ForceField Manual

Amsterdam Modeling Suite 2026.1

www.scm.com

Apr 02, 2026

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 61)]. By default UFF uses non-zero charges for water molecules only.

Other available force fields managed by this engine include Amber95, Tripos 5.2, GAFF and APPLE&P [*9* (page 61)].

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 2024

- *APPLE&P* (page 26) parameters updated to v 1.13. See also the APPLE&P tutorial on ionic liquids.

1.4 What's new in ForceField 2023

- New *APPLE&P* (page 26) polarizable force field [*9* (page 61)] parameters. See also the APPLE&P tutorial on ionic liquids.

1.5 What's new in ForceField 2022

- New *APPLE&P* (page 26) polarizable force field [9 (page 61)], designed for polymers, electrolytes, ionic liquids and energetic materials. See also the APPLE&P tutorial on ionic liquids.
- The GFN-FF force field by Spicher and Grimme. **Note:** GFNFF is technically not part of the ForceField engine. To use GFNFF, you should use the **GFNFF engine** (and not the ForceField engine). See the GFNFF engine manual for more info.

1.6 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.

1.7 What's new in ForceField 2020

1.7.1 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
```

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```
   EndEngine
eor
```

1.8 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.

1.9 Classical force fields

Most force fields require atom typing, as well as atomic charge specifications, see *Examples* (page 63).

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 available 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).

It may be desirable to reuse the atom types and charges from a previous UFF calculation on the same system. This can be done in two ways.

1. By referring to an RKF file
2. By explicitly adding the atom typing information to the input file

For the first option, use the keyword `ReuseTypeInfo` referencing the engine RKF file from the previous UFF calculation (usually named forcefield.rkf).

```
ReuseTypeInfo string
```

ReuseTypeInfo

Type
String

Default value

Description
Path to RKF file with atom typing information (atom types, charges, and - in case of GAFF or APPLE&P - possibly a forcefield (patch) file for the system).

To add the information explicitly to the inputfile one can copy the atomtyping information from the output file. For the addition of atom types and charges to input, see *Adding atom types and charges* (page 11).

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. Note that if some charges are pre-defined by the user, no auto-detection of the water molecules is performed.

2.2 GAFF

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 13)

Using the GAFF forcefield with automatic atomtyping can be done with the `AntechamberIntegration` keyword.

```
GAFF
   AtomTyping
      AntechamberIntegration Yes/No
      AntechamberTask [GeometryOptimization | SinglePoint]
      KeepAntechamberFolder Yes/No
      MolecularCharge
         Charge float
         Region string
      End
   End
End
```

`GAFF`

Type
Block

Description
Specific keywords for the GAFF force field type

`AtomTyping`

Type
Block

Description
Specific keywords for automatic atom typing for the GAFF force field type

`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 invoked to guess atomtypes and charges (GAFF force field), select the task for charge guessing with MOPAC

`KeepAntechamberFolder`

Type
Bool

Default value
No

Description
If atom-typing is performed with antechamber, keep the folder after the call to antechamber

`MolecularCharge`

Type
Block

Recurring
True

Description
Defines a (set of) submolecule(s) with their charge, to be Used in GAFF atomtyping.

`Charge`

Type
Float

Description
Molecular charge of submolecule(s) defined in Region.

`Region`

Type
String

Description
Region name that defines a (set of) submolecule(s).

2.2.1 Molecular charges

When a molecular system consists of multiple molecules, the charges of those molecules default to zero. The user can supply molecular charges by defining regions (see The System block). The regions can then be linked to molecular charges with the keywords `GAFF%AtomTyping%MolecularCharge%Region` and `GAFF%AtomTyping%MolecularCharge%Charge`. Multiple instances of this keyword are allowed. If all the atoms in a single molecule/ion are included in the region, then the charge is applied to it. If the region covers multiple molecules/ions, then all the ions in that region will be assigned the supplied molecular charge.

2.2.2 Reusing type info

For complex molecules atomtyping can take some time. Therefore, it may be desirable to reuse the atom types and charges from a previous GAFF calculation on the same system. This can be done in two ways.

1. By referring to an RKF file
2. By explicitly adding the atom typing information to the input file

For the first option, use the keyword `ReuseTypeInfo` referencing the engine RKF file from the previous GAFF calculation (usually named forcefield.rkf).

```
ReuseTypeInfo string
```

ReuseTypeInfo

Type
String

Default value

Description
Path to RKF file with atom typing information (atom types, charges, and - in case of GAFF or APPLE&P - possibly a forcefield (patch) file for the system).

Adding the atomtyping information for reuse explicitly to the inputfile requires more knowledge of the produced data. Using automatic atomtyping for GAFF produces atom types and charges, and often a parameter patch as well. This is a piece of text that contains additional parameters to the standard GAFF set. All the atomtyping information can be found in the output file. One can then add the types, charges, and parameter patch(es) directly into the GAFF input file. For the addition of atom types and charges to input, see *Adding atom types and charges* (page 11). For the parameter patch, use the keyword `GAFF%ForceFieldParameters`, and insert the patch text directly into the input. The force field patch information can also be passed as a reference to a text file or to the forcefield.rkf file from a previous GAFF calculation, using the keyword *GAFF%ForceFieldPatchFile*.

```
GAFF
   ForceFieldParameters
End
```

GAFF

Type
Block

Description
Specific keywords for the GAFF force field type

ForceFieldParameters

Type
Block

Recurring
True

GUI name

Description
Parameter file text in AMBER format with (additional parameters, missing from main file). Alternative option to ForceFieldPatchFile. The parameter patches provided by antechamber can be used here. Cannot be used when atomtypes are guessed.

```
GAFF
   ForceFieldPatchFile string
End
```

`GAFF`

Type
Block

Description
Specific keywords for the GAFF force field type

`ForceFieldPatchFile`

Type
String

Recurring
True

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.

2.3 APPLE&P

Apple&P atomtyping has to be done prior to an AMS calculation using a separate tool. This tool can be accessed via our graphical user interface (APPLE&P tutorial) or using our general atom typing tool (../AMS/Utilities/AtomTyping.html).

The procedure generates atom types and charges, as well as parameters. After atom typing is complete, an input can be written with the types and charges in the *System* block (*Adding atom types and charges* (page 11)) and the produced parameter file added with the *ForceFielFile* keyword. When the atom typing tool was used, the produced data can also be used in an APPLE&P calculation with the keyword `ReuseTypeInfo`, and a reference to the file *atomtyping.rkf*.

```
ReuseTypeInfo string
```

`ReuseTypeInfo`

Type
String

Default value

Description
Path to RKF file with atom typing information (atom types, charges, and - in case of GAFF or APPLE&P - possibly a forcefield (patch) file for the system).

2.4 Other forcefields

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 13) below. See also the *BondsUsage* (page 19) 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 (https://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:

```
GAFF
   AtomTyping
      AntechamberIntegration Yes/No
      AntechamberTask [GeometryOptimization | SinglePoint]
      KeepAntechamberFolder Yes/No
      MolecularCharge
         Charge float
         Region string
      End
   End
End
```

`GAFF`

Type
Block

Description
Specific keywords for the GAFF force field type

`AtomTyping`

Type
Block

Description
Specific keywords for automatic atom typing for the GAFF force field type

`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 invoked to guess atomtypes and charges (GAFF force field), select the task for charge guessing with MOPAC

`KeepAntechamberFolder`

Type
Bool

Default value
No

Description
If atom-typing is performed with antechamber, keep the folder after the call to antechamber

`MolecularCharge`

Type
Block

Recurring
True

Description
Defines a (set of) submolecule(s) with their charge, to be Used in GAFF atomtyping.

`Charge`

Type
Float

Description
Molecular charge of submolecule(s) defined in Region.

`Region`

Type
String

Description
Region name that defines a (set of) submolecule(s).

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 | APPLE&P | UserDefined]
```

`Type`

Type
Multiple Choice

Default value
UFF

Options
[UFF, Amber95, GAFF, Tripos5.2, APPLE&P, 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 the interaction more aggressively.

```
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 3D-periodic systems, as Ewald summation is used.

It is usually a good idea to add some "skin" to the cutoff above when it's used for computing a neighbor list for changing geometries (e.g. during molecular dynamics or geometry optimization). This way, the neighbor list will not need to be re-computed when atoms move a little. This may save some time because generating a neighbor list can be quite costly. The following option sets the thickness of the "skin":

```
NeighborListSkin float
```

`NeighborListSkin`

Type
Float

Default value
2.5

Unit
Angstrom

Description
Thickness of the buffer region added to the NonBondedCutoff when building a neighbor list.

Note: This option also affects the cutoff used when generating a neighbor list in the real-space part of the Ewald summation but then it is added to the cutoff radius is used there.

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

Unit
1/Angstrom

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 the [Tolerance] and [RealSpaceCutoff] values.

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 if [Alpha] is set on input. Alternatively, if the [RealSpaceCutoff] is set but [Alpha] is not then the [Tolerance] value affects the [Alpha]. 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 in the input to make the results more realistic.

See also example *ChargedMolecules* (page 64).

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 Amber force field options

These options are relevant for the Amber and GAFF 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.

4.4 APPLE&P force field options

The *ForceFieldFile* (page 24) key is mandatory and it should contain path to the APPLE&P forcefield file. This file is usually tailored for each system specifically.

Additionally, the following options are relevant for the APPLE&P force field.

```
DipoleConvergenceThreshold float
```

`DipoleConvergenceThreshold`

Type
Float

Default value
1e-06

Unit
eBohr

Description
Convergence criterion for induced point dipoles, in atomic units. When the length of every atomic delta_mu vector between two iterations becomes below the tolerance, the procedure is considered converged.

The repulsion/dispersion and Coulomb interaction between atoms connected by a bond or by a valence angle are excluded in APPLE&P. Those between atoms connected by a dihedral (the so called 1-4 neighbors) may be scaled down and the scaling factors can be changed using the following options:

```
APPLE&P
   ForceFieldParameters
   LongRangeCorrection Yes/No
   MuMu14Scaling float
   QMu14Scaling float
   QQ14Scaling float
   RD14Scaling float
End
```

`APPLE&P`

Type
Block

Description
Options for the APPLE&P force field.

`ForceFieldParameters`

Type
Block

Recurring
True

GUI name

Description
Forcefield parameter text block, provided as alternative to the general ForceFieldFile keyword. Will be ignored if ForceFieldFile keyword is also present.

`LongRangeCorrection`

Type
Bool

Default value
Yes

GUI name
Add long-range correction

Description
Add a long-range dispersion correction to the energy and pressure for 3D-periodic systems.

