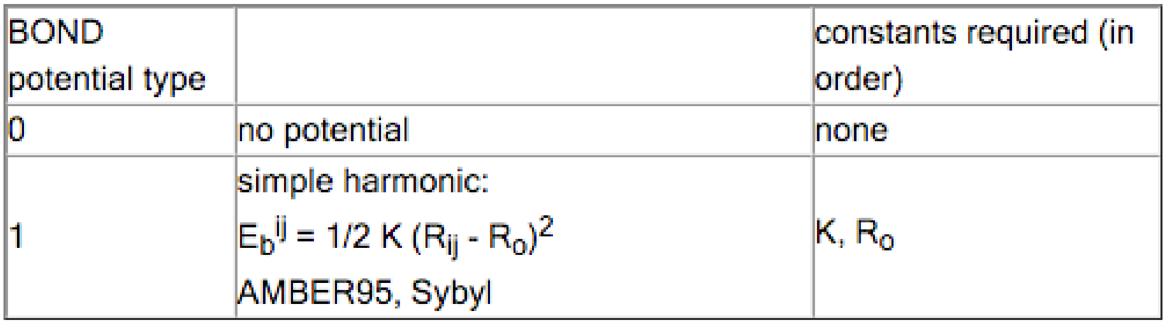
```
HC Zr 0        0.0                 no potential found
================================
```

The first two columns are the atom types (up to four characters long) and the third column is an integer specifying the potential type.

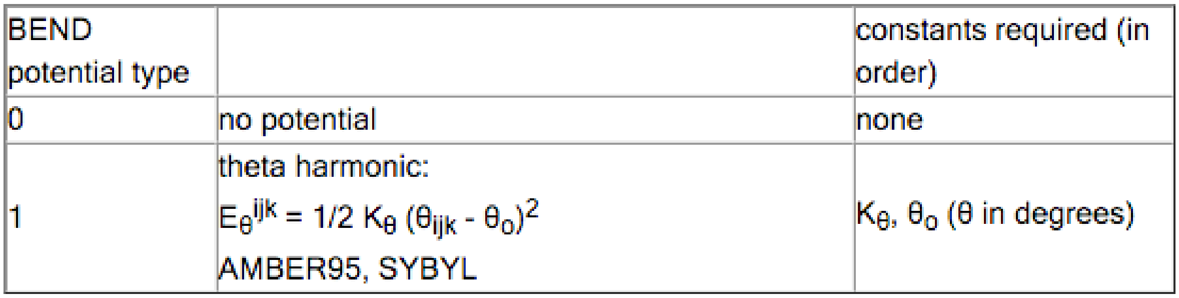


BOND potential type		constants required (in order)
0	no potential	none
1	simple harmonic: $E_b^{ij} = 1/2\ K\ (R_{ij} - R_o)^2$ AMBER95, Sybyl	K, R_o

BENDS Key block (required) This key block specifies the potential type and parameters for each kind of MM bond angle interaction. An example is given below.

```
BENDS
Atoms      pot   k           ao     NOTES
i - j - k type  (kcal/mol)  deg
=================================
*  CA *   1      70.00     120.00 example of wild card
*  CA CA  1     126.00     120.00
CA CA N2  1     140.00     120.10 amber95 N2-CA-CM
CA CA CT  1     140.00     120.00 amber95
=================================
```

