WebFF Documentation

Release 1.0.0

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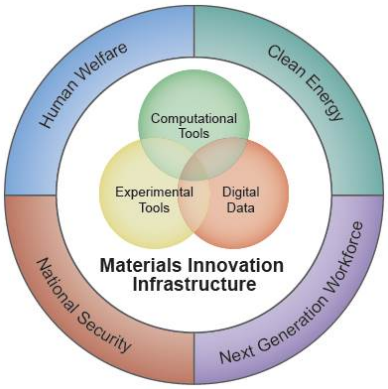
Nov 08, 2019

User Documentation


Human Welfare
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Digital Data
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National Security
Next Generation Workforce

CHAPTER 1

WebFF

WebFF is an open and extensible molecular dynamics force-field (FF) repository, designed to support the Materials Genome Initiative (MGI) for organic and related soft materials. The repository is built using the NIST **Materials Data Curation System (MDCS)** [link] which supports ontology based database descriptions using XML schema.

1.1 Features

Here are some of the main features of WebFF:

- Users interact with the repository through two main portals. The **Data Exploration Portal** [link] supports search for force-field data based on the curated metadata descriptors and download in a number for common formats. We will work with the user community to expand output format coverage per user requests.
- The **Data Curation Portal** [link] supports upload of published force-field data with appropriate metadata descriptors to support provenance based data sharing. New datasets may be curated interactively or using a python based toolset to upload large datasets en masse. Data curation requires an authorized account.
- **The initial release of the repository features three integrated XML schemas:**
    1. Class I organic force-fields in such as OPLS, Amber and CHARMM style representations
    2. Class II style force-fields such as CFF, PCFF, COMPASS and TEAMFF
    3. Coarse-Grained models at various levels of granularity
- For questions, comments and requests please contact: webff@nist.gov

If you use data from WebFF in your work, we ask that you please cite the following:

1. The main source or the data cited in the XML metadata
2. Frederick R. Phelan Jr., Kathleen Mullin, Pablo Garcia Beltran, Gule Teri, Priyanshu Mishra and Huai Sun, "The Web Force-Field (WebFF) Project: Ontology Based Force-Field Repository for Soft Materials at Multiple Levels of Granularity," in preparation (2018).

1.2 External Resources

WebFF-Documentation	
Materials Data Curation System (MDCS)	

CHAPTER 2

Force-Field Data Search

CHAPTER 3

Force-Field Curation to WebFF

3.1 Manual Entry

3.2 Automated Entry

CHAPTER 4

XML Schemas

CHAPTER 5

Python Tools

5.1 WebFF.py Module

5.2 WebFF Data Input: Excel to XML

5.3 WebFF Data Output Tools: XML to MD Format

5.4 Module Index

This module contains functions that translate data between Excel, XML, and molecular dynamics text formats

WebFF.**ReadExcelAnglePotential_CHARMM**(*sheet*, *sub_root*)
Reads in the AnglePotential-CHARMM sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelAnglePotential_COS2**(*sheet*, *sub_root*)
Reads in the AnglePotential-COS2 sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelAnglePotential_Class2**(*sheet*, *sub_root*)
Reads in the AnglePotential-Harmonic sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelAnglePotential_Cosine**(*sheet*, *sub_root*)
Reads in the AnglePotential-Cosine sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelAnglePotential_Harmonic**(*sheet*, *sub_root*)
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WebFF.**ReadExcelAnglePotential_Tabular**(*sheet*, *sub_root*)
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WebFF.**ReadExcelAtomTypeAttributes**(*sheet*, *root*)
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WebFF.**ReadExcelAtomTypeAttributes_DFF**(*sheet*, *root*)
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WebFF.**ReadExcelAtomTypes_Generic**(*sheet*, *root*)
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WebFF.**ReadExcelAutoEquivalenceTable**(*sheet*, *sub_root*)
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WebFF.**ReadExcelBondIncrements**(*sheet*, *sub_root*)
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WebFF.**ReadExcelBondPotential_Class2**(*sheet*, *sub_root*)
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WebFF.**ReadExcelBondPotential_FENE**(*sheet*, *sub_root*)
Reads in the BondPotential-FENE sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelBondPotential_Harmonic**(*sheet*, *sub_root*)
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WebFF.**ReadExcelBondPotential_Morse**(*sheet*, *sub_root*)
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WebFF.**ReadExcelBondPotential_Tabular**(*sheet*, *sub_root*)
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WebFF.**ReadExcelCrossPotential_AngleAngle**(*sheet*, *sub_root*)
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WebFF.**ReadExcelCrossPotential_AngleAngleTorsion**(*sheet*, *sub_root*)
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WebFF.**ReadExcelCrossPotential_AngleTorsion**(*sheet*, *sub_root*)
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WebFF.**ReadExcelCrossPotential_BondBond13**(*sheet*, *sub_root*)
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WebFF.**ReadExcelCrossPotential_EndBondTorsion**(*sheet*, *sub_root*)
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WebFF.**ReadExcelCrossPotential_MiddleBondTorsion**(*sheet*, *sub_root*)
Reads in the BondPotential-Harmonic sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

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WebFF.**ReadExcelDihedralPotential_FourierSimple**(*sheet*, *sub_root*)
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WebFF.**ReadExcelDihedralPotential_Harmonic**(*sheet*, *sub_root*)
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WebFF.**ReadExcelDihedralPotential_Multiharmonic**(*sheet*, *sub_root*)
Reads in the DihedralPotential-Multiharmonic sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelDihedralPotential_OPLS**(*sheet*, *sub_root*)
Reads in the DihedralPotential-OPLS sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

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Reads in the DihedralPotential-Quadratic sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelDihedralPotential_Tabular**(*sheet*, *sub_root*)
Reads in the DihedralPotential-Tabular sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

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WebFF.**ReadExcelEquivalenceTable**(*sheet*, *sub_root*)
Reads in the Equivalence-Table sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelImproperPotential_CHARMM**(*sheet*, *sub_root*)
Reads in the ImporperPotential-CHARMM sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelImproperPotential_COS2**(*sheet*, *sub_root*)
Reads in the ImporperPotential-COS2 sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelImproperPotential_CVFF**(*sheet*, *sub_root*)
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WebFF.**ReadExcelImproperPotential_Class2**(*sheet*, *sub_root*)
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WebFF.**ReadExcelImproperPotential_Fourier**(*sheet*, *sub_root*)
Reads in the ImporperPotential-Fourier sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelImproperPotential_Harmonic**(*sheet*, *sub_root*)
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WebFF.**ReadExcelImproperPotential_Umbrella**(*sheet*, *sub_root*)
Reads in the ImporperPotential-Umbrella sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelMetaData_Header**(*sheet*, *sub_root*)
Reads in the MetaData sheet from the WebFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelMetaData_Keywords**(*sheet*, *root*)
Reads in the Keywords sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelMetaData_References**(*sheet*, *root*)
Reads in the Keywords sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelNonBondPotential_EnergyRenorm**(*sheet*, *sub_root*)
Reads in the NonBondPotential-EnergyRenorm sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelNonBondPotential_LJ**(*sheet*, *sub_root*)
Reads in the NonBondPotential-LJ sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelNonBondPotential_LJ2**(*sheet*, *sub_root*)
Reads in the NonBondPotential-LJ2 sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelNonBondPotential_LJ2AB**(*sheet*, *sub_root*)
Reads in the NonBondPotential-LJ2AB sheet from the WebFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelNonBondPotential_LJ96**(*sheet*, *sub_root*)
Reads in the NonBondPotential-LJRmin sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelNonBondPotential_LJ962**(*sheet*, *sub_root*)
Reads in the NonBondPotential-LJ962 sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelNonBondPotential_LJAB**(*sheet*, *sub_root*)
Reads in the NonBondPotential-LJAB sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelNonBondPotential_LJClass2**(*sheet*, *sub_root*)
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WebFF.**ReadExcelNonBondPotential_LJGROMACS**(*sheet*, *sub_root*)
Reads in the NonBondPotential-LJ-GROMACS sheet from the webFF excel template. Arguments are the sheet and the XML element that is the parent for the data.

WebFF.**ReadExcelNonBondPotential_LJRmin**(*sheet*, *sub_root*)
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WebFF.**ReadExcelNonBondPotential_Mie**(*sheet*, *sub_root*)
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WebFF.**ReadExcelWaterPotential_5Site**(*sheet*, *sub_root*)
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WebFF.**XMLToParamsImproperPotential_Class2**(*root*, *output_file*)

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WebFF.**XMLtoFrcCrossPotential_MiddleBondTorsion**(*root*, *output_file*)

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WebFF.**XMLtoFrcDihedralPotential_Class2**(*root*, *output_file*)

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WebFF.**XMLtoFrcDihedralPotential_Multiharmonic**(*root*, *output_file*)

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WebFF.**XMLtoFrcImproperPotential_COS2**(*root*, *output_file*)

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WebFF.**XMLtoFrcImproperPotential_Class2**(*root*, *output_file*)

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WebFF.**XMLtoFrcImproperPotential_FourierSimple**(*root*, *output_file*)

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WebFF.**XMLtoFrcNonBondPotential_LJ2**(*root*, *output_file*)

WebFF.**XMLtoFrcNonBondPotential_LJ96**(*root*, *output_file*)

WebFF.**XMLtoFrcNonBondPotential_Mie**(*root*, *output_file*)

WebFF.**XMLtoFrcNonBondPotential_Soft**(*root*, *output_file*)

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WebFF.**XMLtoParamsBondPotential_FENE**(*root*, *output_file*)

WebFF.**XMLtoParamsCrossPotential_AngleAngle**(*root*, *output_file*)

WebFF.**XMLtoParamsCrossPotential_AngleAngleTorsion**(*root*, *output_file*)

WebFF.**XMLtoParamsCrossPotential_AngleTorsion**(*root*, *output_file*)

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WebFF.**XMLtoParamsCrossPotential_BondBond**(*root*, *output_file*)

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WebFF.**XMLtoParamsCrossPotential_MiddleBondTorsion**(*root*, *output_file*)

WebFF.**XMLtoParamsNonBondPotential_Weeks_Chandler_Anderson**(*root*, *output_file*)

CHAPTER 6

Importing Data

6.1 WebFF Account

6.2 Self Data Entry

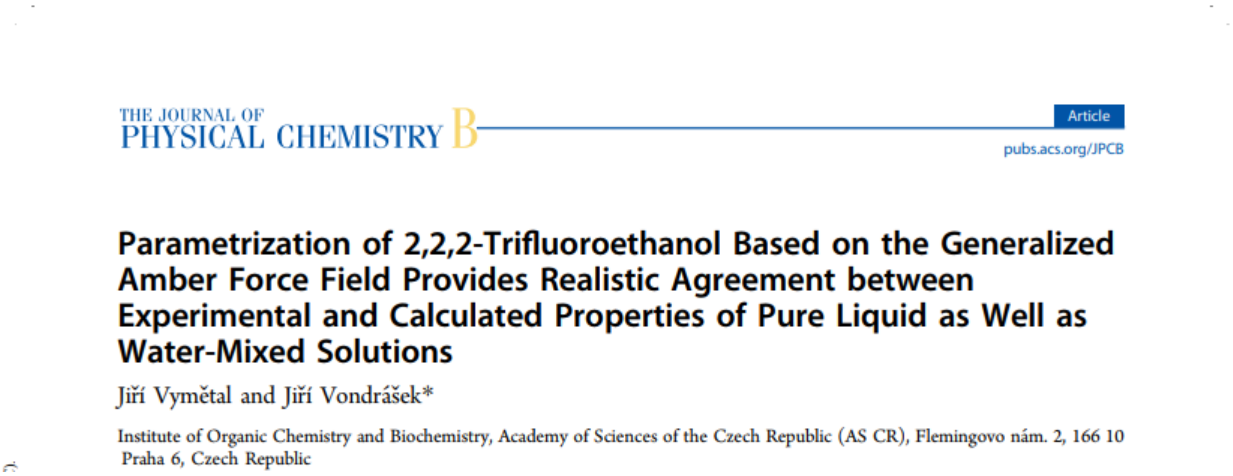
6.3 NIST Data Entry

CHAPTER 7

Tutorial

7.1 Data Curation for Atomistic Force-Field Data

TFE Force-Field Data Source



THE JOURNAL OF PHYSICAL CHEMISTRY B

Article

pubs.acs.org/JPCB

Parametrization of 2,2,2-Trifluoroethanol Based on the Generalized Amber Force Field Provides Realistic Agreement between Experimental and Calculated Properties of Pure Liquid as Well as Water-Mixed Solutions

Jiří Vymětal and Jiří Vondrášek*

Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic (AS CR), Flemingovo nám. 2, 166 10 Praha 6, Czech Republic

Metadata

Atom Types and Attributes

Force-Field Metadata

Instructions	
Schema Version	1.0.0
Force-Field Protocol	Atomistic - Class I
Name	TFE
Description	
Units	Mixed-Metric
Data Source	Jiří Vymětal and Jiří Vondrášek, "Parametrization of 2,2,2-Trifluoroethanol Based on the Generalized Amber Force Field Provides Realistic Agreement between Experimental and Calculated Properties of Pure Liquid as Well as Water-Mixed
» DOI	10.1021/jp505861b
» URL	https://pubs.acs.org/doi/10.1021/jp505861b
» NOTES	
Data Contact (Name)	Jiří Vondrášek
» Affiliation	Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Re
» email	jiri.vondrasek@uochb.cas.cz

Atom-Types

Nomenclature	**DFF**	# Preset			
comment		# Enter data			
AtomType-Name	**Substructure**	*Description*	*Element*	*AtomicNumber*	*AtomicMass*
HC	H[&C]			1	1.0079
HO	H[&O]			1	1.0079
C1	C[&F][&F][&F]			6	12.011
C2	C[&O][&H][&H]			6	12.011
OH	O[&H]			8	15.9994
F	F[&C]			9	18.9984

Atom-Attributes-DFF

Instructions

AtomType-Name	Index	*Coordination*	*Ringsize*	*Aromatic*	*FormalCharge*	*ElementsAllowed*	*ElementsDisallowed*
OH	1	2					
OH	2						
HC	1	1					
HC	2	4					
HO	1	1					
HO	2	4					

Bond Increments

Instructions

AT-I	AT-J	Delta-IJ	Delta-JI	*comment*	*version*	*reference*
F	C1	-0.3218				
HO	OH	0.495				
HC	C2	0.0841				
C1	C2	-0.0589				
OH	C2	-0.1569				

Potentials

Bond Potential

style	**Harmonic**	# Preset
formula	**K*(R-R0)^2**	# Preset
K-units	**kcal/mol/Å^2**	# Choose
R0-units	**Å**	# Choose

AT-1	AT-2	K	R0	*comment*	*version*	*reference*
C1	F	632.3805567	1.344			
C1	C2	526.8674699	1.535			
C2	OH	545.9887827	1.426			
C2	HC	583.8824263	1.093			
OH	HO	642.4615704	0.974			

7.1.1 References

1. Jiří Vymětal and Jiří Vondrášek, “Parametrization of 2,2,2-Trifluoroethanol Based on the Generalized Amber Force Field Provides Realistic Agreement between Experimental and Calculated Properties of Pure Liquid as Well as Water-Mixed Solutions”, J. Phys. Chem. B, 118 (35), pp 10390–10404, (2014).

Angle Potential

style	**Harmonic**	# Preset
formula	**Ka*(Theta-Theta0)^2**	# Preset
Ka-units	**kcal/mol/degrees^2**	# Choose
Theta0-units	**degrees**	# Preset

AT-1	AT-2	AT-3	Ka	Theta0	*precedence*	*comment*	*version*	*reference*
C1	C2	OH	67.7	109.43				
F	C1	F	71.3	107.16				
F	C1	C2	66.2	109.41				
C1	C2	HC	46.4	110.07				
C2	OH	HO	47.1	108.16				
HC	C2	HC	39.2	109.55				
HC	C2	OH	51	109.88				

Dihedral Potential

style	**Fourier**	# Preset
formula	**K1*[1-cos(N1*Phi-D1)]+K2*[1-cos(N2*Phi-D2)]+K3*[1-cos(N3*Phi-D3)]+K4*[1-cos(N4*Phi-D4)]+K5*[1-cos(N5*Phi-D5)]**	# Preset
convention	**cis:right**	# Choose
Kd-units	**kcal**	# Choose
Dd-units	**degrees**	# Preset

AT-1	*AT-2*	*AT-3*	*AT-4*	*K1*	*N1*	*D1*	*K2*	*N2*	*D2*	*K3*	*N3*
F	C1	C2	OH	0.077796367	3	0					
C1	C2	OH	HO	0.214627151	1	0	0.079947419	3	0		
F	C1	C2	HC	0.09500478	1	0	0.077796367	3	0		
HC	C2	OH	HO	0.083293499	3	0					

Non-Bond Potential

style	**Lennard-Jones (12-6)**	# Preset
formula	**4*epsilon*[(sigma/R)^12-(sigma/R)^6]**	# Preset
epsilon-units	**kcal/mol**	# Choose
sigma-units	**Å**	# Choose
Combining-Rule	**Lorentz-Berthelot**	# Choose

AtomType	epsilon	sigma	*comment*	*version*	*reference*
HC	2.774	0.0157			
HO	0.00001	0.00001			
C1	3.816	0.1094			
C2	3.816	0.1094			
OH	3.442	0.2104			
F	3.62753	0.00819			

7.2 Data Curation for Coarse-Grained Force-Field Data

7.2.1 The Martini Coarse-Grained Force-Field

In this tutorial, we show step by step how to curate data for the Martini Coarse-Grained Force-Field into WebFF using the WebFF Excel data template and the WebFF.py Python library.

Martini Force-Field Data Source

7812 J. Phys. Chem. B 2007, 111, 7812−7824

The MARTINI Force Field: Coarse Grained Model for Biomolecular Simulations

Siewert J. Marrink,*,† H. Jelger Risselada,† Serge Yefimov,‡ D. Peter Tieleman,§ and Alex H. de Vries†

Groningen Biomolecular Sciences and Biotechnology Institute & Zernike Institute for Advanced Materials, Department of Biophysical Chemistry, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands, Zernike Institute for Advanced Materials, Department of Applied Physics, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands, and Department of Biological Sciences, University of Calgary, 2500 University Drive NW, Calgary AB T2N 1N4, Canada

Received: February 8, 2007; In Final Form: April 25, 2007

```
; MARTINI FORCEFIELD V2.2
;
; SJ MARRINK (last modified: 04-12-2012 by DdJ)
;
; NOTE 1: Bead definitinions in this file have not been changed with respect to
;         martini_v2.1.itp. This file is purely here for clarity sake. Differences
;         between V2.1 and V2.2 are created by the martinize script and can be found
;         in martini_v2.2_aminoacids.itp.
;
```

WebFF Excel Spreadsheet Data Entry

The data for the Martini force-field was ported to the Excel spreadsheet called: WebFF-DocumentationXMLCoarse-GrainedWebFF-CoarseGrained-DataTemplate.xlsx

Metadata

There are three sections of Metadata to include

Atom Types

The atom types for Martini are general in nature, and each entry can stand for a number of similar but related chemical moeities.