This correction should be enabled only for a homogeneous liquid.

`MuMu14Scaling`

Type
Float

Default value
1.0

GUI name
Mu-Mu 3rd-neighbor scaling

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

`QMu14Scaling`

Type
Float

Default value
0.2

GUI name
Q-Mu 3rd-neighbor scaling

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

`QQ14Scaling`

Type
Float

Default value
1.0

GUI name
Q-Q 3rd-neighbor scaling

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

`RD14Scaling`

Type
Float

Default value
1.0

GUI name
RD 3rd-neighbor scaling

Description
Scaling factor for repulsion/dispersion interactions between atoms connected to 3rd order (via a dihedral).

4.5 Offloading calculations to LAMMPS

The ForceField engine can optionally offload the evaluation of energies and forces to LAMMPS (https://lammps.org/) to accelerate the calculation, possibly leveraging a GPU. In this mode, the engine will still set up all force field parameters as usual, but instead of evaluating the potential directly in AMS, the engine converts the parameters into a a LAMMPS data file and then invokes LAMMPS as an external pipe worker. As of AMS2025, this option is fully supported only for `Type UFF`.

4.5.1 Setting up LAMMPS

The interface between AMS and LAMMPS relies on a modified LAMMPS version that integrates the amspipe library (https://github.com/SCM-NV/amspipe) for communication via the AMSPipe protocol. We intend to make our modification available in upstream LAMMPS (https://github.com/lammps/lammps), but for now the modified version can be obtained from SCM's GitHub page:

https://github.com/SCM-NV/lammps/tree/amspipe

We currently do not distribute binaries for the modified LAMMPS version, but it should be quite easy to build from source. Consult the LAMMPS documentation for a detailed description on building LAMMPS (https://docs.lammps.org/Build.html). For example, the following commands can be used to build LAMMPS including the necessary packages:

```
#!/bin/sh

# 1. build the amspipe library
git clone https://github.com/SCM-NV/amspipe.git
mkdir amspipe/build
cd amspipe/build
cmake -DCMAKE_BUILD_TYPE=Release -DBUILD_SHARED_LIBS=ON -DAMSPIPE_BUILD_DEMOS=OFF ..
cmake --build .
cmake --install . --prefix=../install
cd ../..

# 2. build modified LAMMPS
git clone https://github.com/SCM-NV/lammps.git -b amspipe
mkdir lammps/build
```

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```
cd lammps/build
cmake ../cmake -DPKG_AMSPIPE=yes -Damspipe_ROOT=../../amspipe/install -DBUILD_MPI=no -
↪DBUILD_OMP=yes -DPKG_OPENMP=yes -DPKG_GPU=yes -DPKG_MOLECULE=yes -DPKG_EXTRA-
↪MOLECULE=yes -DPKG_KSPACE=yes
cmake --build .
```

- `-DBUILD_MPI=no -DBUILD_OMP=yes -DPKG_OPENMP=yes` are strongly recommended to enable OpenMP parallelization of the CPU code of LAMMPS. AMS currently cannot use the MPI framework to parallelize LAMMPS and linking to a MPI-enabled library can cause issues.
- `-DPKG_GPU=yes` builds LAMMPS with GPU support. By default this builds the OpenCL version of the GPU package, which runs on both AMD and Nvidia cards. If you are targeting Nvidia cards only, we may consider switching to the Cuda version by adding `-DGPU_API=cuda` (and optionally specifying also `-DGPU_ARCH=sm_XX`). See the instructions for building the LAMMPS GPU package (https://docs.lammps.org/Build_extras.html#gpu-package).
- `-DPKG_MOLECULE=yes -DPKG_EXTRA-MOLECULE=yes -DPKG_KSPACE=yes` enable the potential terms required by UFF.

By default the ForceField engine will look for the modified LAMMPS binary simply as `lmp` on `$PATH`. It is therefore easiest just to extend `$PATH` with the `lammps/build` directory we made above:

```
export PATH="/path/to/modified/lammps/build:$PATH"
```

You may want to put this line into your `$HOME/.profile` file to make this permanent. You can use the `which` command to check that the correct `lmp` binary is picked up:

```
$ which lmp
/path/to/modified/lammps/build/lmp
```

An alternative is to specify the path to the modified `lmp` binary in the input of your job.

```
Engine ForceField
   LAMMPSOffload
      WorkerCommand exec /path/to/modified/lammps/build/lmp
   End
End
```

Note: Prior to AMS2025, the LAMMPS interface in AMS was based on the lammps Python module (https://docs.lammps.org/Python_module.html). This proved to be a performance bottleneck and is no longer supported in AMS2025 in favor of the direct communication with the modified `lmp` binary.

4.5.2 Input options

```
LAMMPSOffload
   Enabled Yes/No
   Input
   UseGPU Yes/No
   UseGPUForKSpace Yes/No
   UseGPUForNeighbor Yes/No
   UseOpenMP Yes/No
   WorkerCommand string
End
```

`LAMMPSOffload`

Type
Block

Description
Offload the calculation to LAMMPS via AMSPipe.

`Enabled`

Type
Bool

Default value
No

Description
Enable offloading the force field evaluation to LAMMPS instead of handling it internally in AMS. This is currently only supported for Type=UFF.

`Input`

Type
Block

Description
Commands to be passed to LAMMPS to set up the calculation. If this is left empty, AMS will generate a set of commands to set LAMMPS up according to the settings of the ForceField engine. Any LAMMPS commands entered in this input block will be used to set LAMMPS up instead of those generated by AMS. To merge the AMS-generated lines with your customizations, include lines like 'AMS somelammpskeyword' anywhere in this block. Any such line will be replaced by the AMS-generated line for 'somelammpskeyword'. Any text after 'somelammpskeyword' will be appended to the generated line verbatim, which can be used to modify the generated command by additional options. A special line 'AMS everything' will be replaced by the entire block of AMS-generated commands, except those overridden anywhere in this input block (defined manually or inserted using 'AMS somelammpskeyword'. Any customized Input block should probably include 'AMS read_data' near or at the end to load the AMS-generated data file defining the system.

`UseGPU`

Type
Bool

Default value
No

Description
Accelerate LAMMPS calculations using a GPU. Requires a LAMMPS library built with the GPU package.

`UseGPUForKSpace`

Type
Bool

Default value
Yes

Description
When UseGPU is enabled, also use the GPU to accelerate reciprocal space electrostatic interactions. Disabling this can improve performance on less powerful GPUs.

`UseGPUForNeighbor`

Type
Bool

Default value
Yes

Description
When UseGPU is enabled, also use the GPU to accelerate neighbor searches. Disabling this can improve performance on less powerful GPUs.

`UseOpenMP`

Type
Bool

Default value
No

Description
Parallelize LAMMPS calculations using OpenMP threading. Requires a LAMMPS library built with the OMP package.

`WorkerCommand`

Type
String

Default value
exec lmp

Description
The command to execute to run the external worker. The command is executed in a subdirectory of the results directory. The LAMMPS input commands will be passed to the worker on standard input.

CHAPTER

FIVE

APPLE&P

APPLE&P is a polarizable forcefield suitable for many electrolytes and polymers.

To use the APPLE&P force field, you need a special license for APPLE&P that you can obtain from SCM.

5.1 APPLE&P use cases

APPLE&P has been specifically parametrized to the below list of molecules. For molecules not on the list, the force field may or may not be reasonable, and it is advised that you do your own testing.

5.1.1 Organic Molecules

- alcohols
- aldehydes
- alkanes, alkenes, alkynes
- amides
- esters
- ethers
- imides
- ketones
- partially fluorinated alkanes
- perfluoroalkanes

5.1.2 Energetic Materials

- FOX-7
- HMX
- hydrazines
- hydroxylammonium nitrate (HAN)
- hydroxylethyl hydrazinium nitrate (HEHN)
- PETN

- RDX
- TATB
- TNT

5.1.3 Polymers

Note: The automatic atom typing may be very slow for large polymers containing the following functional groups: nitro, isocyanate groups, phenyl rings and conjugated rings with carbon and nitrogen (i.e. imidazole), amide, imide and azide groups, as well as phosphorous groups with multiple oxygen atoms (phosphorous oxoacids and derivatives).

- polyimides
- polyamides
- polyesters
- polyethers (e.g., PEO)
- PIB
- PDMS
- PTFE
- polybutadiene
- polyalkanes

5.1.4 Solvents/Additives

- acetone
- alcohols
- cyclic carbonates (e.g., ethylene carbonate)
- ethers (e.g., dimethoxyethane)
- linear carbonates (e.g., dimethyl carbonate)
- nitriles (e.g., acetonitrile, succinonitrile, adiponitrile)
- partially fluorinated carbonates (e.g., FEC)
- partially fluorinated ethers
- perfluoroethers
- sulfones (cyclic and acyclic)
- water

5.1.5 SEI compounds

- dilithium dicarbonates
- lithium carbonates
- LiF
- Li_2CO_3

5.1.6 Cations

- ammoniums
- H_3O^+, hydronium
- hydraziniums
- imidazoliums
- K^+, potassium
- Li^+, lithium
- Mg^{2+}, magnesium
- morpholiniums
- Na^+, sodium
- piperidiniums
- pyrrolidiniums
- Zn^{2+}, zinc

5.1.7 Anions

- $B(CN)_4^-$, tetracyanoborate
- BF_4^-, tetrafluoroborate
- $BF_3CF_3^-$, $CF_3BF_3^-$, trifluoro(trifluoromethyl)borate
- $BF_3CH_3^-$, $CH_3BF_3^-$, methyltrifluoroborate
- BOB, bis(oxalate)borate
- $C(CN)_3^-$, tricyanomethanide
- CN^-, cyanide
- CN_7^-, azidotetrazolate
- CO_3^{2-}, carbonate
- F^-, fluoride
- FSI, bis(fluorosulfonyl)imide
- N_3^-, azide
- $N(CN)_2^-$, dicyanamide
- NO_3^-, nitrate

- OH^-, hydroxide
- PF_6^-, hexafluorophosphate
- $SO_3CF_3^-$, triflate
- TFSI, bistriflimide

5.1.8 Electrodes

Note: The automatic atom typing may be extremely slow for graphite sheets consisting of more than 30-40 atoms.

- graphite
- iridium

5.2 APPLE&P potential shapes

In general, APPLE&P uses similar expressions for the potentials, with some differences. For completeness' sake we list all APPLE&P potentials below.

See also:

Potential shapes (page 55) force other force fields.

- Bond: the same as the stretch potential above.

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

- Bend: the same as the harmonic angle potential above.

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

- Torsion: cyclic.

$$V^{\text{torsion}} = -\sum_{m=1}^{n} c_m \cos(m\phi)$$

- Out-of-plane angle: sum of three harmonic terms, each corresponding to an angle between the R_{ij} bond and the (jkl) plane, where j is the central atom and i, k, l are permutations of the other three atoms.

$$V^{\text{oop}} = \frac{1}{2} f_c (\phi_1^2 + \phi_2^2 + \phi_3^2)$$

- Dispersion: mix of the Buckingham and Lennard-Jones potentials.

$$V^{\text{dispersion}} = Ae^{-Br} - \frac{C}{r^6} + \frac{D}{r^{12}}$$

- Electrostatic potential: charge-charge, charge-dipole and dipole-dipole. Interaction are excluded for the 1-2 and 1-3 neighbors and can be scaled for the 1-4 ones. For each atom, the self-consistent induced dipole moment is computed from its polarizability and the electric field due to other charges and dipoles. The latter includes the Thole damping.

$$V^{\text{elstat}} = \sum_{i>j} \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} + \sum_i \vec{\mu_i} \cdot \vec{E_i}$$

5.3 APPLE&P Python functions

The `scm.appleandp` Python module contains the below functions.

For example usage, see the APPLE&P tutorial

`appleandp_packmol`(*molecules*, *forcefield_file*, ***kwargs*)

molecules: list of Molecule
If they are ions they should have the molecule.properties.charge set to the charge

forcefield_file: str
The force field file will be written here. It will be overwritten if it already exists

`**kwargs`: various options
See the documentation for the `packmol()` function

Returns: a PLAMS Molecule created with packmol

This function differs from the PLAMS implementation of packmol in that it also writes out a force field file for use with APPLE&P.

CHAPTER

SIX

PARAMETER FILES

The parameters of a forcefield are defined via one or more files, automatically set when using a standard *type* (page 17) . 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.

6.1 UFF parameters

The parameter set used by UFF can be changed via the *UFF* (page 25) 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 61)] 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 61)] for details on the parameters.

6.1.1 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.

6.2 AMBER parameters

If you want to use a non-standard forcefield you can specify the *ForceFieldFile* (page 24).

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.

6.2.1 AMBER forcefield file

The format of the AMBER ".dat" files is described here https://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

6.2.2 SCM forcefield file

An example of this is `$AMSHOME/atomicdata/ForceFields/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
========================
```