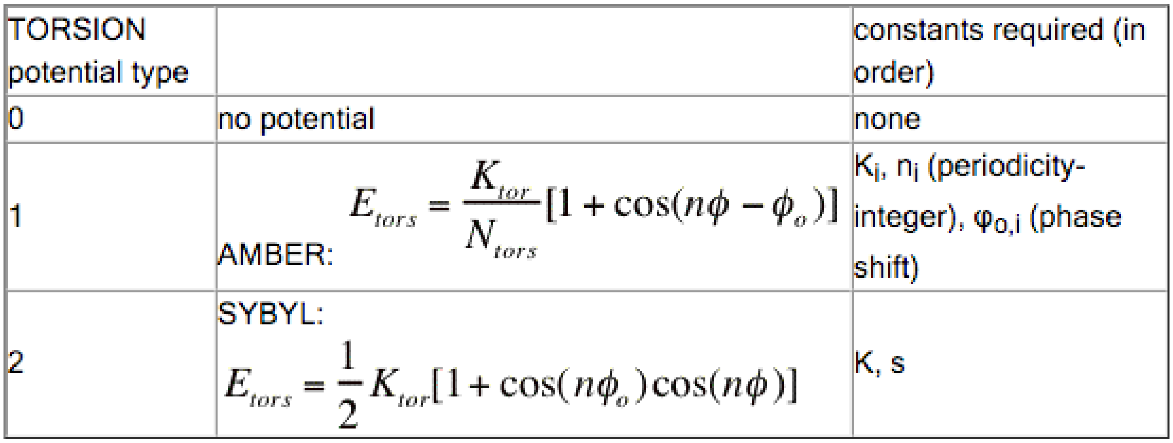
The first three columns specify the atom types and the fourth column is an integer specifying the potential type. The angle bend potential types are described in the table below with the additional constants required.



BEND potential type		constants required (in order)
0	no potential	none
1	theta harmonic: $E_\theta^{ijk} = 1/2\ K_\theta\ (\theta_{ijk} - \theta_o)^2$ AMBER95, SYBYL	K_θ, θ_o (θ in degrees)

Notice that wild cards can be specified for both terminal positions of the bend or just one as in the example above. It is important that the parameters be ordered from the least specific (those containing the most wild cards) to the most specific parameters.

TORSIONS Key block (required) This key block specifies the potential type and parameters for each kind of MM bond torsion interaction. For the bond stretching and bending potentials, only one potential has to date been implemented since both AMBER and SYBYL both use simple harmonic potentials. However, AMBER and SYBYL use different functional forms to represent the torsion potentials, each with their own set of parameters. The AMBER and SYBYL torsional potentials used in this program are defined in the table below.



TORSION potential type		constants required (in order)
0	no potential	none
1	AMBER: $E_{tors} = \frac{K_{tor}}{N_{tors}}[1+\cos(n\phi-\phi_o)]$	K_i, n_i (periodicity-integer), $\varphi_{o,i}$ (phase shift)
2	SYBYL: $E_{tors} = \frac{1}{2}K_{tor}[1+\cos(n\phi_o)\cos(n\phi)]$	K, s

Notice that the two potentials have a different number of parameters. For example, when the program reads 'potential type' number 1, it will expect three parameters K_i , n_i , $\phi_{o,i}$. Further notice that the AMBER torsional potential is a sum of Fourier components (this is what the index i refers to).

Below is an example of the TORSIONS key block, made up of AMBER force field types.

```
TORSIONS
Atoms                   pot            per.  shift
i - j - k - l           type  k        n     to       NOTES
===================================================
*     CV    NB    *     1     2.4000   2     180.0    JCC,7,(1986),230
*     CW    NA    *     1     1.5000   2     180.0    JCC,7,(1986),230
&                             0.1000   3       0.0
C     N     CT    C     1     0.2000   2     180.0
N     CT    C     N     1     0.4000   4     180.0
&                             1.3500   2     180.0
&                             0.7500   1     180.0
CT    CT    N     C     1     0.5000   4     180.0
===================================================
```

Most AMBER torsion potentials are not specific to all four atoms i-j-k-l, but only on the central two, j-k. Wild cards are specified with the '*' symbol as illustrated above. Again, the ordering is important. The parameters should be ordered from least specific (those containing the most wild cards) to most specific. The AMBER torsion potential can be composed of more than one Fourier component for a single torsion potential. Additional Fourier components are specified with the '&' continuation symbol as in the example above. At the moment, up to 6 Fourier components are allowed. Notice that the individual components need not be specified in any particular order. In the above example key block, there are only 5 torsional potentials defined, not 8. Two of the potentials are composed of more than one Fourier component as indicated by the '&' continuation line. Below is an example of the TORSIONS key block for the SYBYL force field. Notice that the potential types are all '2'. There are fewer parameters and no multi component potentials. Also, some potentials are defined with two or only one wild card.

```
TORSIONS
-------------------------------------------
Atoms                   pot
i - j - k - l           type  k        per      NOTES
===============================================
*     C_ar  S_3   *     2     1.0000    3.0     *
*     S_3   S_3   *     2     0.0000    2.0     EXP
C_2   C_2   C_3   *     2     0.1260   -3.0     WHITE_77
C_3   C_2   C_3   *     2     0.1260    3.0     WHITE_77
```