Force-Field Metadata

Instructions	

Schema Version	1.0.0
Force-Field Protocol	Coarse-Grained
Name	Martini v2.2
Description	
Units	Mixed-Metric
Data Source	Siewert J. Marrink, H. Jelger Risselada, Serge Yefimov, D. Peter Tieleman, and Alex H. de Vries, "The MARTINI Force Field: Coarse Grained Model for Biomolecular Simulations," J. Phys. Chem. B, 111 (27), pp 7812–7824, (2007).
» DOI	10.1021/jp071097f
» URL	https://pubs.acs.org/doi/abs/10.1021/jp071097f
» NOTES	
Data Contact (Name)	Siewert J. Marrink
» Affiliation	University of Groningen
» email	s.j.marrink@rug.nl

Keywords

Instructions	

Keywords	*Additional-Keywords*
Biomolecular compounds	Coarse-Grained
- Amino acids	
- Lipids	
- Peptides	
- Proteins	

Additional References

Instructions			
Reference	*DOI*	*URL*	*Notes*
Siewert J. Marrink, Alex H. de Vries, and Alan E. Mark, "The MARTINI Force Field: Coarse Grained Model for Biomolecular Simulations", J. Phys. Chem. B, 108 (2), pp 750-760, (2004).	10.1021/jp036508g	https://pubs.acs.org/doi/abs/10.1021/jp036508g	
Siewart J. Marrink, Alex H. de Vries and Alan E. Mark, "Coarse Grained Model for Semiquantitative Lipid Simulations", J. Phys. Chem. B, 108(2), pp 750-760, (2004).	10.1021/jp036508g	https://pubs.acs.org/doi/10.1021/jp036508g	
L. Monticelli, S. Kandasamy, X. Periole, R. Larson, D.P. Tieleman and S.J. Marrink, "The MARTINI coarse grained force field: extension to proteins.", J. Chem. Th. Comp., 4(5), pp 819-834, (2008).	10.1021/ct700324x	https://pubs.acs.org/doi/10.1021/ct700324x	
Djurre H. de Jong, Gurpreet Singh, W. F. Drew Bennett, Clement Arnarez, Tsjerk A. Wassenaar, Lars V. Schäfer, Xavier Periole, D. Peter Tieleman, and Siewert J. Marrink, "Improved Parameters for the Martini Coarse-Grained Protein Force Field,"	10.1021/ct300646g	https://pubs.acs.org/doi/10.1021/ct300646g	
Martini Coarse Grain Forcefield for Biomolecules		http://www.cgmartini.nl/	
Wikipedia: MARTINI		https://en.wikipedia.org/wiki/MARTINI	
MARTINI FORCEFIELD V2.2		http://www.cgmartini.nl/images/paramete	

Atom-Types

Nomenclature	**?**	# CG Chemistry Nomenclature		
comment	**Version 2.2**	# Enter data		
CG-Name	*CG-Chemistry*	*Description*	*AtomicMass-CG*	*AtomicSize-CG*
P5		Polar	72.0	
P4		Polar	72.0	
P3		Polar	72.0	
P2		Polar	72.0	
P1		Polar	72.0	
Nda		Intermediate Polar	72.0	
Nd		Intermediate Polar	72.0	
Na		Intermediate Polar	72.0	
N0		Intermediate Polar	72.0	

Potentials

Bond Potential

style	**Harmonic**	# Preset
formula	**K*(R-R0)^2**	# Preset
K-units	**kJ/mol/nm^2**	# Choose
R0-units	**nm**	# Choose

AT-1	AT-2	K	R0	*comment*	*version*	*reference*
X	X	625.0	0.47		2.0	

Angle Potential

style	**cosine/squared**	# Preset
formula	**(1/2)*Ka*[cos(Theta)-cos(Theta0)]^2**	# Preset
Ka-units	**kJ/mol**	# Choose
Theta0-units	**degrees**	# Preset

AT-1	AT-2	AT-3	Ka	Theta0	*precedence*	*comment*	*version*	*reference*
X	X	X	25	180		Aliphatic chains		
X	X	X	45	120		Cis double bonds		
X	X	X	45	180		Trans-unsaturated bonds		

Non-Bond Potential

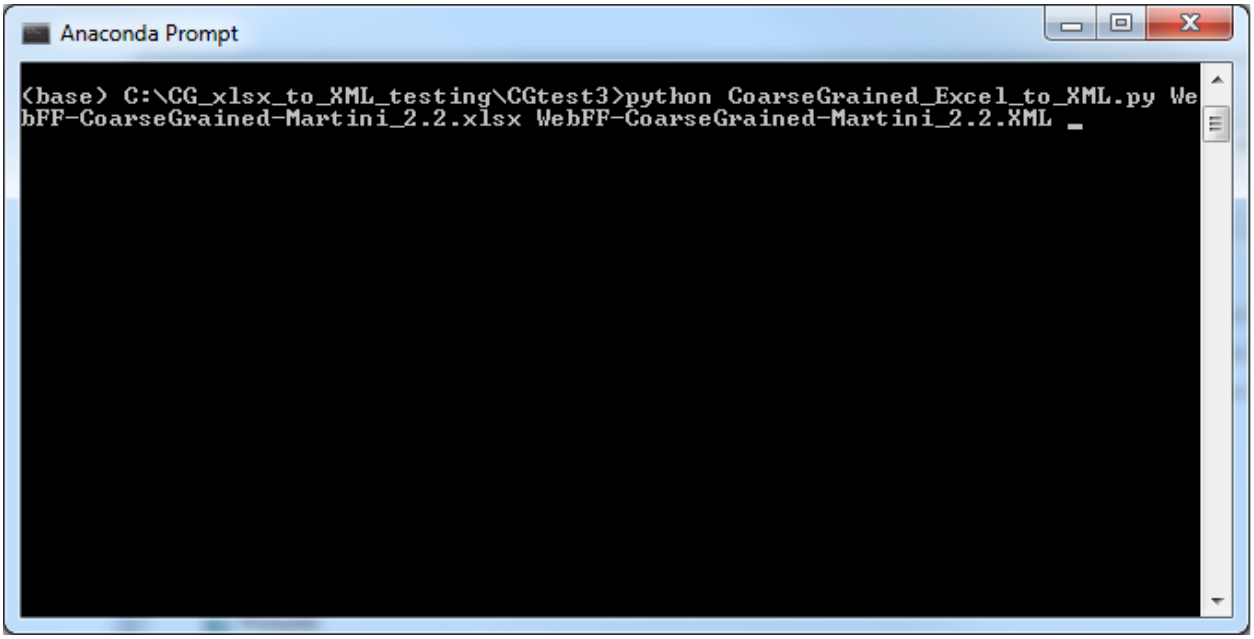
style	**Lennard-Jones (12-6)**	# Preset
formula	**A/(R^12)-B/(R^6)**	# Preset
A-units	**kJ*nm^12/mol**	# Choose
B-units	**kJ*nm^6/mol**	# Choose

AT-1	AT-2	A	B	*comment*	*version*	*reference*
P5	P5	0.0026027	0.24145		2.2	
SP5	SP5	0.00067132	0.1062		2.2	
P4	P4	0.0023238	0.21558		2.2	
BP4	BP4	0.0023238	0.21558		2.2	

Excel to XML Conversion

7.2.2 References

1. Siewert J. Marrink, H. Jelger Risselada, Serge Yefimov, D. Peter Tieleman, and Alex H. de Vries, "The MARTINI Force Field: Coarse Grained Model for Biomolecular Simulations," J. Phys. Chem. B, 111 (27), pp 7812–7824, (2007).
2. Martini v2.2 Force-Field Parameters, http://www.cgmartini.nl/images/parameters/ITP/martini_v2.2.itp



7.3 Data Curation for Water Model Force-Field Data

7.3.1 Water Models

Metadata

Comparison of simple potential functions for simulating liquid water

William L. Jorgensen, Jayaraman Chandrasekhar, and Jeffry D. Madura

Department of Chemistry, Purdue University, West Lafayette, Indiana 47907

Roger W. Impey and Michael L. Klein

Chemistry Division, National Research Council of Canada, Ottawa, Canada K1A OR6

(Received 14 March 1983; accepted 5 April 1983)

3-site

7.3.2 References

1. William L. Jorgensen, Jayaraman Chandrasekhar, Jeffry D. Madura, Roger W. Impey and Michael L. Klein, "Comparison of simple potential functions for simulating liquid water", J. Chem. Phys., 79 (2), pp. 926–935, (1983).

Force-Field Metadata

Instructions	

Schema Version	1.0.0
Force-Field Protocol	Atomistic - Water Model
Name	TIP3P
Description	
Units	Mixed-Metric
Data Source	William L. Jorgensen, Jayaraman Chandrasekhar, Jeffry D. Madura, Roger W. Impey and Michael L. Klein, "Comparison of simple potential functions for simulating liquid water", *J. Chem. Phys.*, 79 (2), pp. 926–935, (1983).
» DOI	10.1063/1.445869
» URL	https://aip.scitation.org/doi/10.1063/1.445869
» NOTES	
Data Contact (Name)	Jorgensen, William L
» Affiliation	Department of Chemistry, Purdue University, West Lafayette, Indiana 47907
» email	william.jorgensen@yale.edu

Keywords

Instructions	

Keywords	*Additional-Keywords*
Water	Rigid Water Model

Water Model

name	**TIP3P**	#Input
formula	**E=E_q+E_LJ**	#Choose
version		#Input
comment		#Input
R-OH-units	**Å**	#Preset
Theta_HOH-units	**degrees**	#Preset
A-units	**x10^-3 (kcal*Å^12**	#Preset
B-units	**(kcal*Å^6)/mol**	#Preset
sigma-units	**Å**	#Choose
epsilon-units	**kJ/mol**	#Choose

R_OH	Theta_HOH	A	B	q_O	q_H	*EnergyDispersion*	*sigma*	*epsilon*
0.9572	104.52	582	595	-0.834	0.417		3.15066	0.63627

CHAPTER 8

Publications

This page will attempt to keep an up-to-date listing of the papers which either use WebFF or used data from WebFF.

8.1 WebFF References

1. Frederick R. Phelan Jr., Kathleen Mullin, Pablo Garcia Beltran, Gule Teri, Priyanshu Mishra and Huai Sun, "The Web Force-Field (WebFF) Project: Ontology Based Force-Field Repository for Soft Materials at Multiple Levels of Granularity," in preparation (2018).

8.2 WebFF Data Publications

Coming Soon

CHAPTER 9

Contacts

- **WebFF Help** Email
- **Dr. Frederick R. Phelan Jr., NIST** NIST Home Page, GitHub
- **Prof. Huai Sun, Shanghai Jiao Tong University** Group Home Page, Department Home Page

CHAPTER 10

Legal

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CHAPTER 11

Metadata

11.1 Force-Field Protocol

11.2 Force-Field Name

11.3 Description

11.4 Data-Source

11.5 Keywords

11.6 Additional Keywords

11.7 WebFF-Scribe

11.8 Additional References

11.9 Attachments

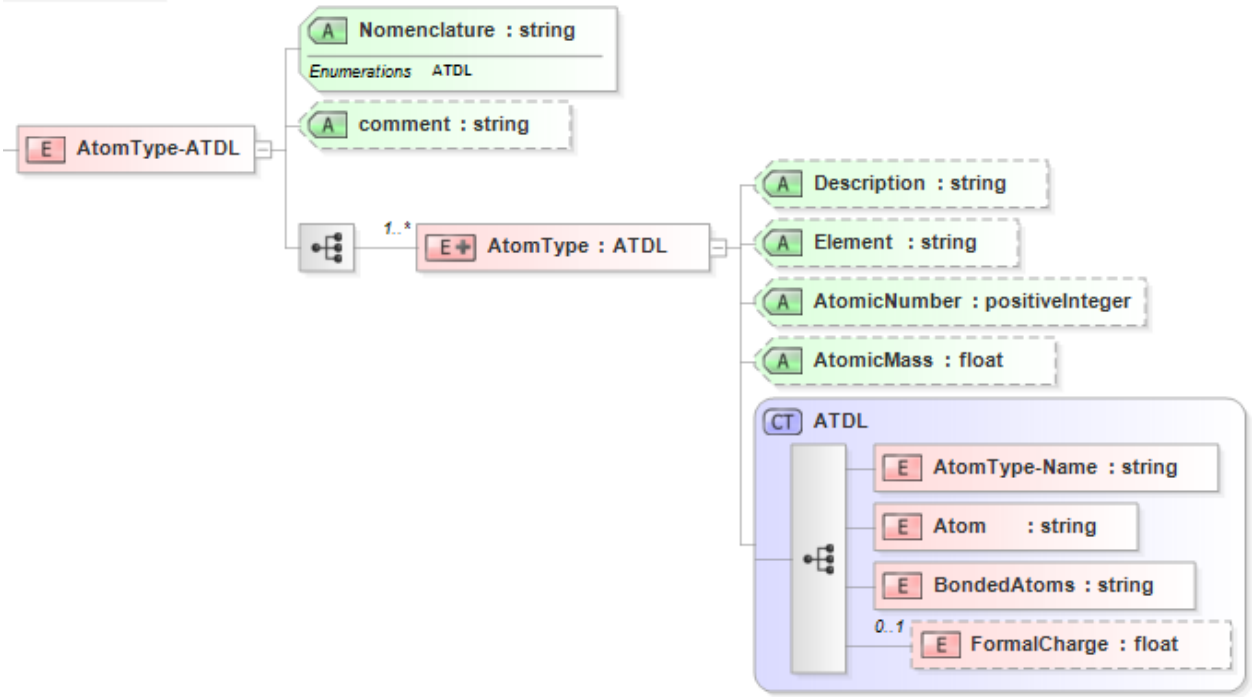
CHAPTER 12

Atom Types

12.1 Atom Type - ATDL

12.1.1 XML Schema

The XML schema for the **Atom Type - ATDL** has the following representation (design mode representation using Liquid XML Studio):



The general attributes (describing the entire set of atoms) are given by:

General Attributes	Cardinality	Value/Definition
Nomenclature	Fixed	ATDL
comment	Optional	Comment attached to set of atoms

The specific attributes (attached to each atom description) are given by:

Specific Attributes	Cardinality	Value/Definition
Description	Required	Description of the atom
Element	Required	Corresponding element of the atom
AtomicNumber	Required	Corresponding atomic number of the atom
AtomicMass	Required	Corresponding atomic mass of the atom

The specific elements (contained within each instance of the atom template) are given by:

Specific Elements	Cardinality	Value/Definition
AtomType-Name	Required	Atom type name
Atom	Required	Atom
BondedAtoms	Required	Bonded atoms
FormalCharge	Optional	Formal charge of the atom

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

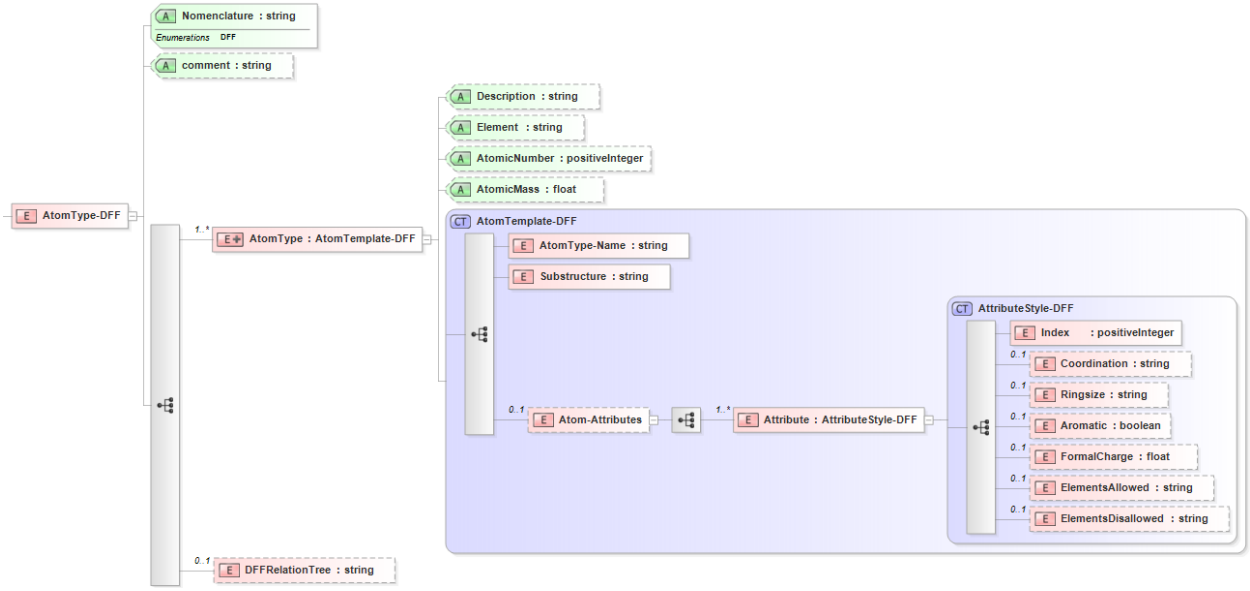
12.1.2 References

1. Atom-type description language.
2. Liquid XML Studio.

12.2 Atom Type - DFF

12.2.1 XML Schema

The XML schema for the **Atom Type - DFF** has the following representation (design mode representation using Liquid XML Studio):



The general attributes (describing the entire set of atoms) are given by:

General Attributes	Cardinality	Value/Definition
Nomenclature	Fixed	DFF
comment	Optional	Comment attached to set of atoms

The general elements (describing the entire set of atoms) are given by:

General Attributes	Cardinality	Value/Definition
DFFRelationTree	Optional	Multiline DFF relation tree

The specific attributes (attached to each atom description) are given by:

Specific Attributes	Cardinality	Value/Definition
Description	Required	Description of the atom
Element	Required	Corresponding element of the atom
AtomicNumber	Required	Corresponding atomic number of the atom
AtomicMass	Required	Corresponding atomic mass of the atom

The specific elements (contained within each instance of the atom template) are given by:

Specific Elements	Cardinality	Value/Definition
AtomType-Name	Required	Atom type name
Substructure	Required	Atom
Index	Required	Index of atom entry
Coordination	Optional	Coordination of the atom
Ringsize	Optional	Ringsize of the atom
Aromatic	Optional	Aromatic (true/false)
FormalCharge	Optional	Formal charge of the atom
ElementsAllowed	Optional	Elements allowed in the atom
ElementsDisallowed	Optional	Elements disallowed in the atom

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

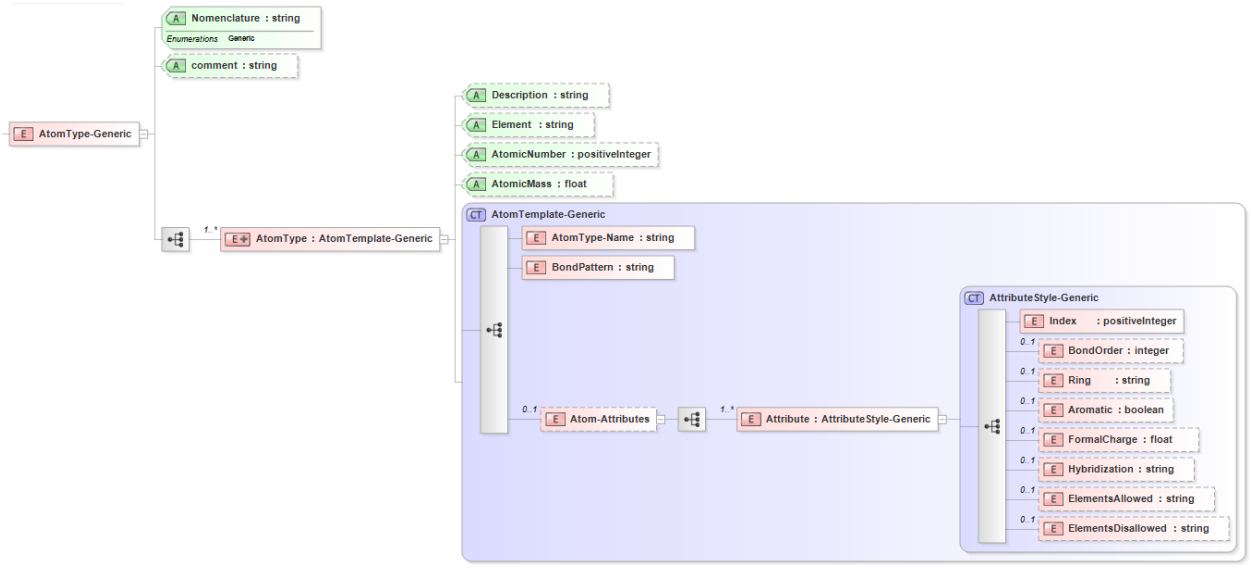
12.2.2 References

1. DFF User Manual.
2. Liquid XML Studio.

12.3 Atom Type - Generic

12.3.1 XML Schema

The XML schema for the **Atom Type - Generic** has the following representation (design mode representation using Liquid XML Studio):



The general attributes (describing the entire set of atoms) are given by:

General Attributes	Cardinality	Value/Definition
Nomenclature	Fixed	Generic
comment	Optional	Comment attached to set of atoms

The specific attributes (attached to each atom description) are given by:

Specific Attributes	Cardinality	Value/Definition
Description	Required	Description of the atom
Element	Required	Corresponding element of the atom
AtomicNumber	Required	Corresponding atomic number of the atom
AtomicMass	Required	Corresponding atomic mass of the atom

The specific elements (contained within each instance of the atom template) are given by:

Specific Elements	Cardinality	Value/Definition
AtomType-Name	Required	Atom type name
BondPattern	Required	Atom
Index	Required	Index of atom entry
BondOrder	Optional	Coordination of the atom
Ring	Optional	Ringsize of the atom
Aromatic	Optional	Aromatic (true/false)
FormalCharge	Optional	Formal charge of the atom
Hybridization	Optional	Hybridization of the atom
ElementsAllowed	Optional	Elements allowed in the atom
ElementsDisallowed	Optional	Elements disallowed in the atom

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

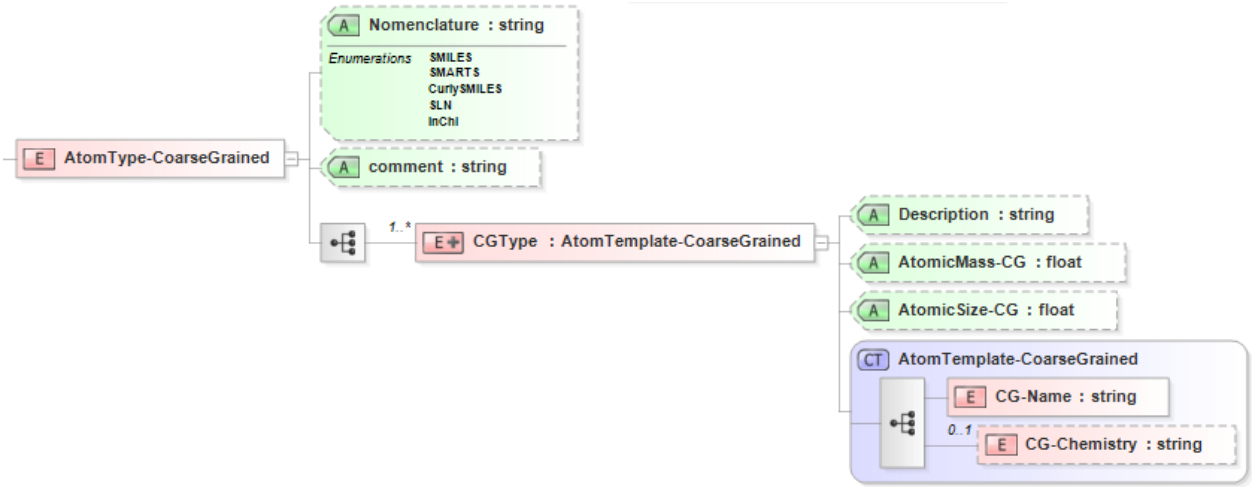
12.3.2 References

1. Liquid XML Studio.

12.4 Atom Type - Coarse Grained

12.4.1 XML Schema

The XML schema for the **Atom Type - Coarse Grained** has the following representation (design mode representation using Liquid XML Studio):