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```
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
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
```

(continues on next page)

(continued from previous page)

```
=========================
*   *   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
=========================

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

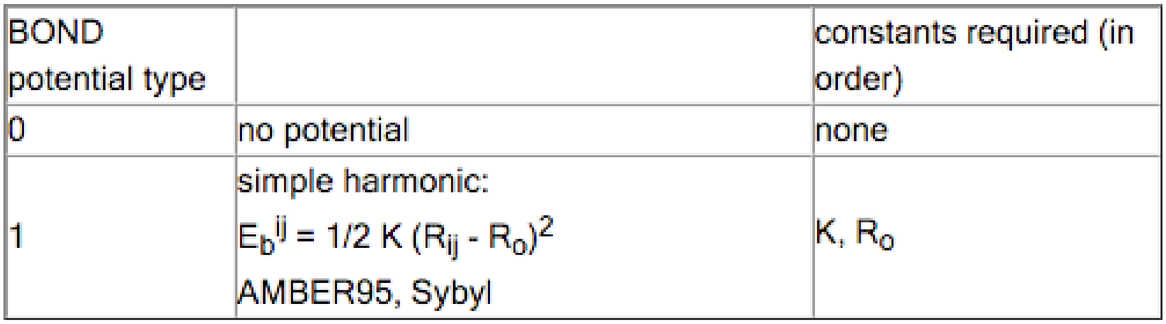
This option is ignored.

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
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.



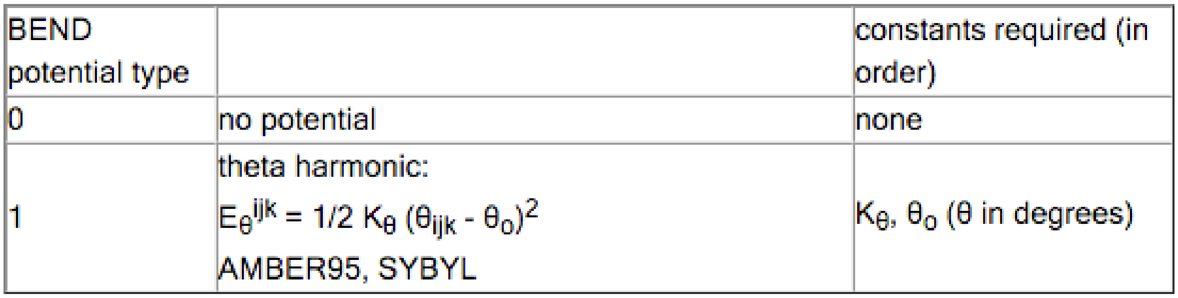
BOND potential type		constants required (in order)
0	no potential	none
1	simple harmonic: $E_b^{ij} = 1/2\ K\ (R_{ij} - R_o)^2$ AMBER95, Sybyl	K, R_o

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.

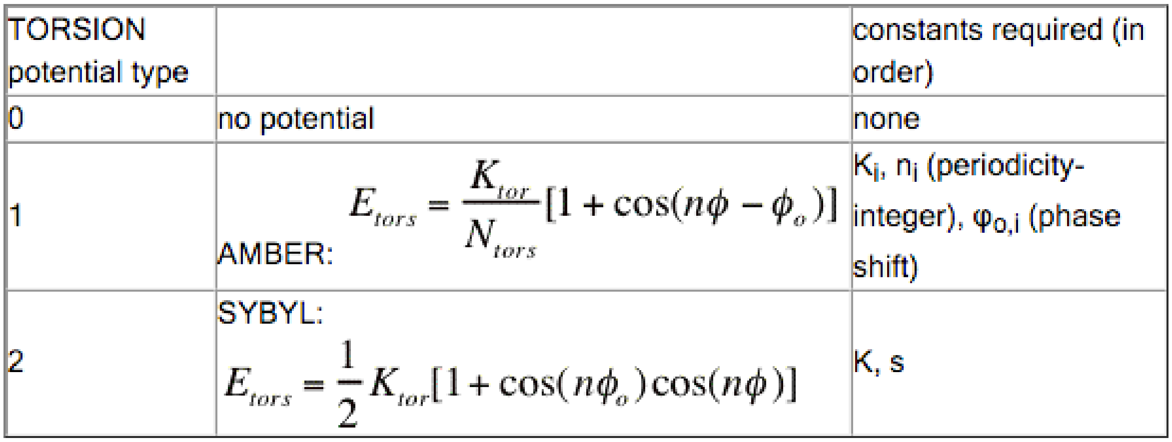


BEND potential type		constants required (in order)
0	no potential	none
1	theta harmonic: $E_\theta^{ijk} = 1/2\ K_\theta\ (\theta_{ijk} - \theta_o)^2$ AMBER95, SYBYL	K_θ, θ_o (θ in degrees)

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), $\varphi_{0,i}$ (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
```

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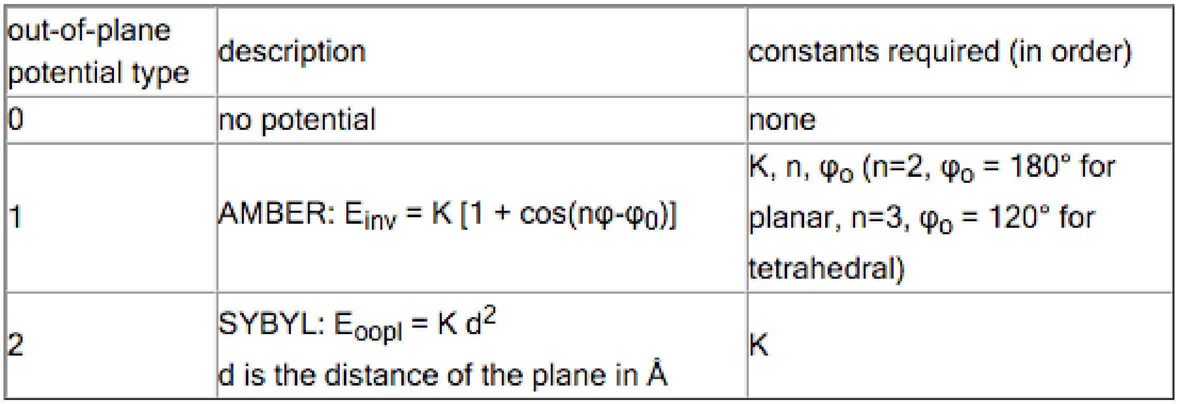
```
i - j - k - l           type  k        per      NOTES
===============================================
*     C_ar  S_3   *     2     1.0000    3.0     *
*     S_3   S_3   *     2     0.0000    2.0     EXP
C_2   C_2   C_3   *     2     0.1260   -3.0     WHITE_77
C_3   C_2   C_3   *     2     0.1260    3.0     WHITE_77
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_o (n=2, φ_o = 180° for planar, n=3, φ_o = 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
```

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```
*     *     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:

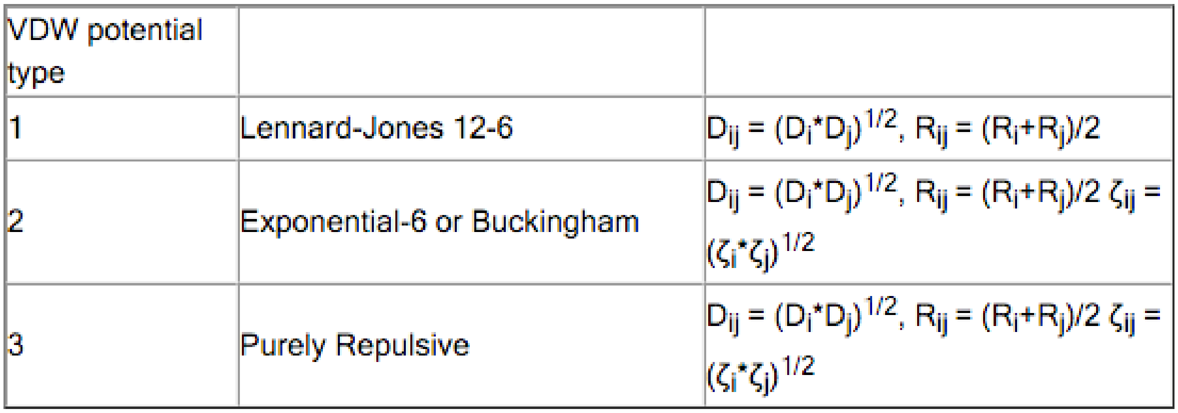
```
atom(s) type  emin   rmin     alpha     NOTES
====================================
CA           -.0860  3.81600  12.00     amber95
HA           -.0150  2.91800  12.00     amber95
Ni - HA  2  -.0480  2.7      12.00     NOTE potential type
Ni - CA  D  -.0480  2.7      12.00     default potential
====================================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

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

6.3 APPLE&P parameters

APPLE&P parameters are generated for a given system and written to a jobname.ff file by AMSinput. The format of this file is similar to that used by the WMI-MD program and consists of seven sections, in this order: repulsion/dispersion (RD) types, non-default RD cross terms, bonds, valence angles (bends), torsions, impropers, and lone pairs (LPs). A line beginning with an asterisk character is a comment and is ignored. Unless otherwise specified all parameters are in the units of electron, kcal/mol, Angstrom, radian and combinations thereof. An RD type name is case-sensitive and it is checked against the atom type specified by the atom's `Forcefield.Type` suffix in the System%Atoms block.