(continues on next page)

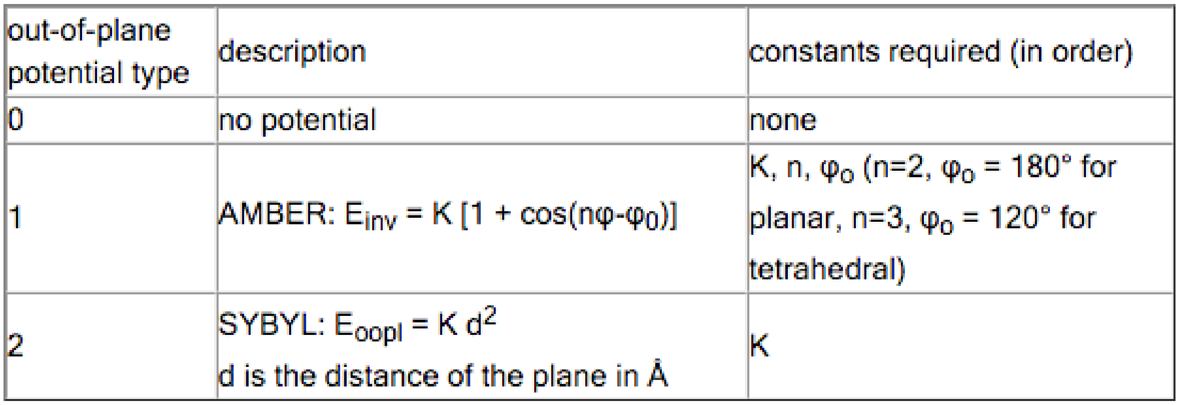
(continued from previous page)

```
H     C_2   C_3   *     2     0.2740    3.0     *
*     C_ar  C_ar  C_ar  2     2.3500   -2.0     *
*     C_2   C_3   C_2   2     0.1260    3.0     WHITE_77
*     C_2   C_3   C_3   2     0.1260    3.0     WHITE_77
*     C_2   C_3   H     2     0.2740    3.0     WHITE_77
*     C_3   C_3   H     2     0.3200    3.0     MC_88
O_2   C_2   C_3   C_3   2     0.7000   -3.0     JL_ES_
O_co  C_2   C_3   C_3   2     0.7000   -3.0     MAC_1
C_2   C_3   C_3   C_2   2     0.0400    3.0     WHITE_77
C_2   C_3   C_3   C_3   2     0.1260    3.0     WHITE_77
================================================
```

One can also mix different potential types within the same force field file, as illustrated below. In this example, three are three potentials. The first two are SYBYL type potentials whereas the last one is a multi component AMBER potential.

```
H  C_2   C_3   *     2  0.2740   3.0
*  C_ar  C_ar  C_ar  2  2.3500   -2.0
N  CT    C     N     1  0.4000   4     180.0
&                       1.3500   2     180.0
&                       0.7500   1     180.0
```

OUT-OF_PLANE Key block (required) This key block specifies the potential type and parameters for each kind of MM out of plane bend. This potential is sometimes referred to as the inversion potential or improper torsions (depending on the force field). The potential types currently supported are provided in the table below.



out-of-plane potential type	description	constants required (in order)
0	no potential	none
1	AMBER: $E_{inv} = K [1 + \cos(n\varphi-\varphi_0)]$	K, n, φ_0 (n=2, φ_0 = 180° for planar, n=3, φ_0 = 120° for tetrahedral)
2	SYBYL: $E_{oopl} = K d^2$ d is the distance of the plane in Å	K

An example of the key block for the AMBER type potentials is given below. It is important to realize that the atom k is the **atom k is the central atom**. (We have adopted the somewhat odd standard of AMBER in this respect).

```
OUT-OF-PLANE
--------------------------
Atoms                    pot
i - j - k - l            type  K       to     NOTES
=============================================
*     *     CA    H4     1      1.10   180.0  bsd.on C6H6 nmodes
*     *     CA    H5     1      1.10   180.0  bsd.on C6H6 nmodes
*     O2    C     O2     1     10.50   180.0  JCC,7,(1986),230
*     N2    CA    N2     1     10.50   180.0  JCC,7,(1986),230
*     CT    N     CT     1      1.00   180.0  JCC,7,(1986),230
CK    CB    N*    CT     1      1.00   180.0
=============================================
```