The general attributes (describing the entire set of atoms) are given by:

General Attributes	Cardinality	Value/Definition
Nomenclature	Fixed	SMILES | SMARTS | CurlySMILES | SLN | InChi
comment	Optional	Comment attached to set of atoms

The specific attributes (attached to each atom description) are given by:

Specific Attributes	Cardinality	Value/Definition
Description	Required	Description of the atom
AtomicMass-CG	Required	Corresponding atomic mass of the atom
AtomicMSize-CG	Required	Corresponding atomic size of the atom

The specific elements (contained within each instance of the atom template) are given by:

Specific Elements	Cardinality	Value/Definition
CG-Name	Required	Atom type name
CG_chemistry	Optional	Chemistry of the atom

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

12.4.2 References

1. Liquid XML Studio.

CHAPTER 13

Bond Potentials

13.1 Class2 Bond

13.1.1 Functional Form

The **class 2 bond potential** has the functional form:

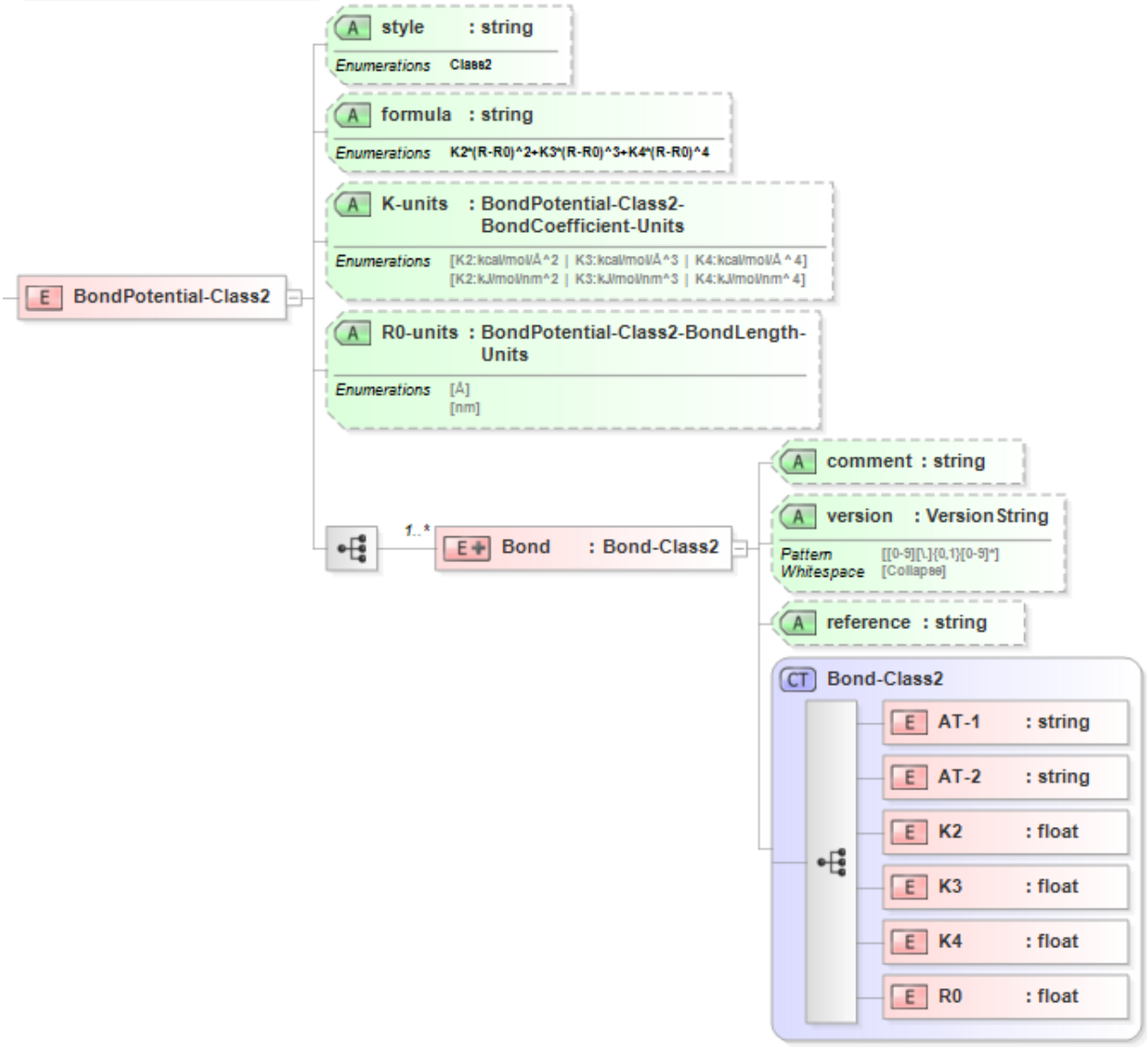
$E = K_{2,ij}(R_{ij} - R_{0,ij})^2 + K_{3,ij}(R_{ij} - R_{0,ij})^3 + K_{4,ij}(R_{ij} - R_{0,ij})^4$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{2,ij}$	Bond coefficient for atoms [i,j] (quadratic term)	energy/length^2
$K_{3,ij}$	Bond coefficient for atoms [i,j] (cubic term)	energy/length^3
$K_{4,ij}$	Bond coefficient for atoms [i,j] (quartic term)	energy/length^4
$R_{0,ij}$	Equilibrium bond length for atoms [i,j]	length

13.1.2 XML Schema

The XML schema for the **class 2 bond potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Bond coefficient for atoms [i,j] (quadratic term)	$K_{2,ij}$	K2
Bond coefficient for atoms [i,j] (cubic term)	$K_{3,ij}$	K3
Bond coefficient for atoms [i,j] (quartic term)	$K_{4,ij}$	K4
Equilibrium bond length for atoms [i,j]	$R_{0,ij}$	R0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Class2
formula	Fixed	K2*(R-R0)^2+K3*(R-R0)^3+K4*(R-R0)^4
K-units	Required	Enumerations specified in schema
R0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

13.1.3 References

1. LAMMPS Class 2 Bond Potential.
2. Liquid XML Studio.

13.2 FENE Bond

13.2.1 Functional Form

The **FENE bond potential** has the functional form:

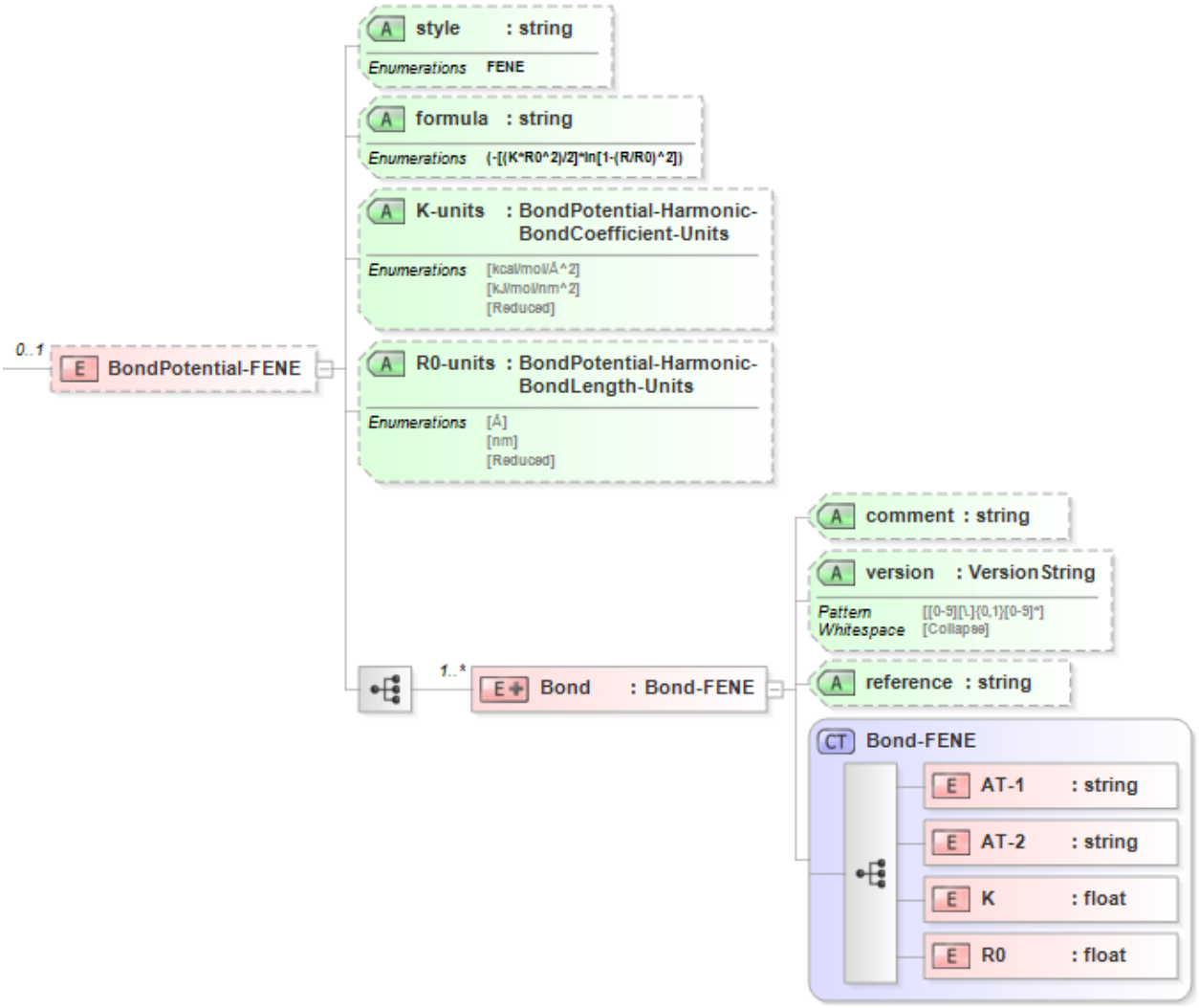
$E = -\frac{1}{2} K_{ij} R_{0,ij}^2 \ln \left[1 - \left(\frac{R_{ij}}{R_{0,ij}} \right)^2 \right]$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
K_{ij}	Bond coefficient for atoms [i,j]	energy/length^2
$R_{0,ij}$	Equilibrium bond length for atoms [i,j]	length

13.2.2 XML Schema

The XML schema for the **FENE bond potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Bond coefficient for atoms [i,j]	K_{ij}	K
Equilibrium bond length for atoms [i,j]	$R_{0,ij}$	R0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	FENE
formula	Fixed	-[(K*R0^2)/2]*ln[1-(R/R0)^2]
K-units	Required	Enumerations specified in schema
R0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

13.2.3 References

1. LAMMPS FENE Bond Potential.
2. GROMACS FENE Bond Potential page 74.
3. Liquid XML Studio.

13.3 Harmonic Bond

13.3.1 Functional Form

The **harmonic bond potential** has the functional form:

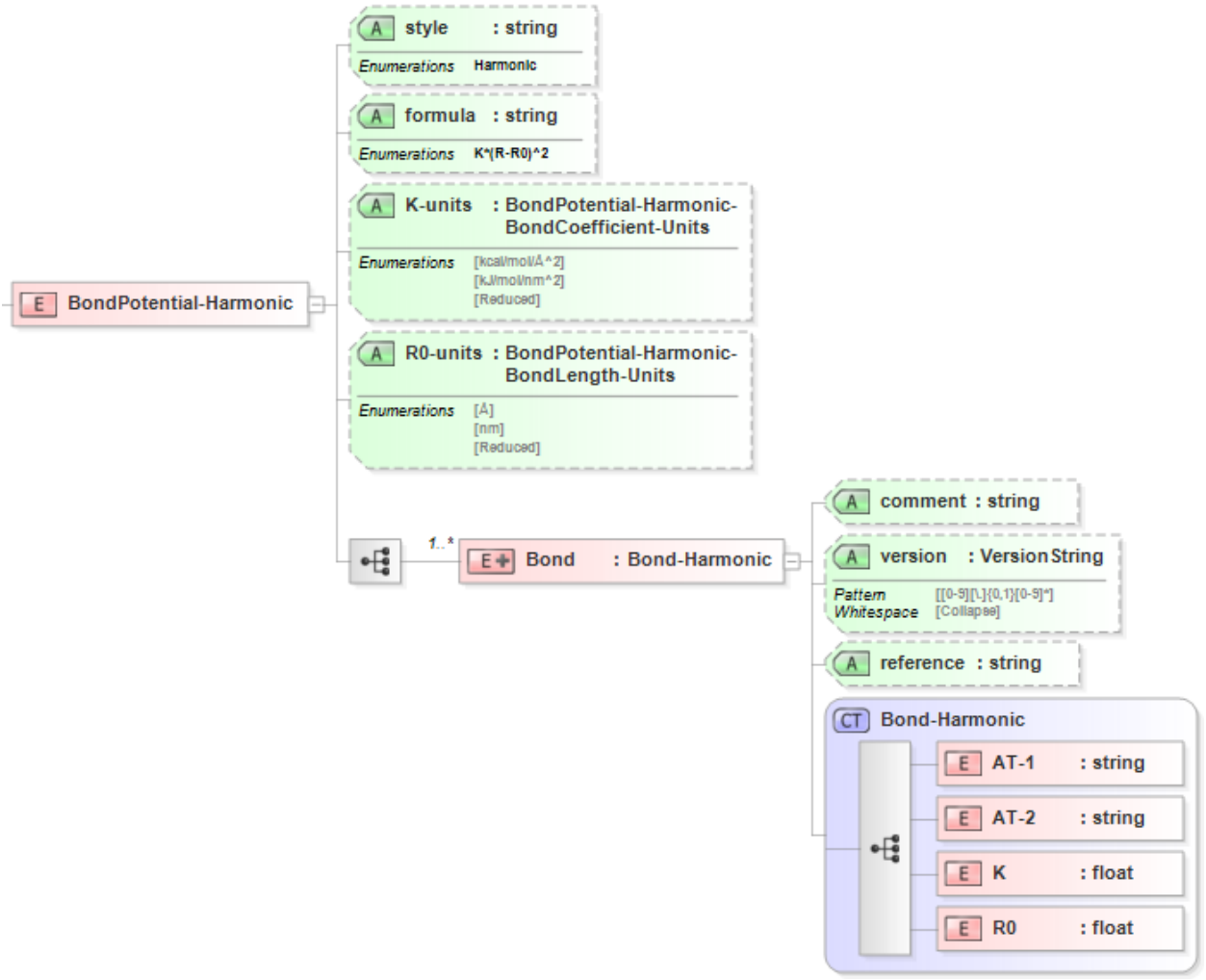
$E = K_{ij} \cdot (R_{ij} - R_{0,ij})^2$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
K_{ij}	Bond coefficient for atoms [i,j]	energy/length^2
$R_{0,ij}$	Equilibrium bond length for atoms [i,j]	length

13.3.2 XML Schema

The XML schema for the **harmonic bond potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Bond coefficient for atoms [i,j]	K_{ij}	K
Equilibrium bond length for atoms [i,j]	$R_{0,ij}$	R0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Harmonic
formula	Fixed	K*(R_R0)^2
K-units	Required	Enumerations specified in schema
R0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

13.3.3 References

1. LAMMPS Harmonic Bond Potential.
2. GROMACS Harmonic Bond Potential page 71.
3. Liquid XML Studio.

13.4 Morse Bond

13.4.1 Functional Form

The **Morse bond potential** has the functional form:

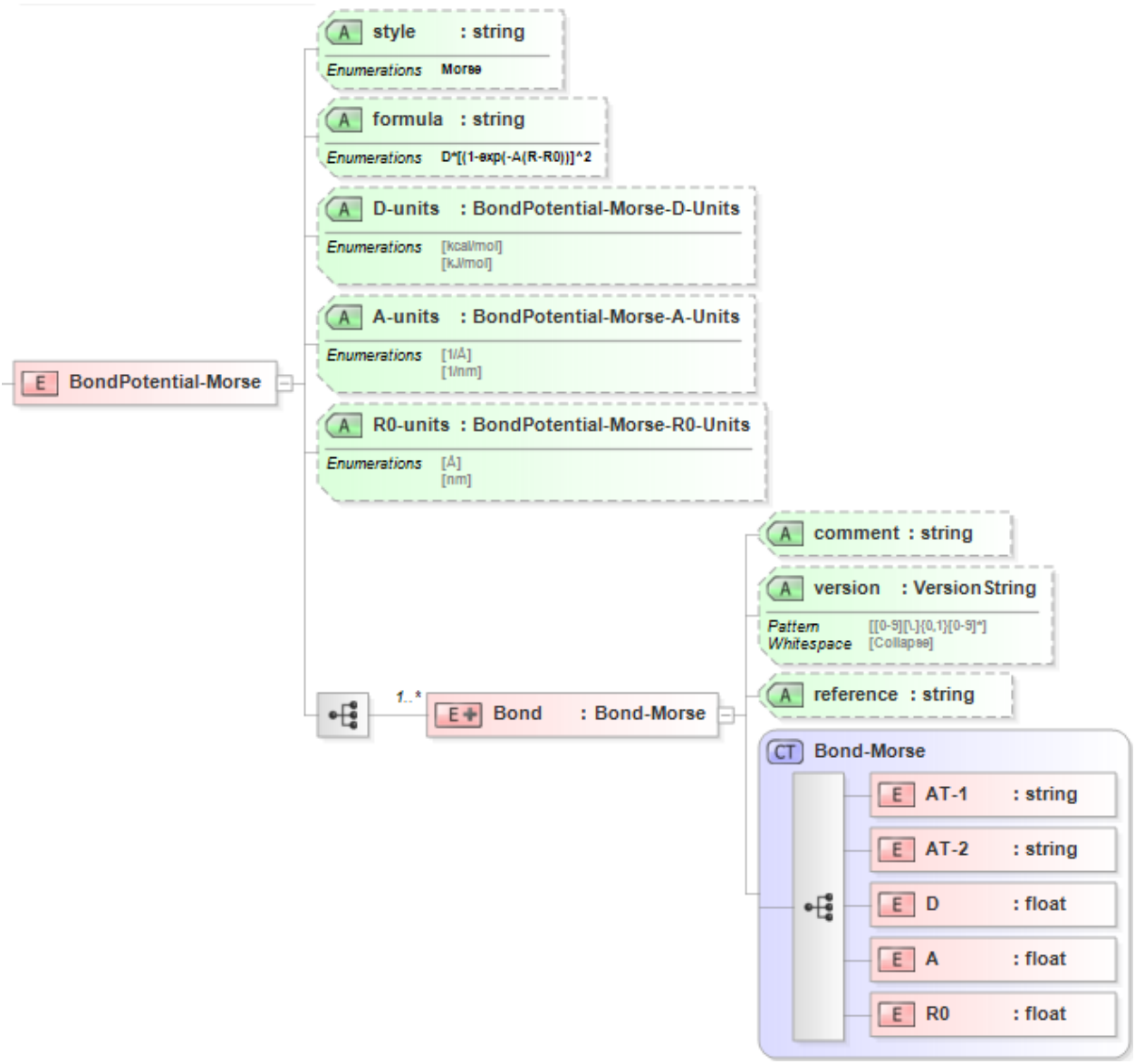
$E = D\left[1 - e^{-\alpha(R_{ij} - R_{0,ij})}\right]^2$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
D	Depth of the potential well	energy
α	Stiffness parameter	inverse length
$R_{0,ij}$	Equilibrium bond length for atoms [i,j]	length

13.4.2 XML Schema

The XML schema for the **Morse bond potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Depth of the potential well	D	D
Stiffness parameter	α	A
Equilibrium bond length for atoms [i,j]	$R_{0,ij}$	R0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Morse
formula	Fixed	D*[(1-exp(-A(R-R0))]^2
D-units	Required	Enumerations specified in schema
A-units	Required	Enumerations specified in schema
R0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

13.4.3 References

1. LAMMPS Morse Bond Potential.
2. GROMACS Morse Bond Potential page 72.
3. Liquid XML Studio.

13.5 Tabular Bond

13.5.1 Tabular Form

The **tabular bond potential** has the parameters:

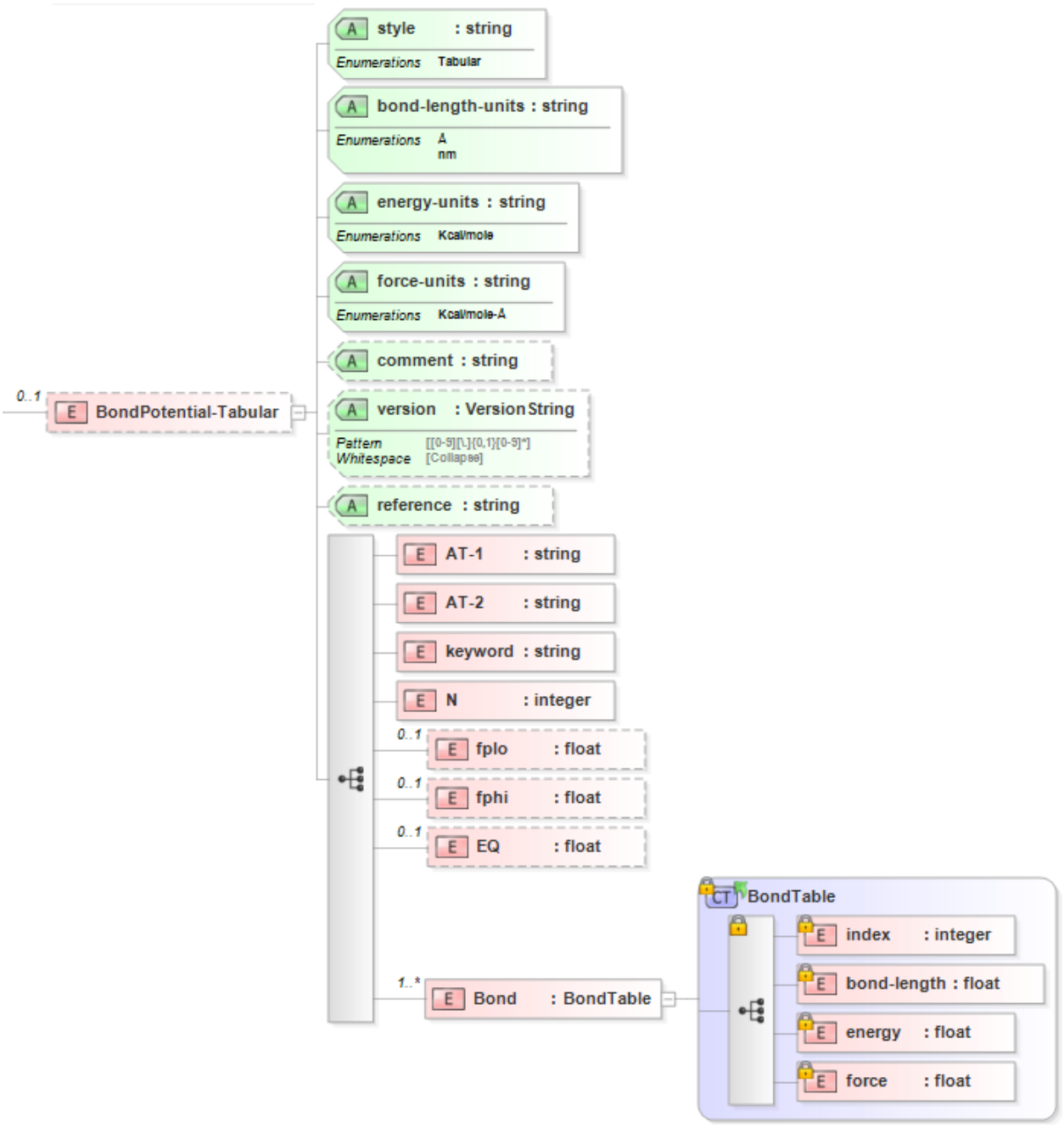
Parameter	Parameter Definition	Units
N	Number of tabulated values	N/A
FP	Derivatives of the force at the innermost (fplo) and outermost (fphi) bond lengths	force/length
EQ	Equilibrium bond length	length

The **tabular bond potential** has the tabulated values:

index	bond-length	energy	force
i_1	bl_1	e_1	f_1
...	...	...	...
i_N	bl_N	e_n	f_N

13.5.2 XML Schema

The XML schema for the **tabular bond potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the parameters/symbols and XML schema notations are given by:

Parameter Definition	Parameter/Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Section identifying keyword	N/A	keyword
Number of tabulated values	N	N
Derivative of the force at the innermost	FP	fplo
Derivative of the force at the outermost	FP	fphi
Equilibrium bond length	EQ	EQ
Index	index	index
Bond length	bond-length	bond-length
Energy	energy	energy
Force	force	force

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Tabular
bond-length-units	Required	Enumerations specified in schema
energy-units	Required	Enumerations specified in schema
force-units	Required	Enumerations specified in schema
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

13.5.3 References

1. LAMMPS Tabular Bond Potential.
2. Liquid XML Studio.

CHAPTER 14

Angle Potentials

14.1 CHARMM Angle

14.1.1 Functional Form

The **CHARMM angle potential** has the functional form:

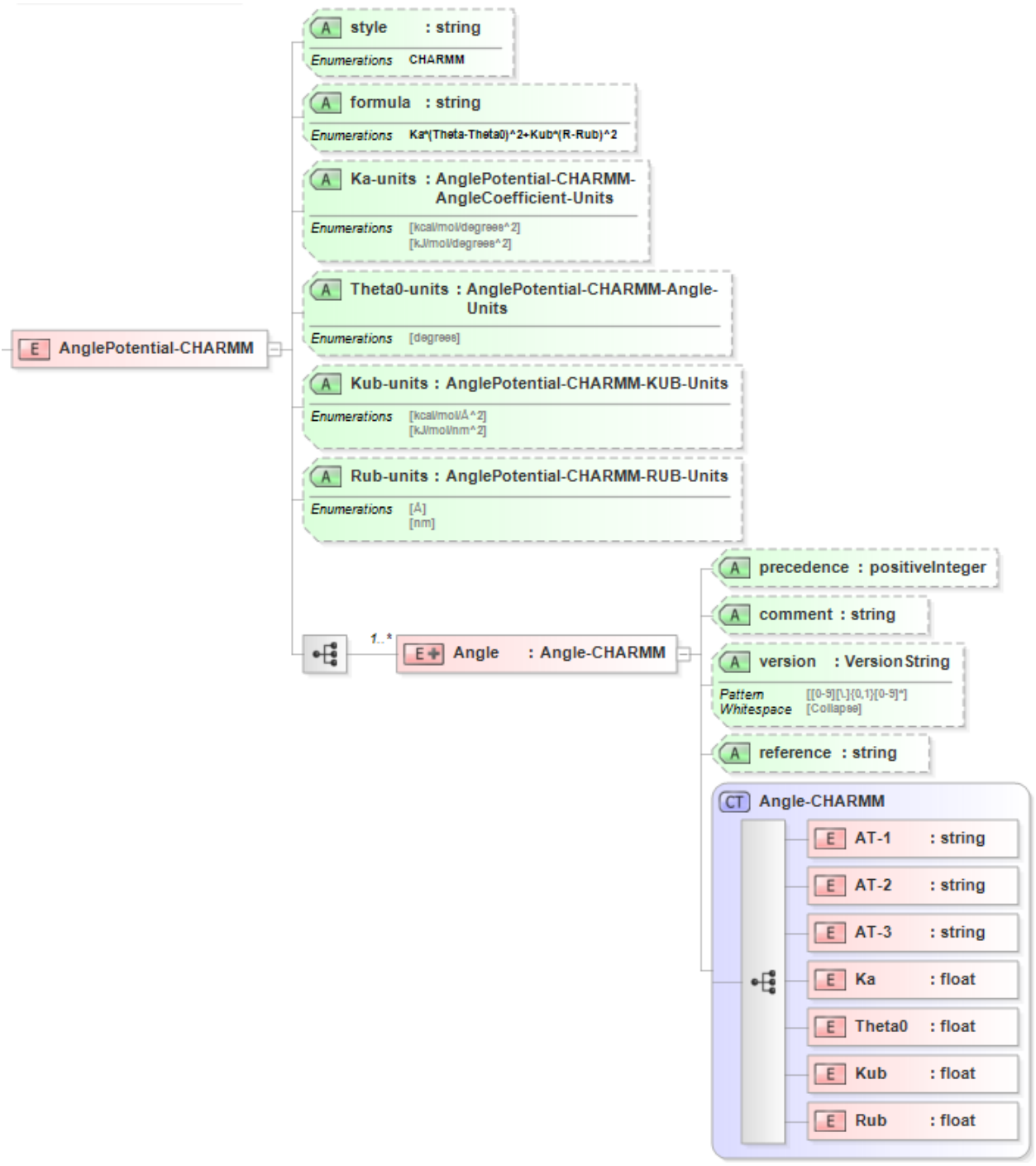
$E = K_{a,ijk}(\theta_{ijk} - \theta_{0,ijk})^2 + K_{ub,ik}(R_{ik} - R_{ub,ik})^2$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{a,ijk}$	Angle coefficient for atoms [i,j,k]	energy/degrees^2
$\theta_{0,ijk}$	Equilibrium angle for atoms [i,j,k]	degrees
$K_{ub,ik}$	Coefficient for Urey-Bradley potential [i,k]	energy/length^2
$R_{ub,ik}$	Equilibrium bond length for Urey-Bradley potential [i,k]	length

14.1.2 XML Schema

The XML schema for the **CHARMM angle potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Angle coefficient for atoms [i,j,k]	$K_{a,ijk}$	Ka
Equilibrium angle for atoms [i,j,k]	$\theta_{0,ijk}$	Theta0
Coefficient for Urey-Bradley potential [i,k]	$K_{ub,ik}$	Kub
Equilibrium bond length for Urey-Bradley potential [i,k]	$R_{ub,ik}$	Rub

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	CHARMM
formula	Fixed	Ka*(Theta-Theta0)^2+Kub*(R-Rub)^2
Ka-units	Required	Enumerations specified in schema
Theta0-units	Required	Enumerations specified in schema
Kub-units	Required	Enumerations specified in schema
Rub-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
precedence	Optional	Precedence of parameter set (where specified)
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

14.1.3 References

1. LAMMPS CHARMM Angle Potential.
2. GROMACS CHARMM (Urey-Bradley) Angle Potential page 76.
3. Liquid XML Studio.

14.2 Class2 Angle

14.2.1 Functional Form

The **class 2 angle potential** has the functional form:

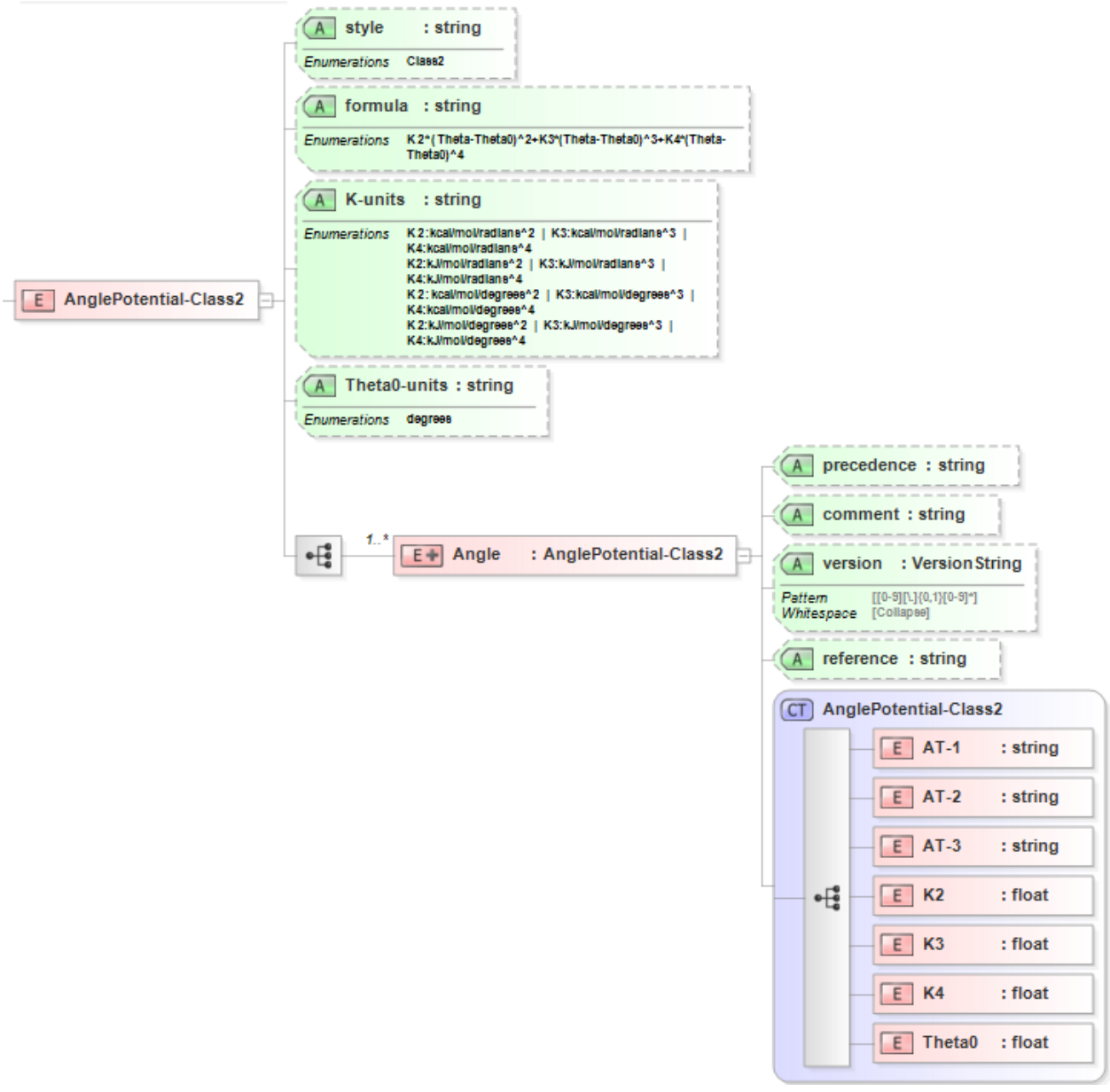
$E = K_{2,ijk}(\theta_{ijk} - \theta_{0,ijk})^2 + K_{3,ijk}(\theta_{ijk} - \theta_{0,ijk})^3 + K_{4,ijk}(\theta_{ijk} - \theta_{0,ijk})^4$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{2,ijk}$	Angle coefficient for atoms [i,j,k] (quadratic term)	energy/degrees^2
$K_{3,ijk}$	Angle coefficient for atoms [i,j,k] (cubic term)	energy/degrees^3
$K_{4,ijk}$	Angle coefficient for atoms [i,j,k] (quartic term)	energy/degrees^4
$\theta_{0,ijk}$	Equilibrium angle for atoms [i,j,k]	degrees

14.2.2 XML Schema

The XML schema for the **class 2 angle potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Angle coefficient for atoms [i,j,k] (quadratic term)	$K_{2,ijk}$	K2
Angle coefficient for atoms [i,j,k] (cubic term)	$K_{3,ijk}$	K3
Angle coefficient for atoms [i,j,k] (quartic term)	$K_{4,ijk}$	K4
Equilibrium angle for atoms [i,j,k]	$\theta_{0,ijk}$	Theta0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Class2
formula	Fixed	K2*(Theta-Theta0)^2+K3*(Theta-Theta0)^3+K4*(Theta-Theta0)^4
K-units	Required	Enumerations specified in schema
Theta0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
precedence	Optional	Precedence of parameter set (where specified)
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

14.2.3 References

1. LAMMPS Class 2 Angle Potential.
2. Liquid XML Studio.

14.3 COS2 Angle

14.3.1 Functional Form

The **COS2 angle potential** has the functional form:

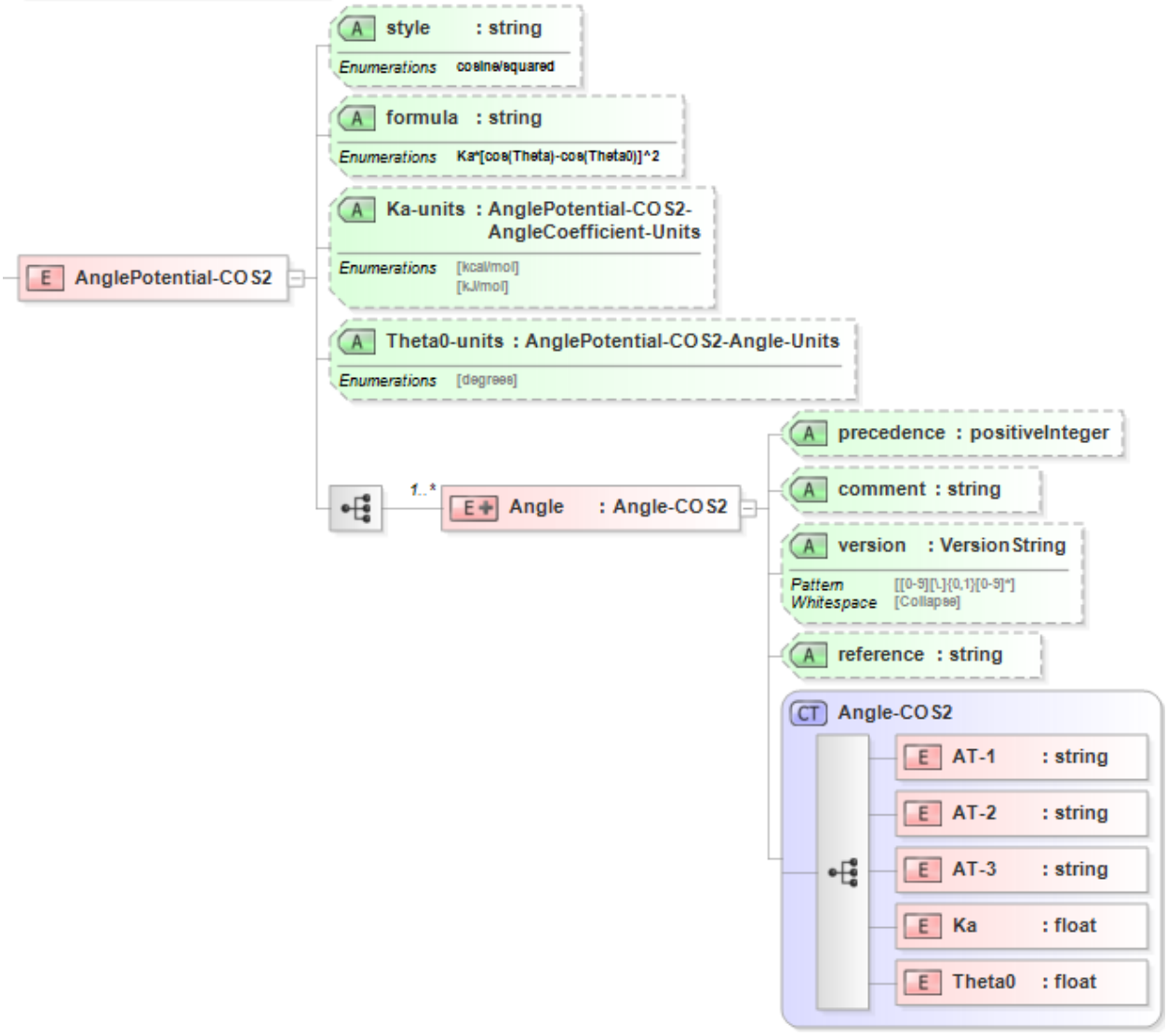
$E = K_{a,ijk}[\cos(\theta_{ijk}) - \cos(\theta_{0,ijk})]^2$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{a,ijk}$	Angle coefficient for atoms [i,j,k]	energy
$\theta_{0,ijk}$	Equilibrium angle for atoms [i,j,k]	degrees

14.3.2 XML Schema

The XML schema for the **COS2 angle potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Angle coefficient for atoms [i,j,k]	$K_{a,ijk}$	Ka
Equilibrium angle for atoms [i,j,k]	$\theta_{0,ijk}$	Theta0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	cosine/squared
formula	Fixed	Ka*[cos(Theta)-cos(Theta0)]^2
Ka-units	Required	Enumerations specified in schema
Theta0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
precedence	Optional	Precedence of parameter set (where specified)
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

14.3.3 References

1. LAMMPS cosine/squared Angle Potential.
2. GROMACS Cosine Based Angle Potential page 96.
3. Liquid XML Studio.

14.4 Cosine Angle

14.4.1 Functional Form

The **cosine angle potential** has the functional form:

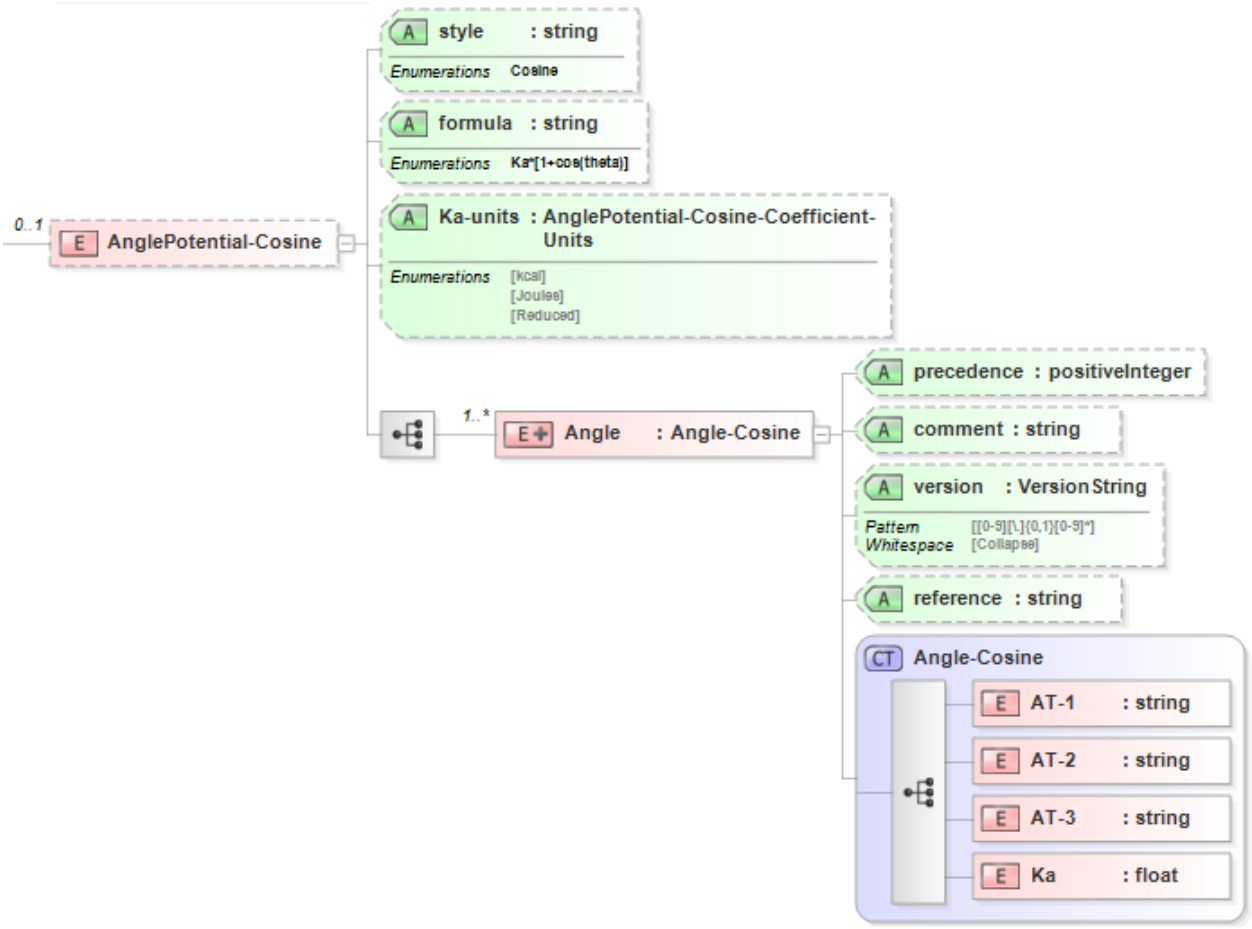
$E = K_{a,ijk} \left[1 + \cos\left(\theta_{ijk}\right)\right]$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{a,ijk}$	Angle coefficient for atoms [i,j,k]	energy