Example force-field file for water:

```
* Repulsion/dispersion types
3
 Hw          0.00    0.0000      0.00   0.5537  0.0000
 Ow     880783.40    0.0000    851.26   0.0000  1.0425
 Lp          0.00    0.0000      0.00  -1.1074  0.0000
* Non-default cross terms
```

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```
 Hw  Ow       0.00    0.0000      0.00
 Hw  Lp       0.00    0.0000      0.00
 Ow  Lp       0.00    0.0000      0.00
!
* Bond potentials
3
 999.00    0.9572    0.9572   T   Ow    Hw
 999.00    1.5140    1.5140   T   Hw    Hw
   0.00    0.2381    0.2381   T   Ow    Lp
* Bend potentials
1
 100.00     104.52    F   Hw   Ow   Hw
* Dihedral potentials (do not make sense for water; provided for illustration)
1
 3  0.00 0.00 20.00 0.00 0.00 0.00   Hw   Ow   Ow   Hw
* Improper/out-of-plane potentials (do not make sense for water; provided for␣
↪illustration)
1
 20.00   Hw   Ow   Hw   Hw
* Lone pair definitions
1
* RD     A       B       C     type   I    J    K
  3     0.5   -0.2381  0.00     1     1    2    1
```

Section Description

`Repulsion/dispersion types`

The block begins with the number of RD types followed by the specified number of lines, one per RD type. Each line begins with the RD type name followed by three dispersion parameters (A’, B’, and C’), atomic charge and polarizability. The (A’, B’, C’) triplet translates to the (A, B, C, D) quartet of the dispersion part of *APPLE&P potentials* (page 33) as follows:

- if B’ is zero then the dispersion potential is converted to pure Lennard-Jones with C = C’ and D = A’.
- if the B’ parameter non-zero then the A’, B’, and C’ parameters translate directly to A, B, and C, while D is set to $0.00005*(12/B')^{12}$.

The atomic charge specified does not include that of the LPs belonging to the atom. In the water example above, the oxygen atom’s charge is carried by its lone pair Lp, so the atomic value is set to zero while the Lp’s value is set to -1.1074 to compensate that of the two hydrogen atoms.

`Non-default RD cross terms`

By default, the cross-term RD parameters are computed from the values in the previous section. For the pure Lennard-Jones (B’ = 0), they are computed as a geometric mean of the corresponding per-type values. For the mixed Buckingham-LJ potential, the expressions are more complicated[1]. Since the A’ parameter has different units in these two cases, then by default there is no dispersion interaction between them. In this case, one should specify the corresponding values in this block. Each line begins with the names of the RD types followed by a (A’, B’, C’) triplet, similar to the previous block. The block ends with line containing a single exclamation mark.

`Bond potentials`

The block begins with the number of bond types followed by the specified number of lines, one per bond type. The parameters are: the force constant, equilibrium distance, constrained distance, constraint flag (T or F), followed by the two RD type names defining the bond. The constrained distance and the constraint flag are currently not used by AMS.

---

[1] O. Borodin, *Polarizable Force Field Development and Molecular Dynamics Simulations of Ionic Liquids*, J. Phys. Chem. B 113, 11463–11478 (2009) (https://doi.org/10.1021/jp905220k)

`Bend potentials`

The block begins with the number of bend types followed by the specified number of lines, one per bend type. The parameters are: the force constant, equilibrium angle in degrees, constraint flag (T or F), followed by the three RD type names defining the angle. The constraint flag is currently not used.

`Dihedral potentials`

The block begins with the number of dihedral types followed by the specified number of lines, one per dihedral type. The parameters are: the number of terms N in the cyclic sum, up to twelve force constant (only the first N will be used), followed by the four RD type names defining the dihedral angle.

`Improper/out-of-plane potentials`

The block begins with the number of improper types followed by the specified number of lines, one per improper type. Each line contains a single parameter, the force constant, followed by the four RD types defining the OOP angle. The second RD type name corresponds to the central atom.

`Lone pair definitions`

The block begins with the number of LP types followed by the specified number of lines, one per LP type. The parameters are: index of RD type corresponding to the LP in the first section, three real parameters (A, B, C), LP type, indices (I, J, K) of the RD types of the atoms used to determine coordinates of the LP(s). The number and the position of the LPs is determined by the its type while the charge and the dispersion parameters are defined by its RD type. A lone pair is a dummy atom that exist only when computing non-bonded (electrostatic and dispersion) interactions and it does not contribute to the bonded interactions in any way. It does not need to (and cannot) be specified in the Atoms block. For each valence angle (ijk) of the RD type I, J, and K, respectively, one or two LPs are created, depending on the type. The position of the LP is fixed with respect to the atoms, thus any force acting on the LP is effectively projected on those atoms.

Currently, there are two LP types defined in AMS: type 1 and type 2. Type 1 is a single LP attached to atom j, lying in the (ijk) plane at the distance abs(B) on the line connecting atom j with the point X on the (ik) line. The parameters A defines the ratio between distances R(iX) and R(ik). Thus, if A=0.5 (a typical value) the type 1 lone pair lies on the median line of the ijk triangle. If B is less than zero then the LP is inside the triangle, otherwise it's outside. For type 2, two LPs are added for each angle: one above the (ijk) plane and one below it. The parameter C defines the distance from the LP to the plane and B defines the distance between atom j and the projection of the LPs onto the (ijk) plane.

CHAPTER SEVEN

POTENTIAL SHAPES

Setting the *Verbosity* (page 18) 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.

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

- 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.

See also: *APPLE&P* (page 33)

CHAPTER
EIGHT

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

NINE

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)

For calculations with the APPLE&P forcefield:

O. Borodin, *Polarizable Force Field Development and Molecular Dynamics Simulations of Ionic Liquids*, J. Phys. Chem. B 113, 11463–11478 (2009) (https://doi.org/10.1021/jp905220k)

9.1 External programs and libraries

Third party software used in the 2026.1 version of the Amsterdam Modeling Suite can be found in the file titled “third-party-software.txt” in the root of your AMS installation.

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)

For calculations with the APPLE&P forcefield:

9. O. Borodin, *Polarizable Force Field Development and Molecular Dynamics Simulations of Ionic Liquids*, J. Phys. Chem. B 113, 11463–11478 (2009) (https://doi.org/10.1021/jp905220k)

CHAPTER

ELEVEN

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.

11.1 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
```

11.2 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 input, 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=0.3120167009638037950E+000
              H 0.497012567535054 0.9247340386709353       -0.7538297483507286  ␣
↪ForceField.Charge=0.1124207547998490870E+000
              H -1.049427360359161 0.0320094307806696      -0.7537906795101232  ␣
↪ForceField.Charge=0.1124258597868739580E+000
              H 1.760678843023289 -1.264262738726653       -0.6572703272452628  ␣
↪ForceField.Charge=0.1124159976242316420E+000
              H 0.2140471968077103 -2.156981931600252      -0.6574882069415752  ␣
↪ForceField.Charge=0.1124199701089378810E+000
              H 1.207324110469442 -0.4308282262683778       -2.854859298860555  ␣
↪ForceField.Charge=0.3120438817503916610E+000
              H -0.2304034502578771 -1.260970512043685      -2.855040966499596  ␣
↪ForceField.Charge=0.3120482437032160990E+000
              H 1.200917269444972 -2.079821003490794        -2.803581935602674  ␣
↪ForceField.Charge=0.3270426757495007440E+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=-0.5710112782050444920E+000
               C -0.003379615065181385 0.005774705419397744 -0.4323726711546611  ␣
↪ForceField.Charge=-0.6282036467199447750E-001
               C 0.7147029862216027 -1.238161594687982      -0.9787933548287219  ␣
↪ForceField.Charge=-0.6288377461831462510E-001
               N 0.7166487936613554 -1.241183181538415       -2.471469363728673  ␣
↪ForceField.Charge=-0.5711255685003771010E+000
               H -0.489254727061788 0.8470579056083724        1.393322418122902  ␣
↪ForceField.Charge=0.1943662472837144330E+000
```

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```
               H 0.9419603270459358 0.02859511576851682       1.443864570589139 ForceField.Charge=0.1944160304581348533E+000
               H -0.4954439060007188 -0.801643243084588       1.443905390218997 ForceField.Charge=0.1944152959160332237E+000
               H 0.497012567535054 0.9247340386709353       -0.7538297483507286 ForceField.Charge=0.2532231311300850044E-001
               H -1.049427360359161 0.0320094307806696      -0.7537906795101232 ForceField.Charge=0.2538013067297969901E-001
               H 1.760678843023289 -1.264262738726653       -0.6572703272452628 ForceField.Charge=0.2535956537939946673E-001
               H 0.2140471968077103 -2.156981931600252      -0.6574882069415752 ForceField.Charge=0.2540605535185176668E-001
               H 1.207324110469442 -0.4308282262683778       -2.854859298860555 ForceField.Charge=0.1943710326917253371E+000
               H -0.2304034502578771 -1.260970512043685      -2.855040966499596 ForceField.Charge=0.1943682070228703332E+000
               H 1.200917269444972 -2.079821003490794        -2.803581935602674 ForceField.Charge=0.1944361081060127751E+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       -2.85485929886055
               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       -2.47146936372867 3  ␣
↪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       -2.85485929886055  ␣
↪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


# this calculation should succeed, ignoring the default zero total charge and using␣
↪the atomic charges instead

export AMS_JOBNAME=C2H10N2++.warning

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
               H 0.2140471968077103 -2.156981931600252      -0.6574882069415752  ␣
↪ForceField.Charge=0.112419970108937881E+000
               H 1.207324110469442 -0.4308282262683778       -2.854859298860555  ␣
```