VAN DER WAALS Key block (required) This key block specifies the potential type and parameters for each kind of MM van der Waals interaction between two atoms. A sample key block is shown below:

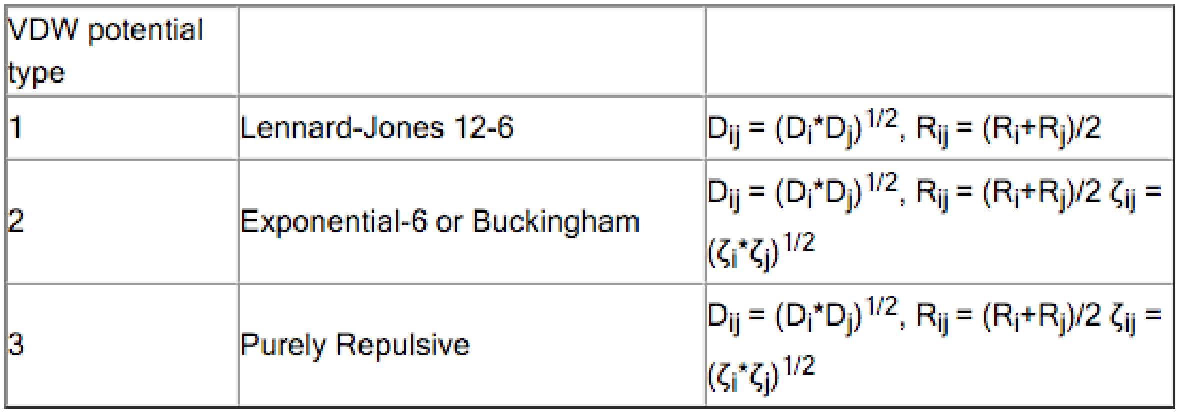
```
atom(s) type  emin    rmin      alpha      NOTES
====================================
CA            -.0860  3.81600   12.00      amber95
HA            -.0150  2.91800   12.00      amber95
Ni - HA  2    -.0480  2.7       12.00      NOTE potential type
Ni - CA  D    -.0480  2.7       12.00      default potential
====================================
```

The van der Waals key block is somewhat different than the previous key blocks, because generally not every atom pair is defined with its own parameters. Rather, the parameters are assigned on a per atom basis and then special combination rules are used to construct the parameters for each atom pair combination. For this reason, the type is defined separately in the FORCE_FIELD_SETTINGS key block, although currently only the Lennard-Jones 6-12 potential is implement, although currently only the Lennard-Jones 6-12 potential is implemented

For each type of van der Waals interaction, the program first scans the key block for pair specific parameters. The three sample lines below specify pair-specific potentials. The two atom types must be separated by a hyphen with spaces between the hyphen and the atom type. Following the specification of the atom pair, the potential type is defined. If D or d is specified here, then this means to use the default potential type. Following the potential type are the parameters needed for that potential type (see above table).

```
CA - CA  1  0.0860   3.81600  12.00 amber95
Ni - HA  0
Ni - CA  D  0.0480   2.7      12.00 default potential type
```

If a pair specific parameter can't be found, then the program looks for individual atom parameters corresponding to each of the atom types in the pair. The pair specific parameters are then constructed from combination of the two individual atom parameters using the following combination rules:



VDW potential type		
1	Lennard-Jones 12-6	$D_{ij} = (D_i*D_j)^{1/2}$, $R_{ij} = (R_i+R_j)/2$
2	Exponential-6 or Buckingham	$D_{ij} = (D_i*D_j)^{1/2}$, $R_{ij} = (R_i+R_j)/2$ $\zeta_{ij} = (\zeta_i*\zeta_j)^{1/2}$
3	Purely Repulsive	$D_{ij} = (D_i*D_j)^{1/2}$, $R_{ij} = (R_i+R_j)/2$ $\zeta_{ij} = (\zeta_i*\zeta_j)^{1/2}$

When individual atom parameters are not used, no potential type is specified since the default potential type is always used. An example is given below.

```
CA 0.0860   3.81600  12.00 amber95
HA 0.0150   2.91800  12.00 amber95
```

The ability to define pair specific parameters is especially useful for those force fields that have different combination rules than used in the program. For example, Jorgensen's TIP3P water force field uses geometric averages for both D_{ij} and R_{ij} .