14.4.2 XML Schema

The XML schema for the **cosine angle potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Angle coefficient for atoms [i,j,k]	$K_{a,ijk}$	Ka

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Cosine
formula	Fixed	Ka*[1+cos(theta)]
Ka-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
precedence	Optional	Precedence of parameter set (where specified)
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

14.4.3 References

1. LAMMPS Cosine Angle Potential.
2. Liquid XML Studio.

14.5 Harmonic Angle

14.5.1 Functional Form

The **harmonic angle potential** has the functional form:

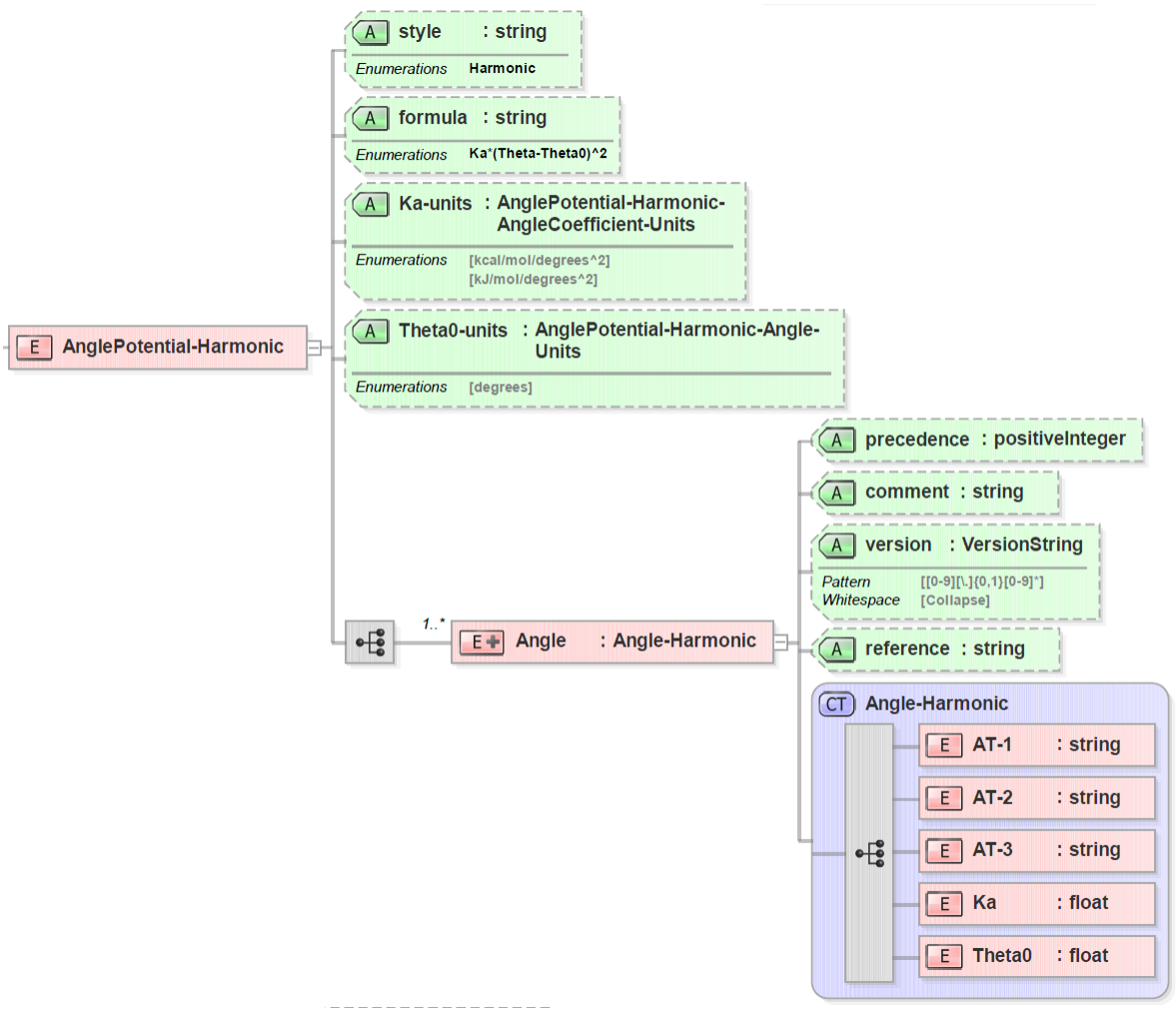
$E = K_{a,ijk} \cdot (\theta_{ijk} - \theta_{0,ijk})^2$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{a,ijk}$	Angle coefficient for atoms [i,j,k]	energy/degrees^2
$\theta_{0,ijk}$	Equilibrium angle for atoms [i,j,k]	degrees

14.5.2 XML Schema

The XML schema for the **harmonic angle potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Angle coefficient for atoms [i,j,k]	$K_{a,ijk}$	Ka
Equilibrium angle for atoms [i,j,k]	$\theta_{0,ijk}$	Theta0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Harmonic
formula	Fixed	Ka*(Theta-Theta0)^2
Ka-units	Required	Enumerations specified in schema
Theta0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
precedence	Optional	Precedence of parameter set (where specified)
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

14.5.3 References

1. LAMMPS Harmonic Angle Potential.
2. GROMACS Harmonic Angle Potential page 74.
3. Liquid XML Studio.

14.6 Tabular Angle

14.6.1 Tabular Form

The **tabular angle potential** has the parameters:

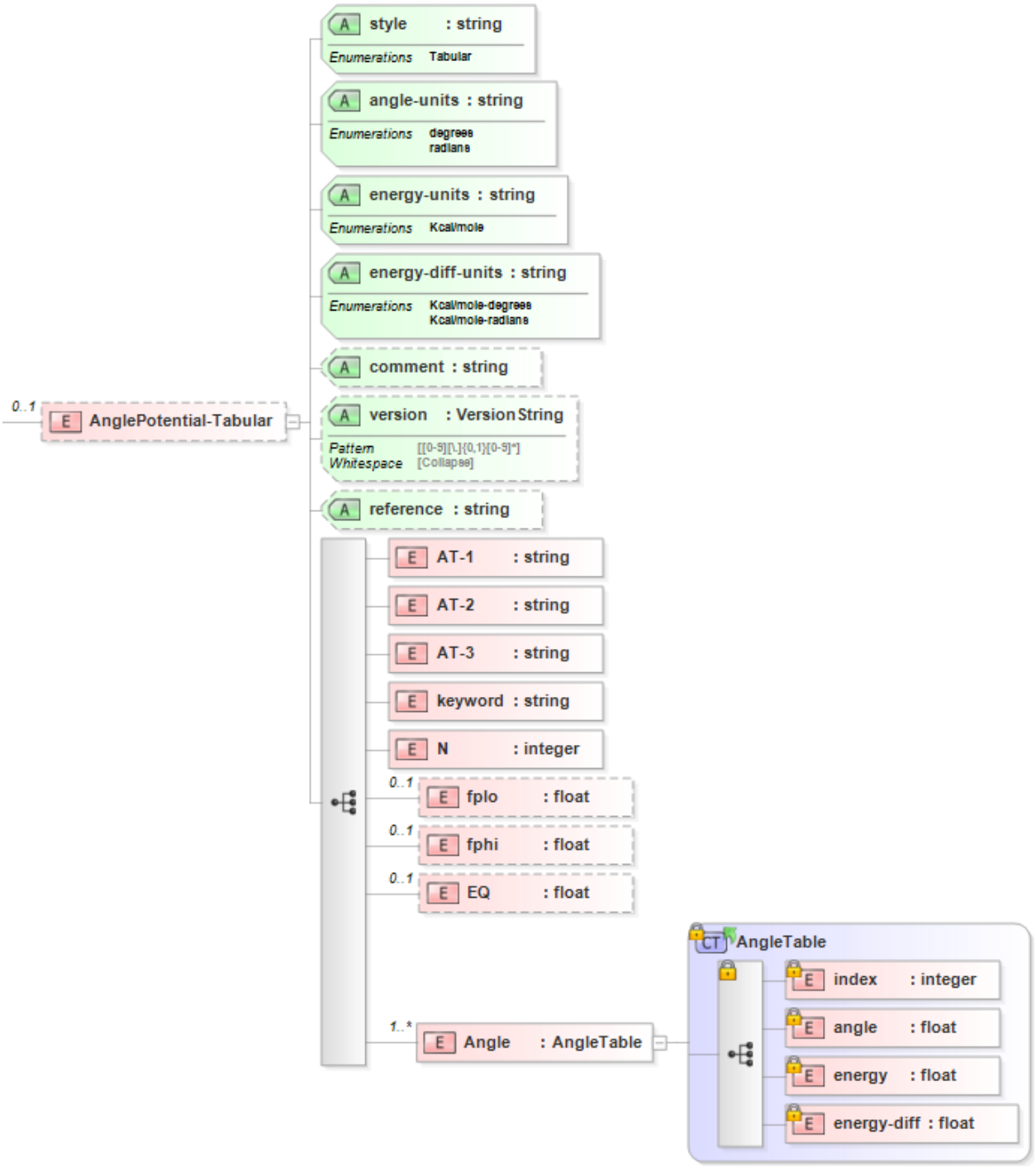
Parameter	Parameter Definition	Units
N	Number of tabulated values	N/A
FP	Derivatives of the force at the innermost (fplo) and outermost (fphi) angles	force/angle
EQ	Equilibrium angle	angle

The **tabular angle potential** has the tabulated values:

index	angle	energy	derivative
i_1	a_1	e_1	de_1
...	...	...	...
i_N	a_N	e_n	de_N

14.6.2 XML Schema

The XML schema for the **tabular angle potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the parameters/symbols and XML schema notations are given by:

Parameter Definition	Parameter/Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Section identifying keyword	N/A	keyword
Number of tabulated values	N	N
Derivative of the force at the innermost	FP	fplo
Derivative of the force at the outermost	FP	fphi
Equilibrium angle	EQ	EQ
Index	index	index
Angle	angle	angle
Energy	energy	energy
Derivate of energy	derivative	energy-diff

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Tabular
angle-units	Required	Enumerations specified in schema
energy-units	Required	Enumerations specified in schema
energy-diff-units	Required	Enumerations specified in schema
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

14.6.3 References

1. LAMMPS Tabular Angle Potential.
2. Liquid XML Studio.

CHAPTER 15

Dihedral Potentials

15.1 CHARMM Dihedral

15.1.1 Functional Form

The **CHARMM dihedral potential** has the functional form:

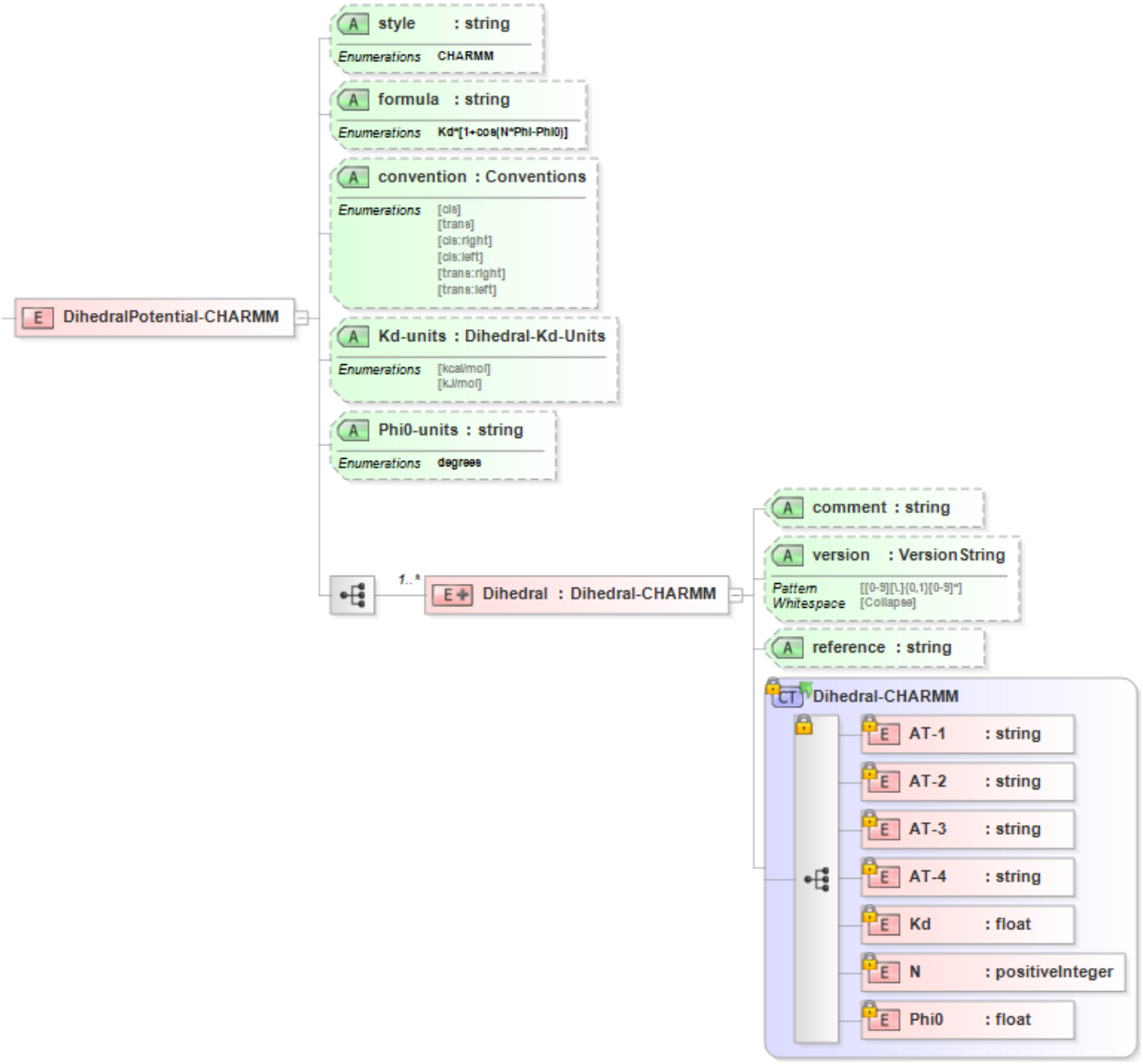
$E = K_{d,ijkl} \left[1 + \cos\left(N\phi_{ijkl} - \phi_{0,ijkl}\right)\right]$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{d,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
N	Nonnegative integer coefficient	N/A
$\phi_{0,ijkl}$	Equilibrium Dihedral for atoms [i,j,k,l]	degrees

15.1.2 XML Schema

The XML schema for the **CHARMM dihedral potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Dihedral coefficient for atoms [i,j,k,l]	$K_{d,ijkl}$	Kd
Nonnegative integer coefficient	N	N
Equilibrium dihedral angle for atoms [i,j,k,l]	$\phi_{0,ijkl}$	Phi0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	CHARMM
formula	Fixed	Kd*[1+cos(N*Phi-Phi0)]
convention	Optional	Enumerations specified in schema
Kd-units	Required	Enumerations specified in schema
Phi0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

15.1.3 References

1. LAMMPS CHARMM Dihedral Potential.
2. Liquid XML Studio.

15.2 Class 2 Dihedral

15.2.1 Functional Form

The **class 2 dihedral potential** has the functional form:

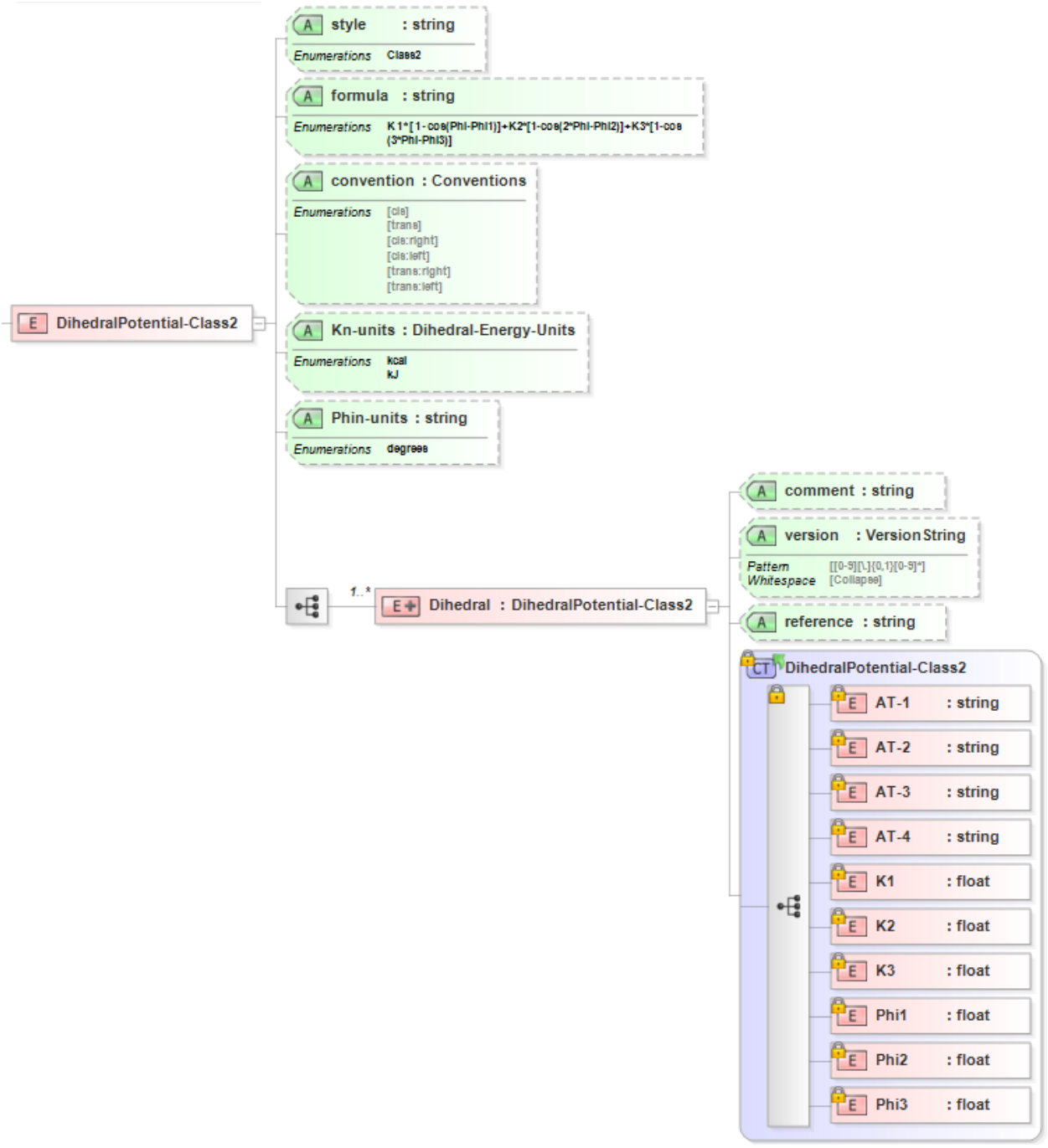
$$E = K_{1,ijkl}\left[1-\cos\left(\phi_{ijkl}-\phi_{1,ijkl}\right)\right] + K_{2,ijkl}\left[1-\cos\left(2\phi_{ijkl}-\phi_{2,ijkl}\right)\right] + K_{3,ijkl}\left[1-\cos\left(3\phi_{ijkl}-\phi_{3,ijkl}\right)\right]$$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{1,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{2,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{3,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$\phi_{1,ijkl}$	Equilibrium Dihedral for atoms [i,j,k,l]	degrees
$\phi_{2,ijkl}$	Equilibrium Dihedral for atoms [i,j,k,l]	degrees
$\phi_{3,ijkl}$	Equilibrium Dihedral for atoms [i,j,k,l]	degrees