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```
↪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


# this calculation should trigger a warning because the explicitly set Charge doesn't␣
↪match

export AMS_JOBNAME=C2H10N2++.warning

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 0.714702986216027 -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
               H 0.2140471968077103 -2.156981931600252      -0.6574882069415752  ␣
```

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```
↪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 1.0
End


Engine ForceField
EndEngine

eor

# finally let us make on purpose an error (total charge not set with strict checking␣
↪enabled)
# 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
```

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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
End


Engine ForceField
    DoChargeCheck True
EndEngine

eor
```

11.3 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
```

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```
  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
  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
```

11.4 Example: calculate some simple properties for water

Download `water_properties.run`

```
#! /bin/sh

$AMSBIN/ams << eor

Task GeometryOptimization

Properties
  BondOrders Yes
  Charges Yes
```

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```
  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"
```

11.5 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

```

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```
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

TWELVE

KEYWORDS

12.1 Links to manual entries

forcefield:

- *APPLE&P* (page 26)
- *AllowMissingParameters* (page 24)
- *BondsUsage* (page 19)
- *CheckDuplicateRules* (page 24)
- *DipoleConvergenceThreshold* (page 26)
- *EnergyTerms* (page 21)
- *EwaldSummation* (page 19)
- *ForceFieldFile* (page 24)
- *GAFF* (page 6)
- *GuessCharges* (page 22)
- *GuessChargesConfig* (page 22)
- *LAMMPSOffload* (page 29)
- *LoadCharges* (page 23)
- *NeighborListSkin* (page 18)
- *NonBondedCutoff* (page 17)
- *ReuseTypeInfo* (page 5)
- *Type* (page 17)
- *UFF* (page 25)
- *Verbosity* (page 18)

12.2 Summary of all keywords

12.2.1 Engine ForceField

`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.

`APPLE&P`

Type
Block

Description
Options for the APPLE&P force field.

`ForceFieldParameters`

Type
Block

Recurring
True

GUI name

Description
Forcefield parameter text block, provided as alternative to the general ForceFieldFile keyword. Will be ignored if ForceFieldFile keyword is also present.

`LongRangeCorrection`

Type
Bool

Default value
Yes

GUI name
Add long-range correction

Description
Add a long-range dispersion correction to the energy and pressure for 3D-periodic systems.

This correction should be enabled only for a homogeneous liquid.

`MuMu14Scaling`

Type
Float

Default value
1.0

GUI name
Mu-Mu 3rd-neighbor scaling

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

`QMu14Scaling`

Type
Float

Default value
0.2

GUI name
Q-Mu 3rd-neighbor scaling

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

`QQ14Scaling`

Type
Float

Default value
1.0

GUI name
Q-Q 3rd-neighbor scaling

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

`RD14Scaling`

Type
Float

Default value
1.0

GUI name
RD 3rd-neighbor scaling

Description
Scaling factor for repulsion/dispersion 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.

`DipoleConvergenceThreshold`

Type
Float

Default value
1e-06

Unit
eBohr

Description
Convergence criterion for induced point dipoles, in atomic units. When the length of every atomic

delta_mu vector between two iterations becomes below the tolerance, the procedure is considered converged.

`DoChargeCheck`

Type
Bool

Default value
No

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.

`EngineConstraints`

Type
Bool

Default value
Yes

Description
Set to false to ignore constraints implied by the engine.

`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

Unit
1/Angstrom

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 the [Tolerance] and [RealSpaceCutoff] values.

`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 if [Alpha] is set on input. Alternatively, if the [RealSpaceCutoff] is set but [Alpha] is not then the [Tolerance] value affects the [Alpha]. 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

`GAFF`

Type
Block

Description
Specific keywords for the GAFF force field type

`AtomTyping`

Type
Block

Description
Specific keywords for automatic atom typing for the GAFF force field type

`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 invoked to guess atomtypes and charges (GAFF force field), select the task for charge guessing with MOPAC

`KeepAntechamberFolder`

Type
Bool

Default value
No

Description
If atom-typing is performed with antechamber, keep the folder after the call to antechamber

`MolecularCharge`

Type
Block

Recurring
True

Description
Defines a (set of) submolecule(s) with their charge, to be Used in GAFF atomtyping.

`Charge`

Type
Float

Description
Molecular charge of submolecule(s) defined in Region.

`Region`

Type
String

Description
Region name that defines a (set of) submolecule(s).

`ForceFieldParameters`

Type
Block

Recurring
True

GUI name

Description
Parameter file text in AMBER format with (additional parameters, missing from main file). Alternative option to ForceFieldPatchFile. The parameter patches provided by antechamber can be used here. Cannot be used when atomtypes are guessed.

`ForceFieldPatchFile`

Type
String

Recurring
True

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

`LAMMPSOffload`

Type
Block

Description
Offload the calculation to LAMMPS via AMSPipe.

`Enabled`

Type
Bool

Default value
No

Description
Enable offloading the force field evaluation to LAMMPS instead of handling it internally in AMS. This is currently only supported for Type=UFF.

`Input`

Type
Block

Description
Commands to be passed to LAMMPS to set up the calculation. If this is left empty, AMS will generate a set of commands to set LAMMPS up according to the settings of the ForceField engine. Any LAMMPS commands entered in this input block will be used to set LAMMPS up instead of those generated by AMS. To merge the AMS-generated lines with your customizations, include lines like 'AMS somelammpskeyword' anywhere in this block. Any such line will be replaced by the AMS-generated line for 'somelammpskeyword'. Any text after 'somelammpskeyword' will be appended to the generated line verbatim, which can be used to modify the generated command by additional options. A special line 'AMS everything' will be replaced by the entire block of AMS-generated commands, except those overridden anywhere in this input block (defined manually or inserted using 'AMS somelammpskeyword'. Any customized Input block should probably include 'AMS read_data' near or at the end to load the AMS-generated data file defining the system.

`UseGPU`

Type
Bool

Default value
No

Description
Accelerate LAMMPS calculations using a GPU. Requires a LAMMPS library built with the GPU package.

`UseGPUForKSpace`

Type
Bool

Default value
Yes

Description
When UseGPU is enabled, also use the GPU to accelerate reciprocal space electrostatic interactions. Disabling this can improve performance on less powerful GPUs.

`UseGPUForNeighbor`

Type
Bool

Default value
Yes

Description
When UseGPU is enabled, also use the GPU to accelerate neighbor searches. Disabling this can improve performance on less powerful GPUs.

`UseOpenMP`

Type
Bool

Default value
No

Description
Parallelize LAMMPS calculations using OpenMP threading. Requires a LAMMPS library built with the OMP package.

`WorkerCommand`

Type
String

Default value
exec lmp

Description
The command to execute to run the external worker. The command is executed in a subdirectory of the results directory. The LAMMPS input commands will be passed to the worker on standard input.

`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

`NeighborListSkin`

Type
Float

Default value
2.5

Unit
Angstrom

Description
Thickness of the buffer region added to the NonBondedCutoff when building a neighbor list.

`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 3D-periodic systems, as Ewald summation is used.

`PairInteractionTapering`

Type
Multiple Choice

Default value
Potential

Options
[None, Potential, Force, CHARMM, CHARMM-Force]

Description
Select a method for smoothing non-bonded pair interactions in the distance range between 90% and 100% of the [NonBondedCutoff] to avoid energy and force jump near the cutoff.

Potential - use a 7th order polynomial switching function that has zero 1st, 2nd and 3rd derivatives at both ends of the interval (force matches the energy derivative).

Force - the same switching function is applied both to the potential and the force (so the force does not match the energy), which may break the total energy conservation during MD.

CHARMM - use a different polynomial that does not have a decaying 2nd derivative at NonBondedCutoff.

CHARMM-Force - use the same switching function as CHARMM but apply it both to the energy and the forces.

`ReuseTypeInfo`

Type
String

Default value

Description
Path to RKF file with atom typing information (atom types, charges, and - in case of GAFF or APPLE&P - possibly a forcefield (patch) file for the system).

`SoftCorePotentials`

Type
Block

Description
When performing free energy perturbation the LJ interactions must be scaled by lambda. To avoid numerical instabilities at small lambda, soft-core potentials need to be used (see DOI:10.1021/ct900587b).

`Alpha`

Type
Float

Default value
0.5

Description
This parameter determines how far the soft-core potential deviates from the scaled regular LJ potential (at zero the expression is a regular LJ expression).

`Enabled`

Type
Bool

Default value
No

Description
Set to True to use the scaled soft-core LJ potentials.

`Lambda`

Type
Float

Default value
1.0

Description
The scaling parameter for the LJ interaction term for free energy perturbation (the window).

`TaperPairInteractions`

Type
Bool

Default value
Yes

Description
Smooth non-bonded pair interactions in the distance range between 90% and 100% of the [NonBondedCutoff] to avoid energy and force jump near the cutoff. See PairInteractionTapering for more precise tuning.

`Type`

Type
Multiple Choice

Default value
UFF

Options
[UFF, Amber95, GAFF, Tripos5.2, APPLE&P, 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.

CHAPTER

THIRTEEN

KF OUTPUT FILES

13.1 Accessing KF files

KF files are Direct Access binary files. KF stands for Keyed File: KF files are keyword oriented, which makes them easy to process by simple procedures. Internally all the data on KF files is organized into sections containing variables, so each datum on the file can be identified by the combination of section and variable.

All KF files can be opened using the KFbrowser GUI program:

```
$AMSBIN/kfbrowser path/to/ams.rkf
```

By default KFbrowser shows a just a curated summary of the results on the file, but you can make it show the raw section and variable structure by switching it to expert mode. To do this, click on **File → Expert Mode** or press **ctrl/cmd + e**.

KF files can be opened and read with Command line tools.

For working with the data from KF files, it is often useful to be able to read them from Python. Using the AMS Python Stack, this can easily be done with the AKFReader class:

```
>>> from scm.akfreader import AKFReader
>>> kf = AKFReader("path/to/ams.rkf")
>>> "Molecule%Coords" in kf
True
>>> kf.description("Molecule%Coords")
{
    '_type': 'float_array',
    '_shape': [3, 'nAtoms'],
    '_comment': 'Coordinates of the nuclei (x,y,z)',
    '_unit': 'Bohr'
}
>>> kf.read("Molecule%Coords")
array([[-11.7770694 ,  -4.19739597,   0.04934546],
       [ -9.37471321,  -2.63234227,  -0.13448698],
        ...
       [ 10.09508738,  -1.06191208,   1.45286913],
       [ 10.11689333,  -1.5080196 ,  -1.87916127]])
```

Tip: For a full overview of the available methods in AKFReader, see the AKFReader API documentation.

13.2 Sections and variables on forcefield.rkf

13.2.1 AMSResults

KF Section: AMSResults

Content: Generic results of the ForceField Engine evaluation.

`AMSResults%AtomicDipoleMoments`

Type

float_array

Description

Atomic dipole moments computed by the engine.

Unit

e*bohr

Shape

[3, Molecule%nAtoms]

`AMSResults%AtomTyping`

Type

subsection

Description

The atom-typing for the ForceField engine.

`AMSResults%AtomTyping.atomIndexToType`

Type

int_array

Description

Array containing the index for the atom type for all the atoms in the system, i.e. iAtomType = atomIndexToType(iAtom).

Shape

[Molecule%nAtoms]

`AMSResults%AtomTyping.atomTypes`

Type

ftl_string_array

Description

Strings defining the atoms types.

Shape

[nAtomTypes]

`AMSResults%AtomTyping.nAtomTypes`

Type

int

Description

The number of distinct force-field atom types.

`AMSResults%BondInfo`

Type
subsection

Description
These aren't written by AMS any more, this subsection is here only for backwards compatibility with old files. FIXME: this section should include the file shared/ArchivedBondInfo.json, but there is a problem: the variable 'BondInfo.LatticeDisplacements@dim ('BondInfo.LatticeDisplacements@dim)' is longer than 32 characters (the KF limit) and this messes up things. For now I'll just ignore all the variables in here…

`AMSResults%Bonds`

Type
subsection

Description
Bond info

`AMSResults%Bonds.Atoms`

Type
archived_int_array

Description
?

`AMSResults%Bonds.CellShifts`

Type
archived_int_array

Description
?

`AMSResults%Bonds.description`

Type
string

Description
A string containing a description of how the bond orders were calculated / where they come from

`AMSResults%Bonds.hasCellShifts`

Type
bool

Description
Whether there are cell shifts (relevant only in case of periodic boundary conditions)

`AMSResults%Bonds.Index`

Type
archived_int_array

Description
index(i) points to the first element of Atoms, Orders, and CellShifts belonging to bonds from atom 'i'. Index(1) is always 1, Index(nAtoms+1) is always nBonds + 1

`AMSResults%Bonds.nLattVec`

Type
int

Description
Number of lattice vectors (0:molecule, 1:chain, 2:slab, 3:bulk). This determines how the lattice displacements for bonds are interpreted.

`AMSResults%Bonds.Orders`

Type
archived_float_array

Description
The bond orders.

`AMSResults%BulkModulus`

Type
float

Description
The Bulk modulus (conversion factor from hartree/bohr^3 to GPa: 29421.026)

Unit
hartree/bohr^3

`AMSResults%Charges`

Type
float_array

Description
Net atomic charges as computed by the engine (for example, the Charges for a water molecule might be [-0.6, 0.3, 0.3]). The method used to compute these atomic charges depends on the engine.

Unit
e

Shape
[Molecule%nAtoms]

`AMSResults%Config`

Type
subsection

Description
Configuration of the ForceField engine.

`AMSResults%DipoleGradients`

Type
float_array

Description
Derivative of the dipole moment with respect to nuclear displacements.

Shape
[3, 3, Molecule%nAtoms]

`AMSResults%DipoleMoment`

Type
float_array

Description
Dipole moment vector (x,y,z)

Unit
e*bohr

Shape
[3]

`AMSResults%ElasticTensor`

Type
float_array

Description
The elastic tensor in Voigt notation (6x6 matrix for 3D periodic systems, 3x3 matrix for 2D periodic systems, 1x1 matrix for 1D periodic systems).

Unit
hartree/bohr^nLatticeVectors

Shape
[:, :]

`AMSResults%Energy`

Type
float

Description
The energy computed by the engine.

Unit
hartree

`AMSResults%Gradients`

Type
float_array

Description
The nuclear gradients.

Unit
hartree/bohr

Shape
[3, Molecule%nAtoms]

`AMSResults%Hessian`

Type
float_array

Description
The Hessian matrix

Unit
hartree/bohr^2

Shape
[3*Molecule%nAtoms, 3*Molecule%nAtoms]

`AMSResults%Molecules`

Type
subsection

Description
Molecules

AMSResults%Molecules.AtCount

Type
archived_int_array

Description
shape=(nMolType), Summary: number of atoms per formula.

AMSResults%Molecules.Atoms

Type
archived_int_array

Description
shape=(nAtoms), atoms(index(i):index(i+1)-1) = atom indices of molecule i

AMSResults%Molecules.Count

Type
archived_int_array

Description
Mol count per formula.

AMSResults%Molecules.Formulas

Type
string

Description
Summary: unique molecule formulas

AMSResults%Molecules.Index

Type
archived_int_array

Description
shape=(nMol+1), index(i) = index of the first atom of molecule i in array atoms(:)

AMSResults%Molecules.Type

Type
archived_int_array

Description
shape=(nMol), type of the molecule, reference to the summary arrays below

AMSResults%PESPointCharacter

Type
string

Description
The character of a PES point.

Possible values
['local minimum', 'transition state', 'stationary point with >1 negative frequencies', 'non-stationary point']

AMSResults%PoissonRatio

Type
float

Description
The Poisson ratio

`AMSResults%ShearModulus`

Type
float

Description
The Shear modulus (conversion factor from hartree/bohr^3 to GPa: 29421.026)

Unit
hartree/bohr^3

`AMSResults%StressTensor`

Type
float_array

Description
The clamped-ion stress tensor in Cartesian notation.

Unit
hartree/bohr^nLatticeVectors

Shape
[:, :]

`AMSResults%YoungModulus`

Type
float

Description
The Young modulus (conversion factor from hartree/bohr^3 to GPa: 29421.026)

Unit
hartree/bohr^3

13.2.2 BZcell(primitive cell)

KF Section: BZcell(primitive cell)
Content: The Brillouin zone of the primitive cell.

`BZcell(primitive cell)%boundaries`

Type
float_array

Description
Normal vectors for the boundaries.

Shape
[ndim, nboundaries]

`BZcell(primitive cell)%distances`

Type
float_array

Description
Distance to the boundaries.

Shape
[nboundaries]

`BZcell(primitive cell)%idVerticesPerBound`

Type
int_array

Description
The indices of the vertices per bound.

Shape
[nvertices, nboundaries]

`BZcell(primitive cell)%latticeVectors`

Type
float_array

Description
The lattice vectors.

Shape
[3, :]

`BZcell(primitive cell)%nboundaries`

Type
int

Description
The nr. of boundaries for the cell.

`BZcell(primitive cell)%ndim`

Type
int

Description
The nr. of lattice vectors spanning the Wigner-Seitz cell.

`BZcell(primitive cell)%numVerticesPerBound`

Type
int_array

Description
The nr. of vertices per bound.

Shape
[nboundaries]

`BZcell(primitive cell)%nvertices`

Type
int

Description
The nr. of vertices of the cell.

`BZcell(primitive cell)%vertices`

Type
float_array

Description
The vertices of the bounds.

Unit
a.u.

Shape
[ndim, nvertices]

13.2.3 DOS_Phonons

KF Section: DOS_Phonons
Content: Phonon Density of States

`DOS_Phonons%DeltaE`

Type
float

Description
The energy difference between sampled DOS energies. When there is no DOS at all a certain energy range can be skipped.

Unit
hartree

`DOS_Phonons%Energies`

Type
float_array

Description
The energies at which the DOS is sampled.

Unit
hartree

Shape
[nEnergies]

`DOS_Phonons%Fermi Energy`

Type
float

Description
The fermi energy.

Unit
hartree

`DOS_Phonons%IntegrateDeltaE`

Type
bool

Description
If enabled it means that the DOS is integrated over intervals of DeltaE. Sharp delta function like peaks cannot be missed this way.

`DOS_Phonons%nEnergies`

Type
int

Description
The nr. of energies to use to sample the DOS.

`DOS_Phonons%nSpin`

Type
int

Description
The number of spin components for the DOS.

Possible values
[1, 2]

`DOS_Phonons%Total DOS`

Type
float_array

Description
The total DOS.

Shape
[nEnergies, nSpin]

13.2.4 General

KF Section: General
Content: General information about the ForceField calculation.

`General%account`

Type
string

Description
Name of the account from the license

`General%engine input`

Type
string

Description
The text input of the engine.

`General%engine messages`

Type
string

Description
Message from the engine. In case the engine fails to solves, this may contains extra information on why.

`General%file-ident`

Type
string

Description
The file type identifier, e.g. RKF, RUNKF, TAPE21…

`General%jobid`

Type
int

Description
Unique identifier for the job.

`General%program`

Type
string

Description
The name of the program/engine that generated this kf file.

`General%release`

Type
string

Description
The version of the program that generated this kf file (including svn revision number and date).

`General%termination status`

Type
string

Description
The termination status. Possible values: 'NORMAL TERMINATION', 'NORMAL TERMINATION with warnings', 'NORMAL TERMINATION with errors', 'ERROR', 'IN PROGRESS'.

`General%title`

Type
string

Description
Title of the calculation.

`General%uid`

Type
string

Description
SCM User ID

`General%version`

Type
int

Description
Version number?

13.2.5 KFDefinitions

KF Section: KFDefinitions

Content: The definitions of the data on this file

`KFDefinitions%json`

Type
string

Description
The definitions of the data on this file in json.

13.2.6 kspace(primitive cell)

KF Section: kspace(primitive cell)

Content: should not be here!!!

`kspace(primitive cell)%avec`

Type
float_array

Description
The lattice stored as a 3xnLatticeVectors matrix. Only the ndimk,ndimk part has meaning.

Unit
bohr

Shape
[3, :]

`kspace(primitive cell)%bvec`

Type
float_array

Description
The inverse lattice stored as a 3x3 matrix. Only the ndimk,ndimk part has meaning.

Unit
1/bohr

Shape
[ndim, ndim]

`kspace(primitive cell)%kt`

Type
int

Description
The total number of k-points used by the k-space to sample the unique wedge of the Brillouin zone.

`kspace(primitive cell)%kuniqu`

Type
int

Description
The number of symmetry unique k-points where an explicit diagonalization is needed. Smaller or equal to kt.

`kspace(primitive cell)%ndim`

Type