MASSES & ATOM LABELS Key block (required) This key block specifies the default masses for each MM atom type and the element label for each MM atom type. The masses are not used by the engine.

A sample key block is shown below:

```
MASSES & ATOM LABELS
=====================================
Ni              Ni              58.70
CM              C               12.011
CA              C               12.011
CT              C               12.011
HC              H                1.0079
HA              H                1.0079
=====================================
```

The first column is the MM atom type, the second is the corresponding atom element and the third column is the mass of the atom type. The atoms do not have to be specified in any particular order.

CHARGES Key block (optional) This key block specifies the parameters for the charges on the atoms by atom type. NOTE: Charges can also be specified on a per atom basis in the `System` block of the AMS input file.

```
CHARGES
atoms        initial
label        charge
========================
OW           -0.8
HW            0.4
========================
```

CHAPTER

EIGHT

POTENTIAL SHAPES

Setting the *Verbosity* (page 10) to Verbose the engine prints the potential formula and the parameters used.

The ForceField engine has a couple of potentials defined.

- Stretch: harmonic

$$V^{\text{stretch/harm}} = \frac{1}{2} f_c (r - r_0)^2$$

- Angle: harmonic and cyclic

$$V^{\text{bend/harm}} = \frac{1}{2} f_c (\phi - \phi_0)^2$$

$$V^{\text{bend/cycl}} = f_c \sum_{m=0}^{n} c_m \cos(m\phi)$$

- Torsions: cyclic, possibly linearly combined. The same torsion occurs more than once in the printed table, and the energies are added.

$$V^{\text{torsion/harm}} = \frac{1}{2} f_c (\phi - \phi_0)^2$$

$$V^{\text{torsion/cycl}} = f_c \sum_{m=0}^{n} c_m \cos(m\phi)$$

- Inversions: either angle or distance based. The angle based one depends on the order of the three atoms connected to the central atom. UFF averages over the three permutations.

$$V^{\text{inversion/harm}} = \frac{1}{2} f_c (\phi - \phi_0)^2$$

$$V^{\text{inversion/cycl}} = f_c \sum_{m=0}^{n} c_m \cos(m\phi)$$

$$V^{\text{inversion/amber}} = f_c (1 + \cos(2\phi - \phi_0))$$

$$V^{\text{inversion/dist}} = f_c \, d^2$$

- Dispersion: Lennard-Jones. Neglect up to second neighbors, possibly scale contribution from third neighbors.

$$V^{\text{dispersion/LJ}} = d \, ((x/r)^{12} - 2 * (x/r)^6)$$

- Coulomb: Neglect up to second neighbors, possibly scale contributions from third neighbors.

In general which formula is used depends on the parameter files. Note that the scaling of the third neighbors contributions is only possible when using .ff parameter files.

CHAPTER

NINE

PERIODIC FORCEFIELD

The forcefield engine can be used to optimize the geometries of periodic systems. When specifying bonds, via the System%Bondorders key block, one should also specify the bonds that pass through a cell boundary. The GUI does this automatically. You can also simply set the key System%GuessBonds to true, and then UFF-guessed bonds will be used.

When you are having charges, Ewald summation will be used to calculate the Coulomb interaction. Currently this will be fairly slow for 1D and 2D periodic systems, as the classical Ewald trick cannot be applied.