15.2.2 XML Schema

The XML schema for the **class 2 dihedral potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Dihedral coefficient for atoms [i,j,k,l]	$K_{1,ijkl}$	K1
Dihedral coefficient for atoms [i,j,k,l]	$K_{2,ijkl}$	K2
Dihedral coefficient for atoms [i,j,k,l]	$K_{3,ijkl}$	K3
Equilibrium dihedral angle for atoms [i,j,k,l]	$\phi_{1,ijkl}$	Phi1
Equilibrium dihedral angle for atoms [i,j,k,l]	$\phi_{2,ijkl}$	Phi2
Equilibrium dihedral angle for atoms [i,j,k,l]	$\phi_{3,ijkl}$	Phi3

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	Class2
formula	Fixed	K1*[1-cos(Phi-Phi1)]+K2*[1-cos(2*Phi-Phi2)]+K3*[1-cos(3*Phi-Phi3)]
convention	Optional	Enumerations specified in schema
Kn-units	Required	Enumerations specified in schema
Phin-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

15.2.3 References

1. LAMMPS Class 2 Dihedral Potential.
2. Liquid XML Studio.

15.3 Fourier Dihedral

15.3.1 Functional Form

The **Fourier dihedral potential** has the functional forms:

$$E = K_{1,ijkl}\left[1+\cos\left(N_1\phi_{ijkl}-D_{1,ijkl}\right)\right] + K_{2,ijkl}\left[1+\cos\left(N_2\phi_{ijkl}-D_{2,ijkl}\right)\right] + K_{3,ijkl}\left[1+\cos\left(N_3\phi_{ijkl}-D_{3,ijkl}\right)\right] + K_{4,ijkl}\left[1+\cos\left(N_4\phi_{ijkl}-D_{4,ijkl}\right)\right] + K_{5,ijkl}\left[1+\cos\left(N_5\phi_{ijkl}-D_{5,ijkl}\right)\right]$$

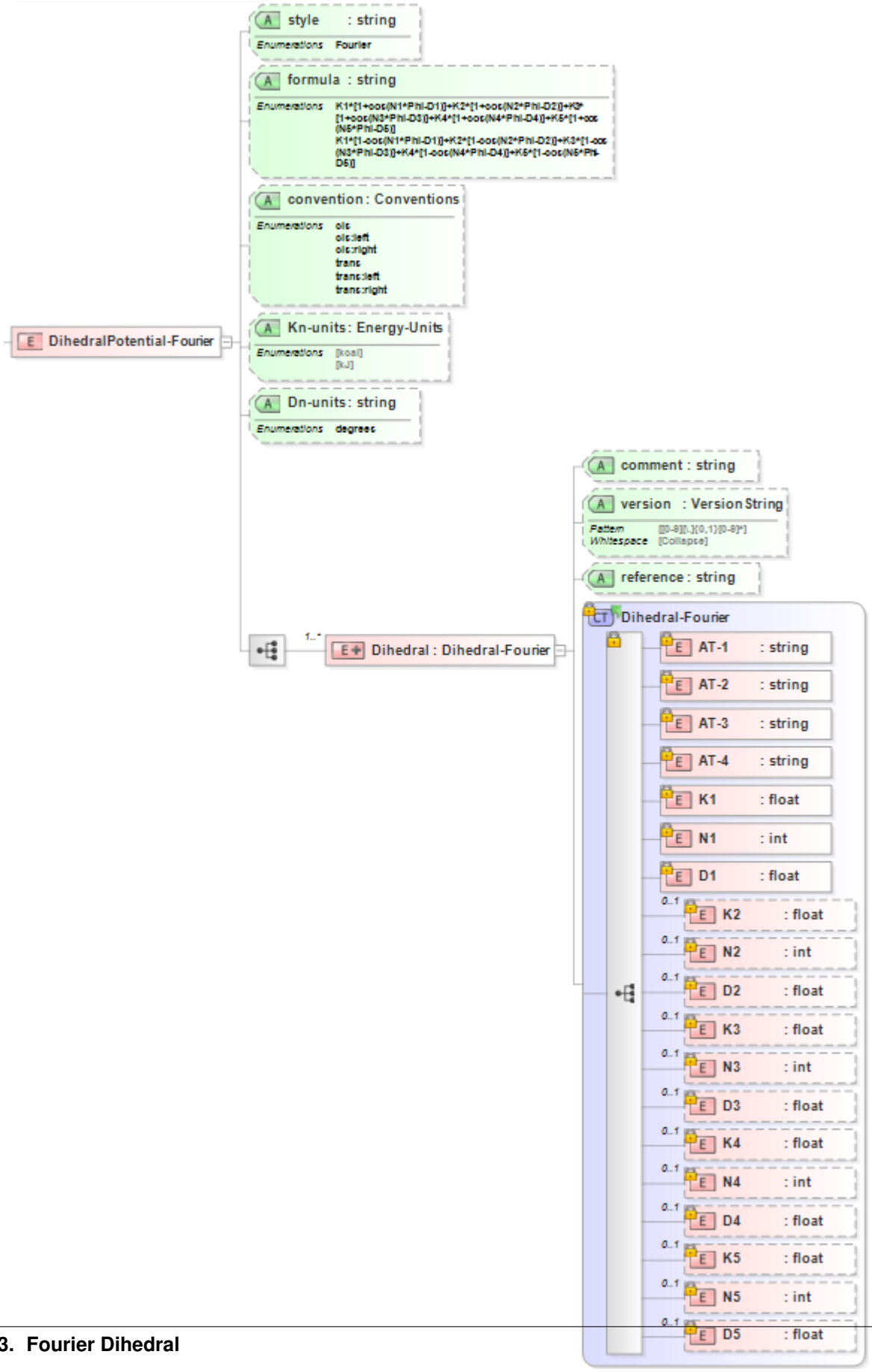
$$E = K_{1,ijkl}\left[1-\cos\left(N_1\phi_{ijkl}-D_{1,ijkl}\right)\right] + K_{2,ijkl}\left[1-\cos\left(N_2\phi_{ijkl}-D_{2,ijkl}\right)\right] + K_{3,ijkl}\left[1-\cos\left(N_3\phi_{ijkl}-D_{3,ijkl}\right)\right] + K_{4,ijkl}\left[1-\cos\left(N_4\phi_{ijkl}-D_{4,ijkl}\right)\right] + K_{5,ijkl}\left[1-\cos\left(N_5\phi_{ijkl}-D_{5,ijkl}\right)\right]$$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{1,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{2,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{3,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{4,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{5,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
N_1	Nonnegative integer coefficient	N/A
N_2	Nonnegative integer coefficient	N/A
N_3	Nonnegative integer coefficient	N/A
N_4	Nonnegative integer coefficient	N/A
N_5	Nonnegative integer coefficient	N/A
$D_{1,ijkl}$	Equilibrium Dihedral for atoms [i,j,k,l]	degrees
$D_{2,ijkl}$	Equilibrium Dihedral for atoms [i,j,k,l]	degrees
$D_{3,ijkl}$	Equilibrium Dihedral for atoms [i,j,k,l]	degrees
$D_{4,ijkl}$	Equilibrium Dihedral for atoms [i,j,k,l]	degrees
$D_{5,ijkl}$	Equilibrium Dihedral for atoms [i,j,k,l]	degrees

15.3.2 XML Schema

The XML schema for the **Fourier dihedral potential** has the following representation (design mode representation using Liquid XML Studio):


style : string
Enumerations Fourier
formula : string
Enumerations K1*[1+cos(N1*Phi-D1)]+K2*[1+cos(N2*Phi-D2)]+K3*[1+cos(N3*Phi-D3)]+K4*[1+cos(N4*Phi-D4)]+K5*[1+cos(N5*Phi-D5)]
K1*[1-cos(N1*Phi-D1)]+K2*[1-cos(N2*Phi-D2)]+K3*[1-cos(N3*Phi-D3)]+K4*[1-cos(N4*Phi-D4)]+K5*[1-cos(N5*Phi-D5)]
convention : Conventions
Enumerations cis
cis:left
cis:right
trans
trans:left
trans:right
DihedralPotential-Fourier
Kn-units : Energy-Units
Enumerations [kcal]
[kJ]
Dn-units : string
Enumerations degrees
comment : string
version : VersionString
Pattern [[0-9][.-][0,1][0-9]*]
Whitespace [Collapse]
reference : string
1..*
Dihedral : Dihedral-Fourier
Dihedral-Fourier
AT-1 : string
AT-2 : string
AT-3 : string
AT-4 : string
K1 : float
N1 : int
D1 : float
0..1
K2 : float
N2 : int
D2 : float
K3 : float
N3 : int
D3 : float
K4 : float
N4 : int
D4 : float
K5 : float
N5 : int
D5 : float

The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Dihedral coefficient for atoms [i,j,k,l]	$K_{1,ijkl}$	K1
Dihedral coefficient for atoms [i,j,k,l]	$K_{2,ijkl}$	K2
Dihedral coefficient for atoms [i,j,k,l]	$K_{3,ijkl}$	K3
Dihedral coefficient for atoms [i,j,k,l]	$K_{4,ijkl}$	K4
Dihedral coefficient for atoms [i,j,k,l]	$K_{5,ijkl}$	K5
Nonnegative integer coefficient	N_1	N1
Nonnegative integer coefficient	N_2	N2
Nonnegative integer coefficient	N_3	N3
Nonnegative integer coefficient	N_4	N4
Nonnegative integer coefficient	N_5	N5
Equilibrium dihedral angle for atoms [i,j,k,l]	$D_{1,ijkl}$	D1
Equilibrium dihedral angle for atoms [i,j,k,l]	$D_{2,ijkl}$	D2
Equilibrium dihedral angle for atoms [i,j,k,l]	$D_{3,ijkl}$	D3
Equilibrium dihedral angle for atoms [i,j,k,l]	$D_{4,ijkl}$	D4
Equilibrium dihedral angle for atoms [i,j,k,l]	$D_{5,ijkl}$	D5

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	Fourier
formula	Fixed	Enumerations specified in schema
convention	Optional	Enumerations specified in schema
Kn-units	Required	Enumerations specified in schema
Dn-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

15.3.3 References

1. LAMMPS Fourier Dihedral Potential.
2. Liquid XML Studio.

15.4 Fourier (Simple) Dihedral

15.4.1 Functional Form

The **Fourier (Simple) dihedral potential** has the functional forms:

$E = K_{1,ijkl}\left[1 + \cos\left(\phi_{ijkl}\right)\right] + K_{2,ijkl}\left[1 + \cos\left(\phi_{ijkl}\right)\right] + K_{3,ijkl}\left[1 + \cos\left(\phi_{ijkl}\right)\right] \quad + K_{4,ijkl}\left[1 + \cos\left(\phi_{ijkl}\right)\right] + K_{5,ijkl}\left[1 + \cos\left(\phi_{ijkl}\right)\right]$

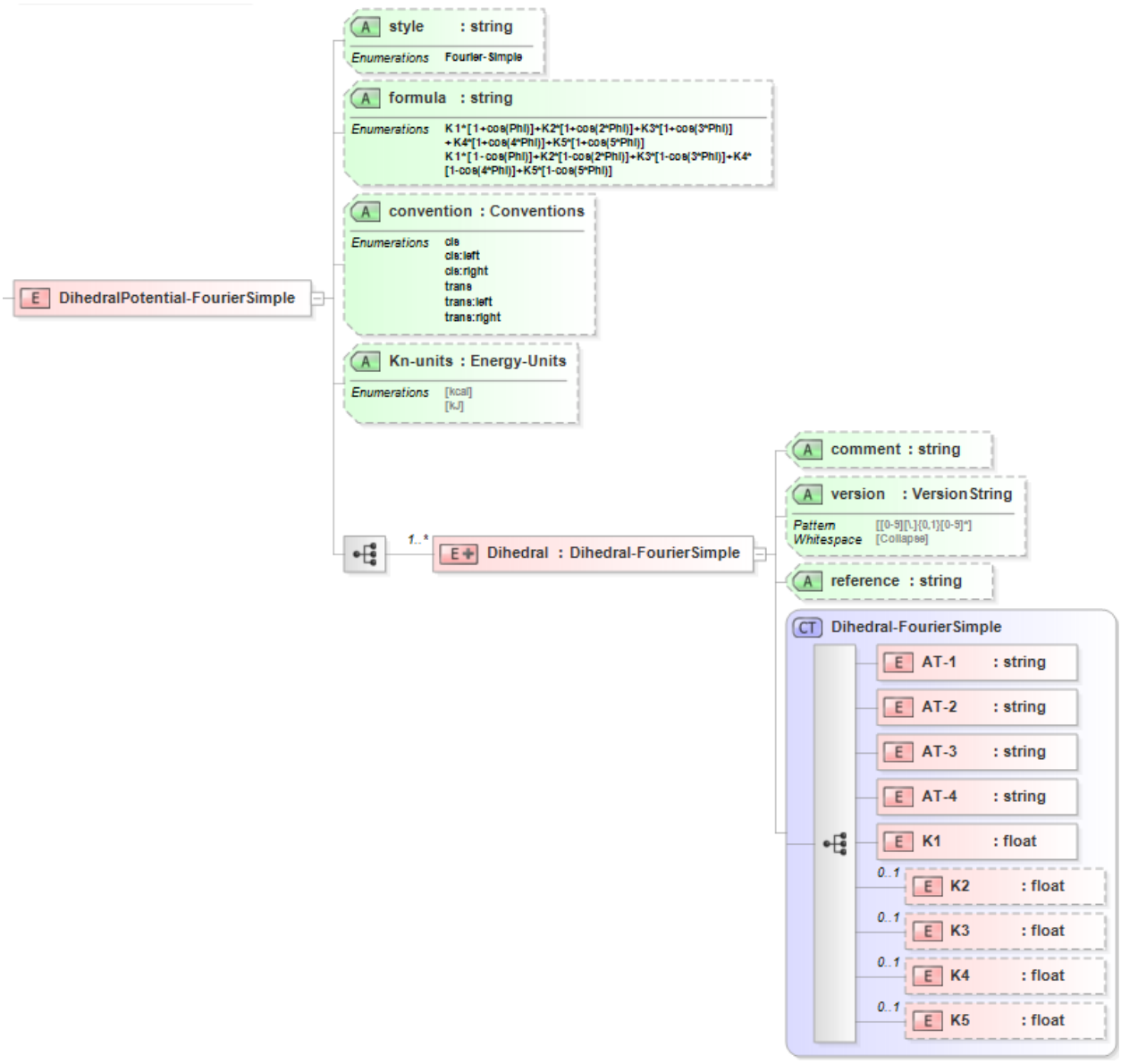
$E = K_{1,ijkl}\left[1 - \cos\left(\phi_{ijkl}\right)\right] + K_{2,ijkl}\left[1 - \cos\left(\phi_{ijkl}\right)\right] + K_{3,ijkl}\left[1 - \cos\left(\phi_{ijkl}\right)\right] \quad + K_{4,ijkl}\left[1 - \cos\left(\phi_{ijkl}\right)\right] + K_{5,ijkl}\left[1 - \cos\left(\phi_{ijkl}\right)\right]$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{1,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{2,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{3,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{4,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{5,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy

15.4.2 XML Schema

The XML schema for the **Fourier (Simple) dihedral potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Dihedral coefficient for atoms [i,j,k,l]	$K_{1,ijkl}$	K1
Dihedral coefficient for atoms [i,j,k,l]	$K_{2,ijkl}$	K2
Dihedral coefficient for atoms [i,j,k,l]	$K_{3,ijkl}$	K3
Dihedral coefficient for atoms [i,j,k,l]	$K_{4,ijkl}$	K4
Dihedral coefficient for atoms [i,j,k,l]	$K_{5,ijkl}$	K5

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	Fourier
formula	Fixed	Enumerations specified in schema
convention	Optional	Enumerations specified in schema
Kn-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

15.4.3 References

1. LAMMPS Fourier Dihedral Potential.
2. GROMACS Fourier (Simple) Dihedral Potential page 80.
3. Liquid XML Studio.

15.5 Harmonic Dihedral

15.5.1 Functional Form

The **harmonic dihedral potential** has the functional form:

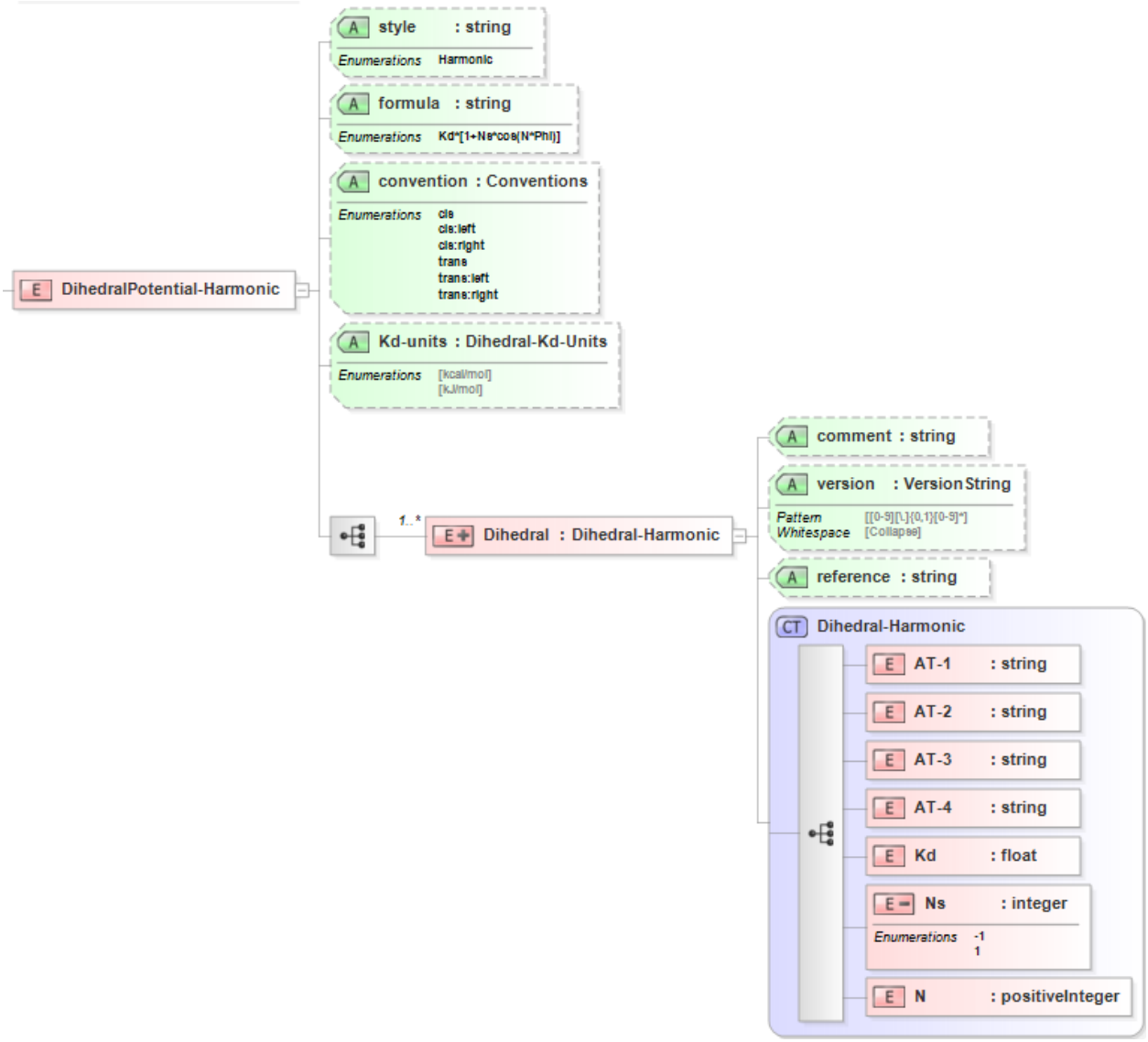
$E = K_{d,ijkl} \left[1 + N_s \cos\left(N\phi_{ijkl}\right)\right]$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{d,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
N_s	Determines sign convention (-1 or +1)	N/A
N	Nonnegative integer coefficient	N/A

15.5.2 XML Schema

The XML schema for the **harmonic dihedral potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Dihedral coefficient for atoms [i,j,k,l]	$K_{d,ijkl}$	Kd
Determines sign convention (-1 or +1)	N_S	Ns
Nonnegative integer coefficient	N	N

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	Harmonic
formula	Fixed	Kd*[1+Ns*cos(N*Phi)]
convention	Optional	Enumerations specified in schema
Kd-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

15.5.3 References

1. LAMMPS Harmonic Dihedral Potential.
2. Liquid XML Studio.

15.6 OPLS Dihedral

15.6.1 Functional Form

The **OPLS dihedral potential** has the functional forms:

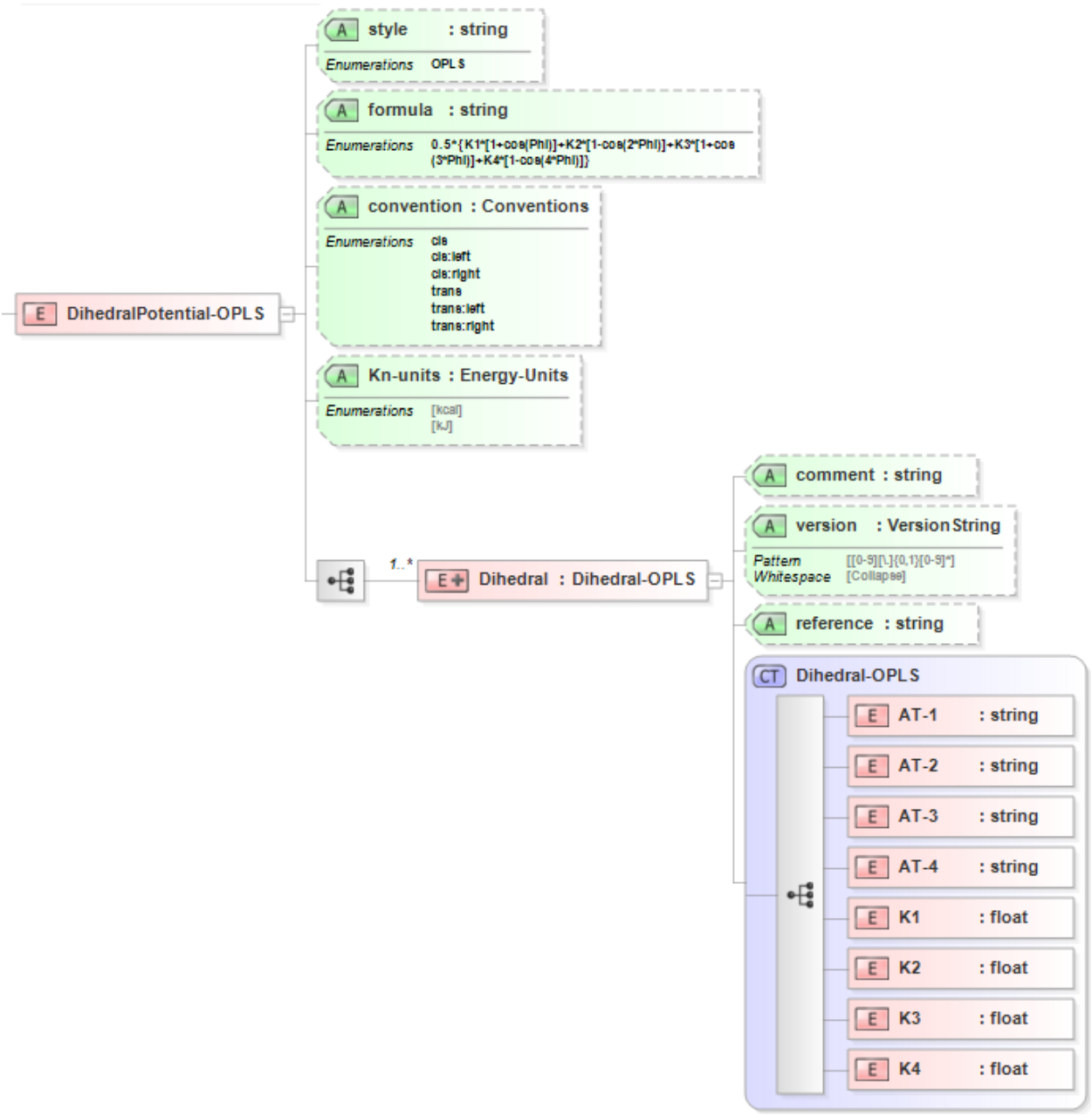
$E = \frac{1}{2}K_{1,ijkl}\left[1+\cos\left(\phi_{ijkl}\right)\right] + \frac{1}{2}K_{2,ijkl}\left[1-\cos\left(2\phi_{ijkl}\right)\right] + \frac{1}{2}K_{3,ijkl}\left[1+\cos\left(3\phi_{ijkl}\right)\right] + \frac{1}{2}K_{4,ijkl}\left[1-\cos\left(4\phi_{ijkl}\right)\right]$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{1,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{2,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{3,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$K_{4,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy

15.6.2 XML Schema

The XML schema for the **OPLS dihedral potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Dihedral coefficient for atoms [i,j,k,l]	$K_{1,ijkl}$	K1
Dihedral coefficient for atoms [i,j,k,l]	$K_{2,ijkl}$	K2
Dihedral coefficient for atoms [i,j,k,l]	$K_{3,ijkl}$	K3
Dihedral coefficient for atoms [i,j,k,l]	$K_{4,ijkl}$	K4

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	OPLS
formula	Fixed	0.5*{K1*[1+cos(Phi)]+K2*[1-cos(2*Phi)]+K3*[1+cos(3*Phi)]+K4*[1-cos(4*Phi)]}
convention	Optional	Enumerations specified in schema
Kn-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

15.6.3 References

1. LAMMPS OPLS Dihedral Potential.
2. GROMACS OPLS Dihedral Potential page 81.
3. Liquid XML Studio.

15.7 Quadratic Dihedral

15.7.1 Functional Form

The **quadratic dihedral potential** has the functional form:

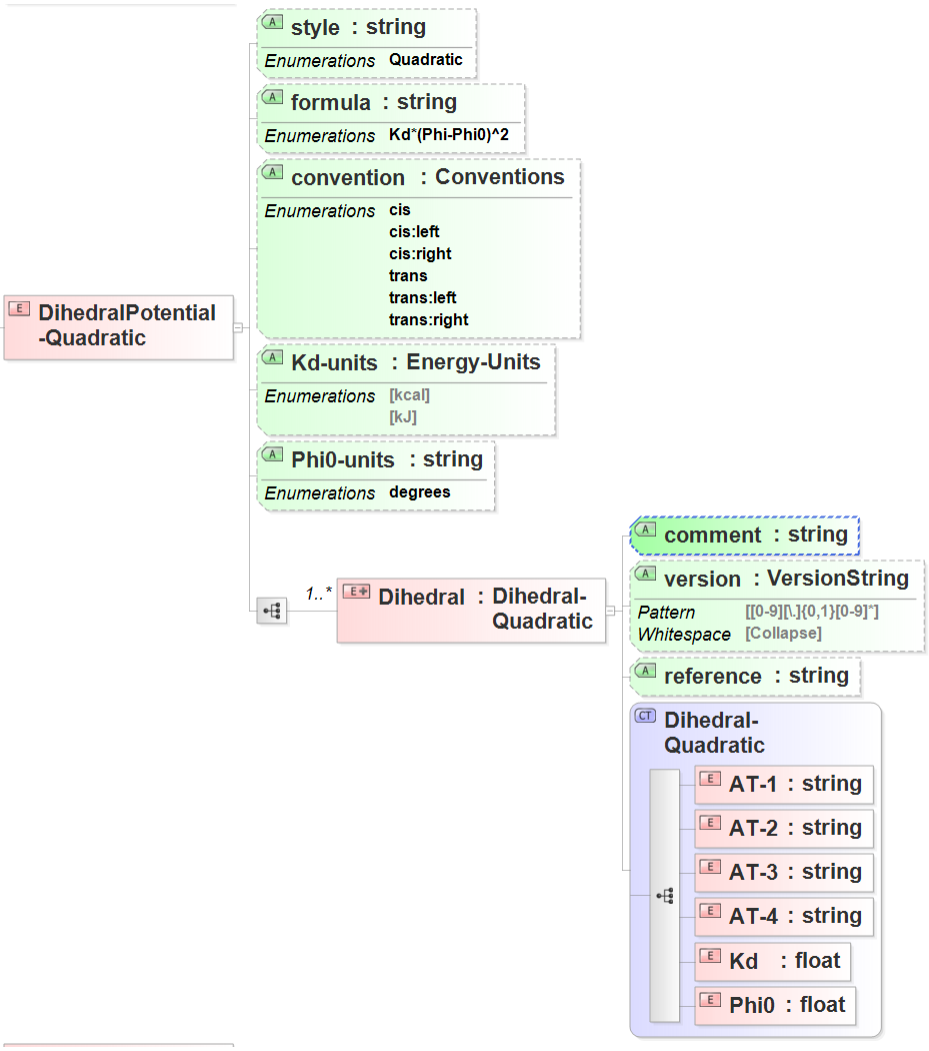
$E = K_{d,ijkl} \cdot (\phi_{ijkl} - \phi_{0,ijkl})^2$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{d,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy/degrees^2
$\phi_{0,ijkl}$	Equilibrium Dihedral for atoms [i,j,k,l]	degrees

15.7.2 XML Schema

The XML schema for the **quadratic dihedral potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Dihedral coefficient for atoms [i,j,k,l]	$K_{d,ijkl}$	Kd
Equilibrium dihedral angle for atoms [i,j,k,l]	$\phi_{0,ijkl}$	Phi0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	Quadratic
formula	Fixed	Kd*(Phi_Phi0)^2
convention	Optional	Enumerations specified in schema
Kd-units	Required	Enumerations specified in schema
Phi0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

15.7.3 References

1. LAMMPS Quadratic Dihedral Potential.
2. **'GROMACS Quadratic Dihedral Potential'_**.
3. Liquid XML Studio.

15.8 Multi-Harmonic Dihedral

15.8.1 Functional Form

The **Multi-Harmonic dihedral potential** has the functional form:

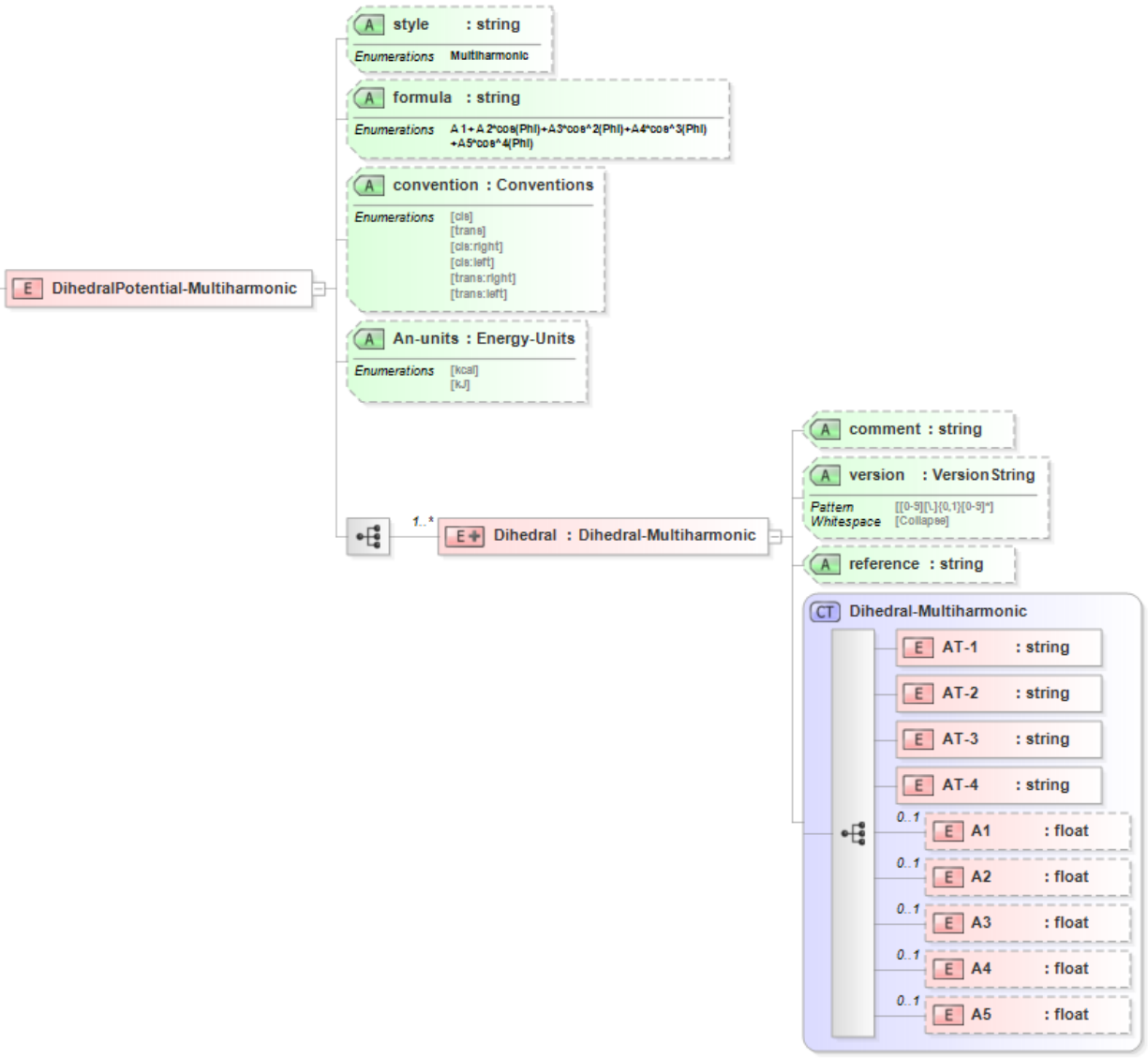
$E = A_{1,ijkl} + A_{2,ijkl}\cos\left(\phi_{ijkl}\right) + A_{3,ijkl}\cos^2\left(\phi_{ijkl}\right) + A_{4,ijkl}\cos^3\left(\phi_{ijkl}\right) + A_{5,ijkl}\cos^4\left(\phi_{ijkl}\right)$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$A_{1,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$A_{2,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$A_{3,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$A_{4,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
$A_{5,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy

15.8.2 XML Schema

The XML schema for the **Fourier dihedral potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Dihedral coefficient for atoms [i,j,k,l]	$A_{1,ijkl}$	A1
Dihedral coefficient for atoms [i,j,k,l]	$A_{2,ijkl}$	A2
Dihedral coefficient for atoms [i,j,k,l]	$A_{3,ijkl}$	A3
Dihedral coefficient for atoms [i,j,k,l]	$A_{4,ijkl}$	A4
Dihedral coefficient for atoms [i,j,k,l]	$A_{5,ijkl}$	A5

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	Fourier
formula	Fixed	Enumerations specified in schema
convention	Optional	Enumerations specified in schema
An-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

15.8.3 References

1. **'LAMMPS Multi-Harmonic Dihedral Potential'_**.
2. Liquid XML Studio.

15.9 Tabular Dihedral

15.9.1 Tabular Form

The **tabular dihedral potential** has the parameters:

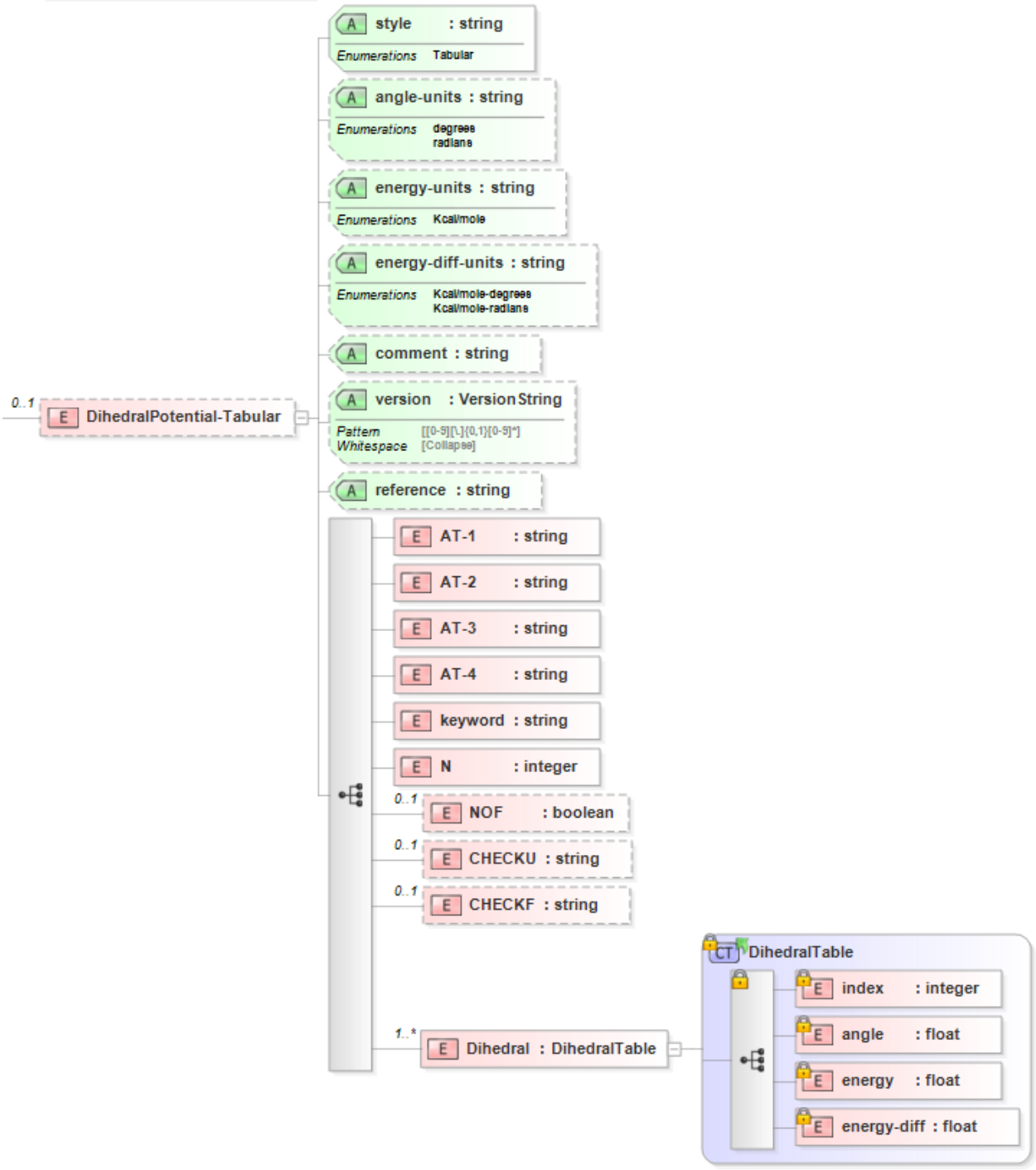
Parameter	Parameter Definition	Units
N	Number of tabulated values	N/A
NOF	Allows omission of forces (energy derivatives) in the table	N/A
DEGREES	Specify degrees as units for the angles	N/A
RADIANS	Specify radians as units for the angles	N/A
CHECKU	File to save interpolated energy table	N/A
CHECKF	File to save interpolated force table	N/A

The **tabular dihedral potential** has the tabulated values:

index	angle	energy	derivative
i_1	a_1	e_1	de_1
...	...	...	...
i_N	a_N	e_n	de_N

15.9.2 XML Schema

The XML schema for the **tabular dihedral potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the parameters/symbols and XML schema notations are given by:

Parameter Definition	Parameter/Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Section identifying keyword	N/A	keyword
Number of tabulated values	N	N
Allows omission of forces in the table	NOF	NOF
Specify degrees as units for the angles	DEGREES	angle-units
Specify radians as units for the angles	RADIANS	angle-units
File to save interpolated energy table	CHECKU	CHECKU
File to save interpolated force table	CHECKF	CHECKF
Index	index	index
Angle	angle	angle
Energy	energy	energy
Derivate of energy	derivative	energy-diff

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Tabular
angle-units	Required	Enumerations specified in schema
energy-units	Required	Enumerations specified in schema
energy-diff-units	Required	Enumerations specified in schema
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

15.9.3 References

1. LAMMPS Tabular Dihedral Potential.
2. Liquid XML Studio.

CHAPTER 16

Improper Potentials

16.1 CHARMM Improper

16.1.1 Functional Form

The **CHARMM improper potential** has the functional forms:

$E = K_{d,ijkl}\left[1 + \cos\left(N\phi_{ijkl} - \phi_{0,ijkl}\right)\right]$

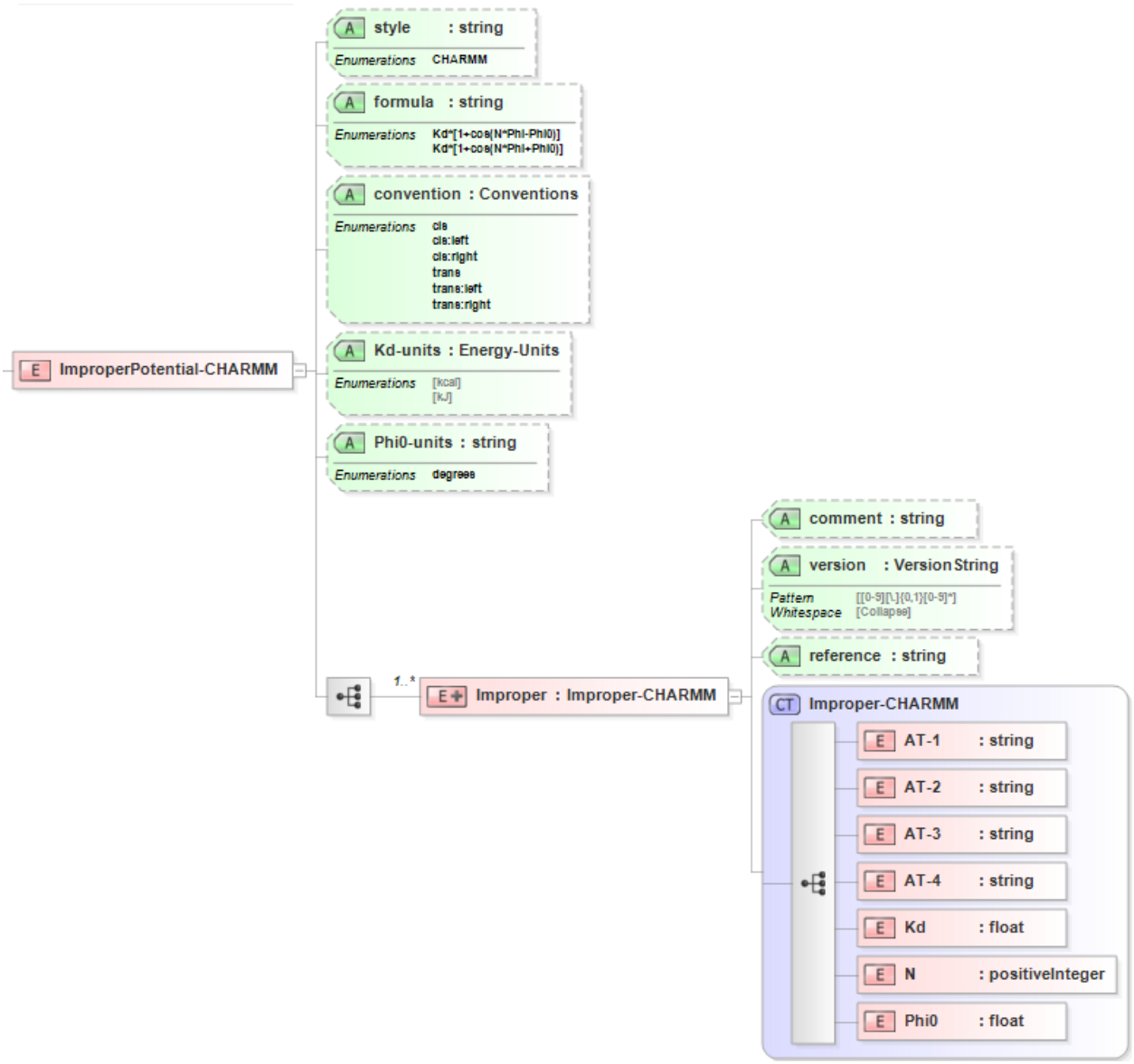
$E = K_{d,ijkl}\left[1 + \cos\left(N\phi_{ijkl} + \phi_{0,ijkl}\right)\right]$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{d,ijkl}$	Improper coefficient for atoms [i,j,k,l]	energy
N	Nonnegative integer coefficient	N/A
$\phi_{0,ijkl}$	Equilibrium improper angle for atoms [i,j,k,l]	degrees