int

Description
The nr. of lattice vectors.

`kspace(primitive cell)%ndimk`

Type
int

Description
The nr. of dimensions used in the k-space integration.

`kspace(primitive cell)%xyzpt`

Type
float_array

Description
The coordinates of the k-points.

Unit
1/bohr

Shape
[ndimk, kt]

13.2.7 Low Frequency Correction

KF Section: Low Frequency Correction
Content: Configuration for the Head-Gordon Dampener-powered Free Rotor Interpolation.

`Low Frequency Correction%Alpha`

Type
float

Description
Exponent term for the Head-Gordon dampener.

`Low Frequency Correction%Frequency`

Type
float

Description
Frequency around which interpolation happens, in 1/cm.

`Low Frequency Correction%Moment of Inertia`

Type
float

Description
Used to make sure frequencies of less than ca. 1 1/cm don’t overestimate entropy, in kg m^2.

13.2.8 Mobile Block Hessian

KF Section: Mobile Block Hessian

Content: Mobile Block Hessian.

`Mobile Block Hessian%Coordinates Internal`

Type

float_array

Description

?

`Mobile Block Hessian%Free Atom Indexes Input`

Type

int_array

Description

?

`Mobile Block Hessian%Frequencies in atomic units`

Type

float_array

Description

?

`Mobile Block Hessian%Frequencies in wavenumbers`

Type

float_array

Description

?

`Mobile Block Hessian%Input Cartesian Normal Modes`

Type

float_array

Description

?

`Mobile Block Hessian%Input Indexes of Block #`

Type

int_array

Description

?

`Mobile Block Hessian%Intensities in km/mol`

Type

float_array

Description

?

`Mobile Block Hessian%MBH Curvatures`

Type

float_array

Description
?

`Mobile Block Hessian%Number of Blocks`

Type
int

Description
Number of blocks.

`Mobile Block Hessian%Sizes of Blocks`

Type
int_array

Description
Sizes of the blocks.

Shape
[Number of Blocks]

13.2.9 Molecule

KF Section: Molecule
Content: The input molecule of the calculation.

`Molecule%AtomicNumbers`

Type
int_array

Description
Atomic number ‘Z’ of the atoms in the system

Shape
[nAtoms]

`Molecule%AtomMasses`

Type
float_array

Description
Masses of the atoms

Unit
a.u.

Values range
[0, ‘\infinity’]

Shape
[nAtoms]

`Molecule%AtomSymbols`

Type
string

Description
The atom’s symbols (e.g. ‘C’ for carbon)

Shape
[nAtoms]

Molecule%bondOrders

Type
float_array

Description
The bond orders for the bonds in the system. The indices of the two atoms participating in the bond are defined in the arrays 'fromAtoms' and 'toAtoms'. e.g. bondOrders[1]=2, fromAtoms[1]=4 and toAtoms[1]=7 means that there is a double bond between atom number 4 and atom number 7

Molecule%Charge

Type
float

Description
Net charge of the system

Unit
e

Molecule%Coords

Type
float_array

Description
Coordinates of the nuclei (x,y,z)

Unit
bohr

Shape
[3, nAtoms]

Molecule%eeAttachTo

Type
int_array

Description
UNUSED IN AMS>=2026. A multipole may be attached to an atom. This influences the energy gradient.

Molecule%eeChargeWidth

Type
float

Description
If charge broadening was used for external charges, this represents the width of the charge distribution.

Molecule%eeEField

Type
float_array

Description
The external homogeneous electric field.

Unit
hartree/(e*bohr)

Shape
[3]

`Molecule%eeLatticeVectors`

Type
float_array

Description
UNUSED IN AMS>=2026. The lattice vectors used for the external point- or multipole-charges.

Unit
bohr

Shape
[3, eeNLatticeVectors]

`Molecule%eeMulti`

Type
float_array

Description
The values of the external point- or multipole- charges.

Unit
a.u.

Shape
[eeNZlm, eeNMulti]

`Molecule%eeNLatticeVectors`

Type
int

Description
UNUSED IN AMS>=2026. The number of lattice vectors for the external point- or multipole-charges.

`Molecule%eeNMulti`

Type
int

Description
The number of external point- or multipole- charges.

`Molecule%eeNZlm`

Type
int

Description
When external point- or multipole- charges are used, this represents the number of spherical harmonic components. E.g. if only point charges were used, eeNZlm=1 (s-component only). If point charges and dipole moments were used, eeNZlm=4 (s, px, py and pz).

`Molecule%eeUseChargeBroadening`

Type
bool

Description
Whether or not the external charges are point-like or broadened.

`Molecule%eeXYZ`

Type
float_array

Description
The position of the external point- or multipole- charges.

Unit
bohr

Shape
[3, eeNMulti]

`Molecule%EngineAtomicInfo`

Type
string_fixed_length

Description
Atom-wise info possibly used by the engine.

`Molecule%fromAtoms`

Type
int_array

Description
Index of the first atom in a bond. See the bondOrders array

`Molecule%latticeDisplacements`

Type
int_array

Description
The integer lattice translations for the bonds defined in the variables bondOrders, fromAtoms and toAtoms.

`Molecule%LatticeVectors`

Type
float_array

Description
Lattice vectors

Unit
bohr

Shape
[3, nLatticeVectors]

`Molecule%nAtoms`

Type
int

Description
The number of atoms in the system

`Molecule%nAtomsTypes`

Type
int

Description
The number different of atoms types

`Molecule%nLatticeVectors`

Type
int

Description
Number of lattice vectors (i.e. number of periodic boundary conditions)

Possible values
[0, 1, 2, 3]

`Molecule%toAtoms`

Type
int_array

Description
Index of the second atom in a bond. See the bondOrders array

13.2.10 MoleculeSuperCell

KF Section: MoleculeSuperCell
Content: The system used for the numerical phonon super cell calculation.

`MoleculeSuperCell%AtomicNumbers`

Type
int_array

Description
Atomic number ‘Z’ of the atoms in the system

Shape
[nAtoms]

`MoleculeSuperCell%AtomMasses`

Type
float_array

Description
Masses of the atoms

Unit
a.u.

Values range
[0, ‘\infinity’]

Shape
[nAtoms]

`MoleculeSuperCell%AtomSymbols`

Type
string

Description
The atom's symbols (e.g. 'C' for carbon)

Shape
[nAtoms]

`MoleculeSuperCell%bondOrders`

Type
float_array

Description
The bond orders for the bonds in the system. The indices of the two atoms participating in the bond are defined in the arrays 'fromAtoms' and 'toAtoms'. e.g. bondOrders[1]=2, fromAtoms[1]=4 and toAtoms[1]=7 means that there is a double bond between atom number 4 and atom number 7

`MoleculeSuperCell%Charge`

Type
float

Description
Net charge of the system

Unit
e

`MoleculeSuperCell%Coords`

Type
float_array

Description
Coordinates of the nuclei (x,y,z)

Unit
bohr

Shape
[3, nAtoms]

`MoleculeSuperCell%eeAttachTo`

Type
int_array

Description
UNUSED IN AMS>=2026. A multipole may be attached to an atom. This influences the energy gradient.

`MoleculeSuperCell%eeChargeWidth`

Type
float

Description
If charge broadening was used for external charges, this represents the width of the charge distribution.

`MoleculeSuperCell%eeEField`

Type
float_array

Description
The external homogeneous electric field.

Unit
hartree/(e*bohr)

Shape
[3]

`MoleculeSuperCell%eeLatticeVectors`

Type
float_array

Description
UNUSED IN AMS>=2026. The lattice vectors used for the external point- or multipole-charges.

Unit
bohr

Shape
[3, eeNLatticeVectors]

`MoleculeSuperCell%eeMulti`

Type
float_array

Description
The values of the external point- or multipole- charges.

Unit
a.u.

Shape
[eeNZlm, eeNMulti]

`MoleculeSuperCell%eeNLatticeVectors`

Type
int

Description
UNUSED IN AMS>=2026. The number of lattice vectors for the external point- or multipole-charges.

`MoleculeSuperCell%eeNMulti`

Type
int

Description
The number of external point- or multipole- charges.

`MoleculeSuperCell%eeNZlm`

Type
int

Description
When external point- or multipole- charges are used, this represents the number of spherical harmonic components. E.g. if only point charges were used, eeNZlm=1 (s-component only). If point charges and dipole moments were used, eeNZlm=4 (s, px, py and pz).

`MoleculeSuperCell%eeUseChargeBroadening`

Type
bool

Description
Whether or not the external charges are point-like or broadened.

`MoleculeSuperCell%eeXYZ`

Type
float_array

Description
The position of the external point- or multipole- charges.

Unit
bohr

Shape
[3, eeNMulti]

`MoleculeSuperCell%EngineAtomicInfo`

Type
string_fixed_length

Description
Atom-wise info possibly used by the engine.

`MoleculeSuperCell%fromAtoms`

Type
int_array

Description
Index of the first atom in a bond. See the bondOrders array

`MoleculeSuperCell%latticeDisplacements`

Type
int_array

Description
The integer lattice translations for the bonds defined in the variables bondOrders, fromAtoms and toAtoms.

`MoleculeSuperCell%LatticeVectors`

Type
float_array

Description
Lattice vectors

Unit
bohr

Shape
[3, nLatticeVectors]

`MoleculeSuperCell%nAtoms`

Type
int

Description
The number of atoms in the system

`MoleculeSuperCell%nAtomsTypes`

Type
int

Description
The number different of atoms types

`MoleculeSuperCell%nLatticeVectors`

Type
int

Description
Number of lattice vectors (i.e. number of periodic boundary conditions)

Possible values
[0, 1, 2, 3]

`MoleculeSuperCell%toAtoms`

Type
int_array

Description
Index of the second atom in a bond. See the bondOrders array

13.2.11 phonon_curves

KF Section: phonon_curves
Content: Phonon dispersion curves.

`phonon_curves%brav_type`

Type
string

Description
Type of the lattice.

`phonon_curves%Edge_#_bands`

Type
float_array

Description
The band energies

Shape
[nBands, nSpin, :]

`phonon_curves%Edge_#_direction`

Type
float_array

Description
Direction vector.

Shape
[nDimK]

`phonon_curves%Edge_#_kPoints`

Type
float_array

Description
Coordinates for points along the edge.

Shape
[nDimK, :]

`phonon_curves%Edge_#_labels`

Type
lchar_string_array

Description
Labels for begin and end point of the edge.

Shape
[2]

`phonon_curves%Edge_#_lGamma`

Type
bool

Description
Is gamma point?

`phonon_curves%Edge_#_nKPoints`

Type
int

Description
The nr. of k points along the edge.

`phonon_curves%Edge_#_vertices`

Type
float_array

Description
Begin and end point of the edge.

Shape
[nDimK, 2]

`phonon_curves%Edge_#_xFor1DPlotting`

Type
float_array

Description
x Coordinate for points along the edge.

Shape
[:]

`phonon_curves%indexLowestBand`

Type
int

Description
?

`phonon_curves%nBands`

Type
int

Description
Number of bands.

`phonon_curves%nBas`

Type
int

Description
Number of basis functions.

`phonon_curves%nDimK`

Type
int

Description
Dimension of the reciprocal space.

`phonon_curves%nEdges`