CHAPTER TEN

REFERENCES

1. A.K. Rappe, C.J. Casewit, K.S. Colwell, W.A. Goddard III, and W. M. Skiff, *UFF, a Full Periodic Table Force Field for Molecular Dynamics Simulations*, Journal of the American Chemical Society 114, 10024-10035 (1992). (https://doi.org/10.1021/ja00051a040)
2. A.K. Rappe, W.A. Goddard III, *Charge Equilibration for Molecular Dynamics Simulations*, The Journal of Physical Chemistry 95, 3358-3363 (1991). (https://doi.org/10.1021/j100161a070)
3. M. O'Keeffe and N.E. Brese, *Atom sizes and bond lengths in Molecules and Crystals*, Journal of the American Chemical Society 113, 3226-3229 (1991). (https://doi.org/10.1021/ja00009a002)
4. S.L. Mayo, B.D. Olafson, W.A. Goddard III, *DREIDING: A Generic Force Field for Molecular Simulations*, The Journal of Physical Chemistry 94, 8897-8909 (1990). (https://doi.org/10.1021/j100389a010)
5. C.J. Casewit, K.S. Colwell, A.K. Rappe, *Applications of a Universal Force Field to Main Group Compounds*, Journal of the American Chemical Society 114, 10046-10053 (1992). (https://doi.org/10.1021/ja00051a042)
6. C.J. Casewit, K.S. Colwell, A.K. Rappe, *Application of a Universal Force Field to Organic Molecules*, Journal of the American Chemical Society 114, 10035-10046 (1992). (https://doi.org/10.1021/ja00051a041)

For calculations with the UFF4MOF parameters:

7. M.A. Addicoat, N. Vankova, I.F. Akter, and T. Heine, *An extension of the Universal Force Field to Metal-Organic Frameworks*, J. Chem. Theory Comput. 10, 880-891 (2013) (https://doi.org/10.1021/ct400952t)

For calculations with the UFF4MOFII parameters:

8. D.E. Coupry, M.A. Addicoat, and T. Heine, *An Extension of the Universal Force Field for Metal-Organic Frameworks*, J. Chem. Theory Comput. 12, 5215-5225 (2016) (https://doi.org/10.1021/acs.jctc.6b00664)

CHAPTER

ELEVEN

KEYWORDS

11.1 Links to manual entries

forcefield:

- *AllowMissingParameters* (page 14)
- *AntechamberIntegration* (page 7)
- *AntechamberTask* (page 7)
- *BondsUsage* (page 10)
- *CheckDuplicateRules* (page 14)
- *EnergyTerms* (page 11)
- *EwaldSummation* (page 10)
- *ForceFieldFile* (page 14)
- *GuessCharges* (page 13)
- *GuessChargesConfig* (page 13)
- *LoadCharges* (page 13)
- *NonBondedCutoff* (page 9)
- *Type* (page 9)
- *UFF* (page 14)
- *Verbosity* (page 10)

11.2 Summary of all keywords

`AllowMissingParameters`

Type Bool

Default value No

Description When parameters are not found for bonds, angles, dihedrals, or inversions, the first entry in the database will be used.

`AntechamberIntegration`

Type Bool

Default value No

GUI name Automatic atom typing

Description EXPERIMENTAL: Use the Antechamber program to automatically determine atom types for the GAFF force field. This may run a geometry optimization with MOPAC under the hood in order to determine the charges (see keyword AntechamberTask), which might not work for very large systems.

AntechamberTask

Type Multiple Choice

Default value GeometryOptimization

Options [GeometryOptimization, SinglePoint]

Description If antechamber is envoked to guess atomtypes and charges (GAFF force field), select the task for charge guessing with MOPAC

APPLEnP

Type Block

Description Option for the APPLEnP force filed.

ThirdNeighborScaling

Type Float

Default value 0.8

Description Scaling factor for non-bonded interactions between atoms connected to 3rd order (via a dihedral).

BondsUsage

Type Multiple Choice

Default value Auto

Options [Input, None, Guess, Auto]

Description Controls what bonds are used by the engine. The choice auto means: guess in case there are no bonds. Guessing only happens at the first MD step, or first geometry optimization step.

CheckDuplicateRules

Type Bool

Default value Yes

Description The database could contain duplicate entries. For torsions this is a feature, and the potentials will be added. For all other terms this is no allowed, and if detected the program stops. One should fix the database or set the checking to false. As always the last entry will be used.

DoChargeCheck

Type Bool

Default value Yes

Description Check that the sum of atomic (partial) charges equals the total charge of the system.

EnergyTerms

Type Block

Description expert key, that allows you to disable specific energy terms.

Angle

Type Bool

Default value Yes

Description Whether to use angle (bend) energy.