Type
int

Description
The number of edges. An edge is a line-segment through k-space. It has a begin and end point and possibly points in between.

`phonon_curves%nEdgesInPath`

Type
int

Description
A path is built up from a number of edges.

`phonon_curves%nSpin`

Type
int

Description
Number of spin components.

Possible values
[1, 2]

`phonon_curves%path`

Type
int_array

Description
If the (edge) index is negative it means that the vertices of the edge abs(index) are swapped e.g. path = (1,2,3,0,-3,-2,-1) goes though edges 1,2,3, then there's a jump, and then it goes back.

Shape
[nEdgesInPath]

`phonon_curves%path_source`

Type
string

Description
Source or program used to generate the path.

Possible values
['input', 'kpath', 'seekpath']

`phonon_curves%path_type`

Type
string

Description
?

13.2.12 Phonons

KF Section: Phonons

Content: Information on the numerical phonons (super cell) setup. NB: the reciprocal cell of the super cell is smaller than the reciprocal primitive cell.

`Phonons%Modes`

Type
float_array

Description
The normal modes with the translational symmetry of the super cell.

Shape
[3, nAtoms, 3, NumAtomsPrim, nK]

`Phonons%nAtoms`

Type
int

Description
Number of atoms in the super cell.

`Phonons%nK`

Type
int

Description
Number of gamma-points (of the super cell) that fit into the primitive reciprocal cell.

`Phonons%NumAtomsPrim`

Type
int

Description
Number of atoms in the primitive cell.

`Phonons%xyzKSuper`

Type
float_array

Description
The coordinates of the gamma points that fit into the primitive reciprocal cell.

Shape
[3, nK]

13.2.13 Properties

KF Section: Properties

Content: Generic container for properties. The program band uses different rules for Types and Subtypes.

`Properties%nEntries`

Type
int

Description
Number of properties.

`Properties%Subtype(#)`

Type
string_fixed_length

Description
Extra detail about the property. For a charge property this could be Mulliken.

`Properties%Type(#)`

Type
string

Description
Type of the property, like energy, gradients, charges, etc.

`Properties%Value(#)`

Type
float_array

Description
The value(s) of the property.

13.2.14 Thermodynamics

KF Section: Thermodynamics

Content: Thermodynamic properties computed from normal modes.

`Thermodynamics%Enthalpy`

Type
float_array

Description
Enthalpy.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Entropy rotational`

Type
float_array

Description
Rotational contribution to the entropy.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Entropy total`

Type
float_array

Description
Total entropy.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Entropy translational`

Type
float_array

Description
Translational contribution to the entropy.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Entropy vibrational`

Type
float_array

Description
Vibrational contribution to the entropy.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Gibbs free Energy`

Type
float_array

Description
Gibbs free energy.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Heat Capacity rotational`

Type
float_array

Description
Rotational contribution to the heat capacity.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Heat Capacity total`

Type
float_array

Description
Total heat capacity.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Heat Capacity translational`

Type
float_array

Description
Translational contribution to the heat capacity.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Heat Capacity vibrational`

Type
float_array

Description
Vibrational contribution to the heat capacity.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Inertia direction vectors`

Type
float_array

Description
Inertia direction vectors.

Shape
[3, 3]

`Thermodynamics%Internal Energy rotational`

Type
float_array

Description
Rotational contribution to the internal energy.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Internal Energy total`

Type
float_array

Description
Total internal energy.

Unit
a.u.

`Thermodynamics%Internal Energy translational`

Type
float_array

Description
Translational contribution to the internal energy.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Internal Energy vibrational`

Type
float_array

Description
Vibrational contribution to the internal energy.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%lowFreqEntropy`

Type
float_array

Description
Entropy contributions from low frequencies (see 'lowFrequencies').

Unit
a.u.

Shape
[nLowFrequencies]

`Thermodynamics%lowFreqHeatCapacity`

Type
float_array

Description
Heat capacity contributions from low frequencies (see 'lowFrequencies').

Unit
a.u.

Shape
[nLowFrequencies]

`Thermodynamics%lowFreqInternalEnergy`

Type
float_array

Description
Internal energy contributions from low frequencies (see 'lowFrequencies').

Unit
a.u.

Shape
[nLowFrequencies]

`Thermodynamics%lowFrequencies`

Type
float_array

Description
Frequencies below 20 cm^-1 (contributions from frequencies below 20 cm^-1 are not included in vibrational sums, and are saved separately to 'lowFreqEntropy', 'lowFreqInternalEnergy' and 'lowFreqInternalEnergy'). Note: this does not apply to RRHO-corrected quantities.

Unit
cm^-1

Shape
[nLowFrequencies]

`Thermodynamics%Moments of inertia`

Type
float_array

Description
Moments of inertia.

Unit
a.u.

Shape
[3]

`Thermodynamics%nLowFrequencies`

Type
int

Description
Number of elements in the array lowFrequencies.

`Thermodynamics%nTemperatures`

Type
int

Description
Number of temperatures.

`Thermodynamics%Pressure`

Type
float

Description
Pressure used.

Unit
atm

`Thermodynamics%RRHOCorrectedHeatCapacity`

Type
float_array

Description
Heat capacity T*S corrected using the ‘low vibrational frequency free rotor interpolation corrections’.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%RRHOCorrectedInternalEnergy`

Type
float_array

Description
Internal energy T*S corrected using the 'low vibrational frequency free rotor interpolation corrections'.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%RRHOCorrectedTS`

Type
float_array

Description
T*S corrected using the 'low vibrational frequency free rotor interpolation corrections'.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%Temperature`

Type
float_array

Description
List of temperatures at which properties are calculated.

Unit
a.u.

Shape
[nTemperatures]

`Thermodynamics%TS`

Type
float_array

Description
T*S, i.e. temperature times entropy.

Unit
a.u.

Shape
[nTemperatures]

13.2.15 Vibrations

KF Section: Vibrations

Content: Information related to molecular vibrations.

`Vibrations%ExcitedStateLifetime`

Type
float

Description
Raman excited state lifetime.

Unit
hartree

`Vibrations%ForceConstants`

Type
float_array

Description
The force constants of the vibrations.

Unit
hartree/bohr^2

Shape
[nNormalModes]

`Vibrations%Frequencies[cm-1]`

Type
float_array

Description
The vibrational frequencies of the normal modes.

Unit
cm^-1

Shape
[nNormalModes]

`Vibrations%Intensities[km/mol]`

Type
float_array

Description
The intensity of the normal modes.

Unit
km/mol

Shape
[nNormalModes]

`Vibrations%IrReps`

Type
lchar_string_array

Description
Symmetry symbol of the normal mode.

Shape
[nNormalModes]

`Vibrations%ModesNorm2`

Type
float_array

Description
Norms of the rigid motions.

Shape
[nNormalModes+nRigidModes]

`Vibrations%ModesNorm2*`

Type
float_array

Description
Norms of the rigid motions (for a given irrep…?).

Shape
[nNormalModes+nRigidModes]

`Vibrations%nNormalModes`

Type
int

Description
Number of normal modes.

`Vibrations%NoWeightNormalMode(#)`

Type
float_array

Description
?.

Shape
[3, Molecule%nAtoms]

`Vibrations%NoWeightRigidMode(#)`

Type
float_array

Description
?

Shape
[3, Molecule%nAtoms]

`Vibrations%nRigidModes`

Type
int

Description
Number of rigid modes.

`Vibrations%nSemiRigidModes`

Type
int

Description
Number of semi-rigid modes.

`Vibrations%PVDOS`

Type
float_array

Description
Partial vibrational density of states.

Values range
[0.0, 1.0]

Shape
[nNormalModes, Molecule%nAtoms]

`Vibrations%RamanDepolRatioLin`

Type
float_array

Description
Raman depol ratio (lin).

Shape
[nNormalModes]

`Vibrations%RamanDepolRatioNat`

Type
float_array

Description
Raman depol ratio (nat).

Shape
[nNormalModes]

`Vibrations%RamanIncidentFreq`

Type
float

Description
Raman incident light frequency.

Unit
hartree

`Vibrations%RamanIntens[A^4/amu]`

Type
float_array

Description
Raman intensities

Unit
A^4/amu

Shape
[nNormalModes]

`Vibrations%ReducedMasses`

Type
float_array

Description
The reduced masses of the normal modes.

Unit
a.u.

Values range
[0, '\infinity']

Shape
[nNormalModes]

`Vibrations%RotationalStrength`

Type
float_array

Description
The rotational strength of the normal modes.

Shape
[nNormalModes]

`Vibrations%TransformationMatrix`

Type
float_array

Description
?

Shape
[3, Molecule%nAtoms, nNormalModes]

`Vibrations%VROACIDBackward`

Type
float_array

Description
VROA Circular Intensity Differential: Backward scattering.

Unit
10¯3

Shape
[nNormalModes]

`Vibrations%VROACIDDePolarized`

Type
float_array

Description
VROA Circular Intensity Differential: Depolarized scattering.

Unit
10¯3

Shape
[nNormalModes]

`Vibrations%VROACIDForward`

Type
float_array

Description
VROA Circular Intensity Differential: Forward scattering.

Unit
10¯3

Shape
[nNormalModes]

`Vibrations%VROACIDPolarized`

Type
float_array

Description
VROA Circular Intensity Differential: Polarized scattering.

Unit
10¯3

Shape
[nNormalModes]

`Vibrations%VROADeltaBackward`

Type
float_array

Description
VROA Intensity: Backward scattering.

Unit
10¯3 A^4/amu

Shape
[nNormalModes]

`Vibrations%VROADeltaDePolarized`

Type
float_array

Description
VROA Intensity: Depolarized scattering.

Unit
10¯3 A^4/amu

Shape
[nNormalModes]

`Vibrations%VROADeltaForward`

Type
float_array

Description
VROA Intensity: Forward scattering.

Unit
10¯3 A^4/amu

Shape
[nNormalModes]

`Vibrations%VROADeltaPolarized`

Type
float_array

Description
VROA Intensity: Polarized scattering.

Unit
10¯3 A^4/amu

Shape
[nNormalModes]

`Vibrations%ZeroPointEnergy`

Type
float

Description
Vibrational zero-point energy.

Unit
hartree

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