`Coulomb`

Type Bool

Default value Yes

Description Whether to use coulomb energy.

`Dispersion`

Type Bool

Default value Yes

Description Whether to use dispersion energy.

`Inversion`

Type Bool

Default value Yes

Description Whether to use inversion energy.

`Stretch`

Type Bool

Default value Yes

Description Whether to use stretch energy.

`Torsion`

Type Bool

Default value Yes

Description Whether to use torsion energy.

`EwaldSummation`

Type Block

Description Configures the details of the particle mesh Ewald (PME) summation of the Coulomb interaction.

`Alpha`

Type Float

Default value -1.0

Description This parameter shifts the workload from real space (smaller alpha) to reciprocal space (larger alpha). Using a larger [Alpha] without decreasing [GridSpacing] may increase the error in the reciprocal-space contribution. Set to zero to disable the reciprocal-space Ewald part. Negative value means the [Alpha] will be determined automatically from [Tolerance].

`Enabled`

Type Bool

Default value Yes

Description Set to false to use real-space pair summation instead of the Ewald, which is the default and the only option for molecules, 1D and 2D periodic systems.

`GridSpacing`

Type Float

Default value 0.5

Unit Angstrom

Description Grid spacing in the particle mesh Ewald method. Smaller grid spacing will make the reciprocal energy calculation more accurate but slower. Using a larger [Alpha] value may require a smaller GridSpacing to be accurate.

`RealSpaceCutoff`

Type Float

Default value 0.0

Unit Angstrom

Description Set the cutoff value for the real-space summation. Zero means the internal defaults will be used depending on the [Alpha] (if Alpha=0 then the cutoff will be set to 50 Bohr, otherwise to 20 Bohr).

`Tolerance`

Type Float

Default value 1e-10

Description Value of the error function that should be used to determine the cutoff radius for real-space Ewald summation. Larger values will make the real-space summation faster but less accurate.

`ForceFieldFile`

Type String

Default value

GUI name Force field library

Description Path to the force field parameter file

`ForceFieldPatchFile`

Type String

Default value

GUI name Force field patch file

Description Path to the force field patch parameter file (additional parameters, missing from main file). Cannot be used when atomtypes are guessed.

`GuessCharges`

Type Bool

Default value No

Description Use another engine to calculate/guess the charges to be used by the force field.

`GuessChargesConfig`

Type Block

Description Guess charges to be used by the forcefield

EngineType

Type String

Default value dftb

Description Engine that can calculate or guess charges

LinearizationEnergyForRepulsion

Type Float

Default value 3.0

Unit Hartree

Description The Lennard Jones potential becomes extremely repulsive at short distances. The distance is determined where the potential reaches this threshold, for smaller distances a linear expression is used, reducing the repulsion.

LoadCharges

Type Block

Description Load charges from a file to be used as forcefield charges

File

Type String

Description Name of the (kf) file

Section

Type String

Default value AMSResults

Description Section name of the kf file

Variable

Type String

Default value Charges

Description variable name of the kf file

NonBondedCutoff

Type Float

Default value 15.0

Unit Angstrom

Description Distance beyond which the non-bonded pair interactions (Coulomb and Van der Waals) will be ignored. The interactions are smoothly damped starting from 0.9*NonBondedCutoff. Has no effect on the Coulomb term for periodic systems, as Ewald summation is used.

Type

Type Multiple Choice

Default value UFF

Options [UFF, Amber95, GAFF, Tripos5.2, UserDefined]

Description Type of force field to be used

`UFF`

Type Block

Description Option for the UFF force filed.

`AtomTypesFile`

Type String

Default value mmatomtypes_db

Description Expert option: Select the file that defines how UFF determines the atom types

`Database`

Type String

Default value general_db

Description Expert option: Select the file that defines the UFF parameters per atom type

`ElementsFile`

Type String

Default value elements_db

Description Expert option: Select the file that defines the elements known to UFF

`Library`

Type Multiple Choice

Default value UFF

Options [UFF, UFF4MOF, UFF4MOF-II]

GUI name Force field library

Description Selects the used parameter library.

`Verbosity`

Type Multiple Choice

Default value Silent

Options [Silent, Normal, Verbose, VeryVerbose]

Description Controls the verbosity of the engine.

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