16.1.2 XML Schema

The XML schema for the **CHARMM improper potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Improper coefficient for atoms [i,j,k,l]	$K_{d,ijkl}$	Kd
Nonnegative integer coefficient	N	N
Equilibrium improper angle for atoms [i,j,k,l]	$\phi_{0,ijkl}$	Phi0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	CHARMM
formula	Fixed	Kd*[1+cos(N*Phi-Phi0)], Kd*[1+cos(N*Phi+Phi0)]
convention	Optional	Enumerations specified in schema
Kd-units	Required	Enumerations specified in schema
Phi0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

16.1.3 References

1. Liquid XML Studio.

16.2 Class 2 Improper

16.2.1 Functional Form

The **class 2 improper potential** has the functional form:

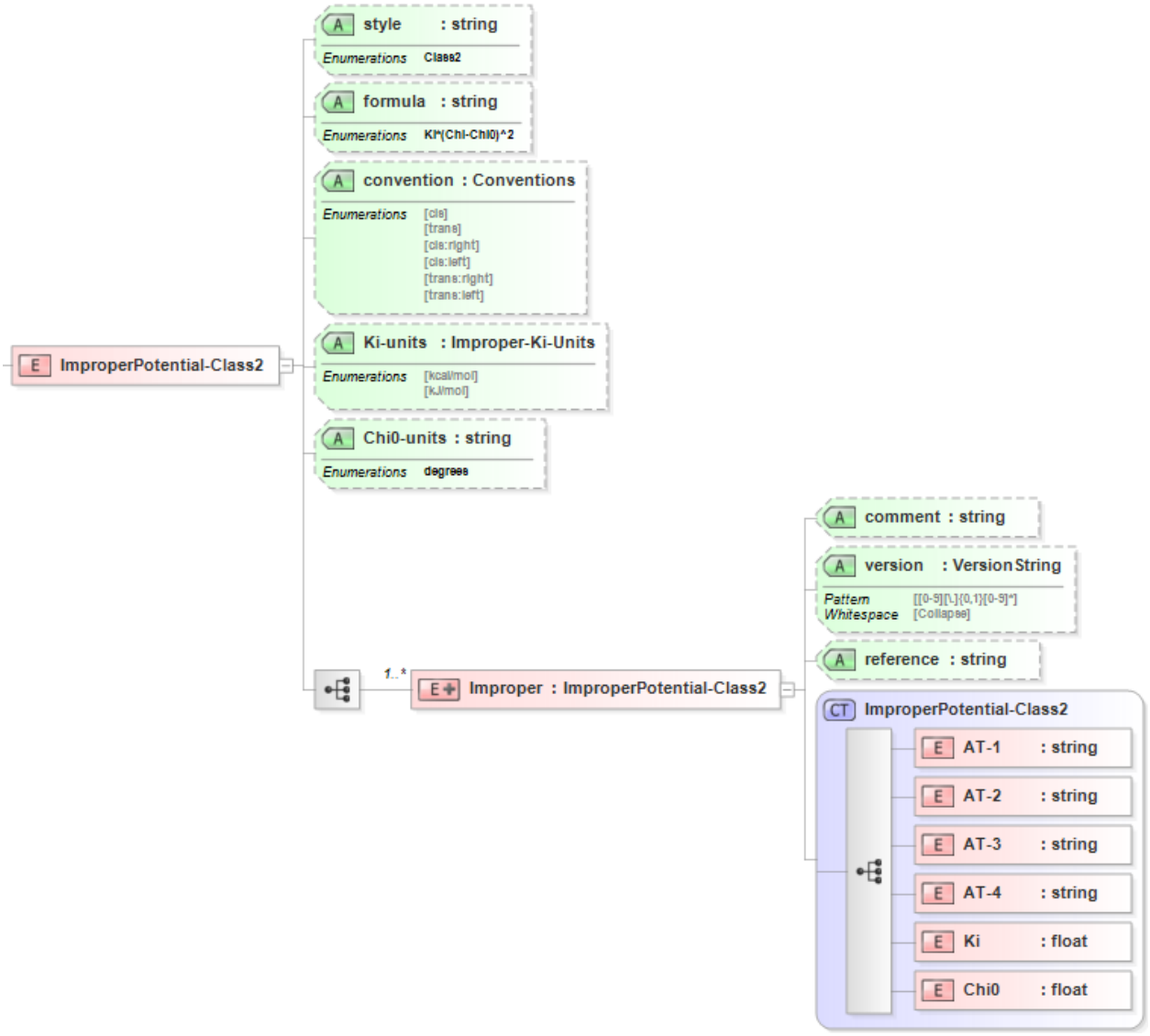
$E = K_{i,ijkl} \cdot (\chi_{ijkl} - \chi_{0,ijkl})^2$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{i,ijkl}$	Improper coefficient for atoms [i,j,k,l]	energy/degrees^2
$\chi_{0,ijkl}$	Equilibrium improper angle for atoms [i,j,k,l]	degrees

16.2.2 XML Schema

The XML schema for the **class 2 improper potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Improper coefficient for atoms [i,j,k,l]	$K_{i,ijkl}$	Ki
Equilibrium improper angle for atoms [i,j,k,l]	$\chi_{0,ijkl}$	Chi0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	Class2
formula	Fixed	Ki*(Chi-Chi0)^2
convention	Optional	Enumerations specified in schema
Ki-units	Required	Enumerations specified in schema
Chi0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

16.2.3 References

1. LAMMPS Harmonic Improper Potential.
2. GROMACS Harmonic Improper Potential page 77.
3. Liquid XML Studio.

16.3 COS2 Improper

16.3.1 Functional Form

The **COS2 improper potential** has the functional form:

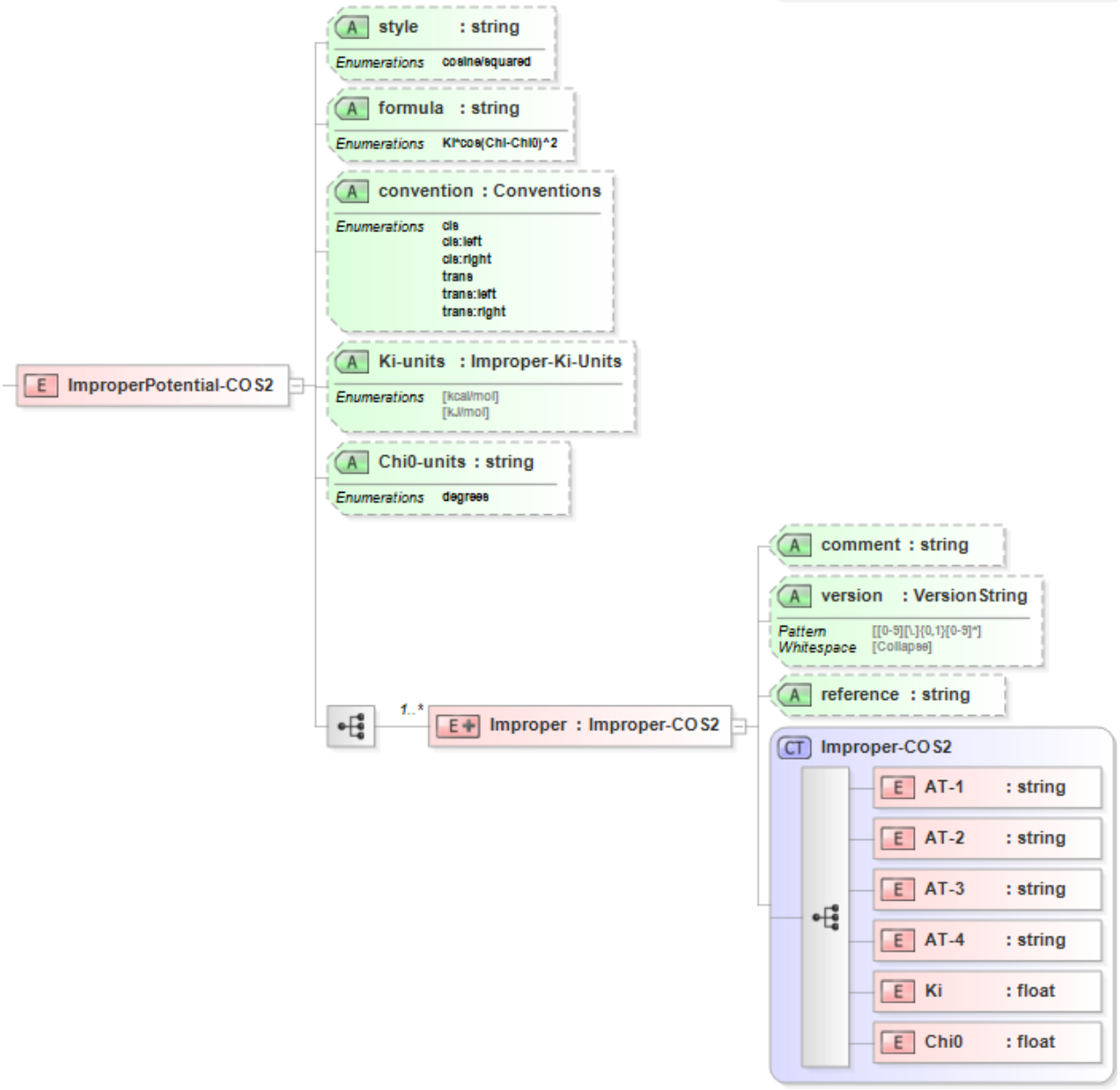
$E = K_{i,ijkl}\cos^2\left(\chi_{ijkl} - \chi_{0,ijkl}\right)$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{i,ijkl}$	Improper coefficient for atoms [i,j,k,l]	energy
$\chi_{0,ijkl}$	Equilibrium improper angle for atoms [i,j,k,l]	degrees

16.3.2 XML Schema

The XML schema for the **COS2 improper potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Improper coefficient for atoms [i,j,k,l]	$K_{i,ijkl}$	Ki
Equilibrium improper angle for atoms [i,j,k,l]	$\chi_{0,ijkl}$	Chi0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	cosine/squared
formula	Fixed	Ki*cos(Chi-Chi0)^2
convention	Optional	Enumerations specified in schema
Ki-units	Required	Enumerations specified in schema
Chi0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

16.3.3 References

1. LAMMPS COS2 Improper Potential.
2. Liquid XML Studio.

16.4 CVFF Improper

16.4.1 Functional Form

The **CVFF improper potential** has the functional form:

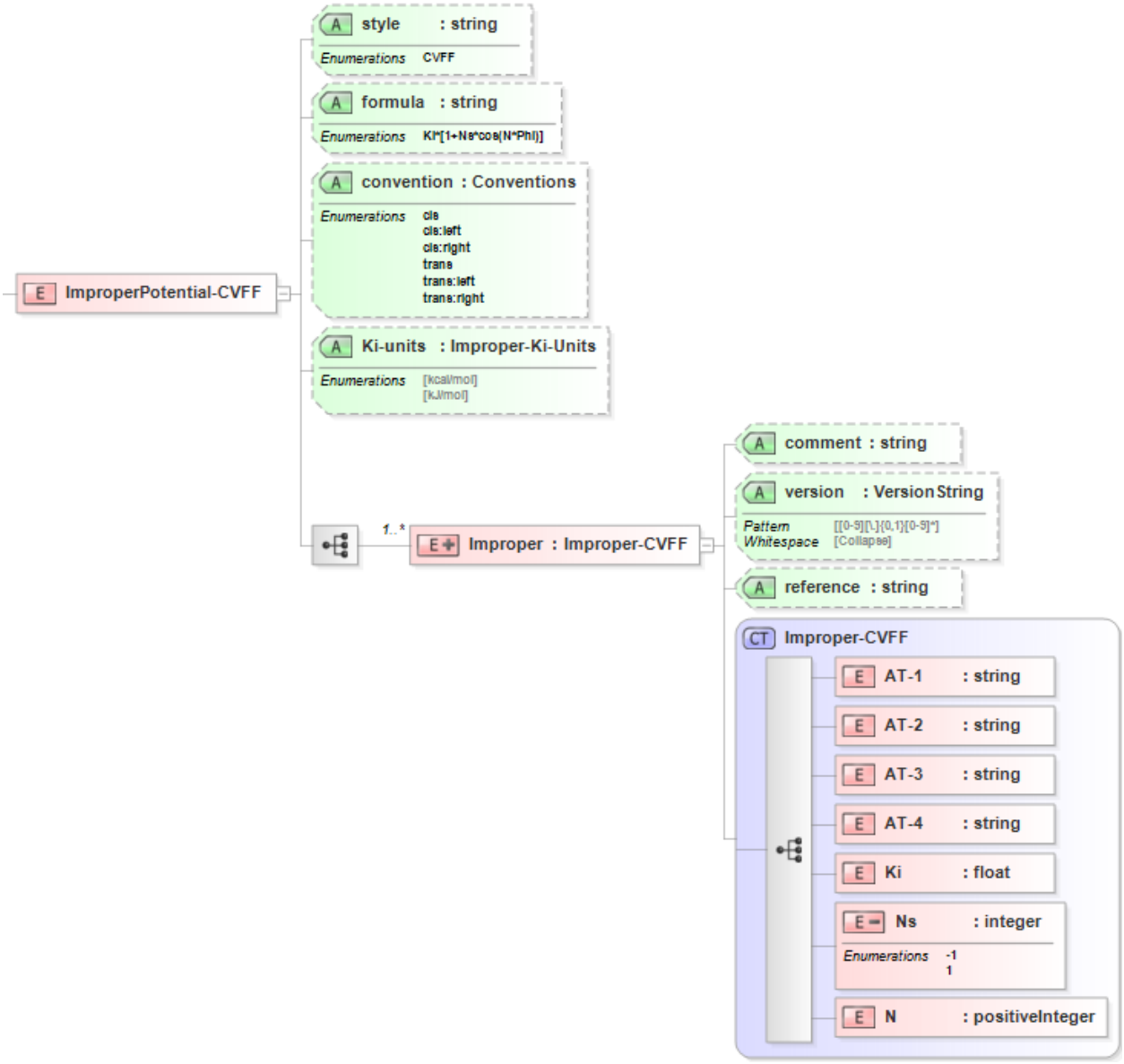
$E = K_{i,ijkl} \left[1 + N_s \cos\left(N\phi_{ijkl}\right)\right]$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{i,ijkl}$	Dihedral coefficient for atoms [i,j,k,l]	energy
N_s	Determines sign convention (-1 or +1)	N/A
N	Nonnegative integer coefficient	N/A

16.4.2 XML Schema

The XML schema for the **CVFF improper potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Dihedral coefficient for atoms [i,j,k,l]	$K_{i,ijkl}$	K1
Determines sign convention (-1 or +1)	N_S	Ns
Nonnegative integer coefficient	N	N

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	CVFF
formula	Fixed	Ki*[1+Ns*cos(N*Phi)]
convention	Optional	Enumerations specified in schema
Ki-units	Required	Enumerations specified in schema
Chi0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

16.4.3 References

1. LAMMPS CVFF Improper Potential.
2. Liquid XML Studio.

16.5 Fourier Improper

16.5.1 Functional Form

The **Fourier improper potential** has the functional form:

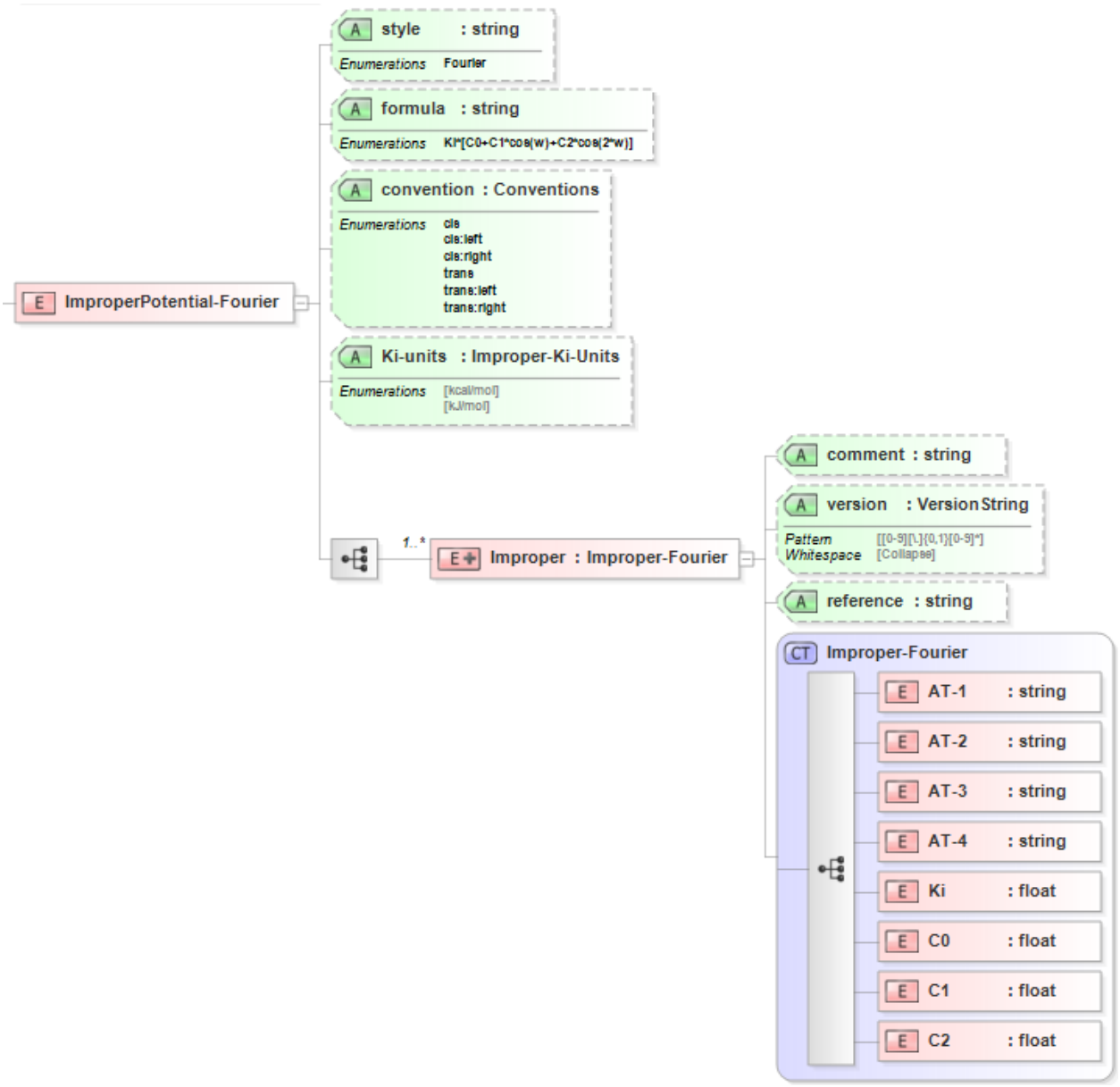
$E = K_{i,ijkl} \left[C_{0,ijkl} + C_{1,ijkl} \cos\left(\omega_{ijkl}\right) + C_{2,ijkl} \cos\left(2\omega_{ijkl}\right) \right]$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{i,ijkl}$	Improper coefficient for atoms [i,j,k,l]	energy
$C_{0,ijkl}$	Real coefficient for cosine term #0 [i,j,k,l]	N/A
$C_{1,ijkl}$	Real coefficient for cosine term #1 [i,j,k,l]	N/A
$C_{2,ijkl}$	Real coefficient for cosine term #2 [i,j,k,l]	N/A

16.5.2 XML Schema

The XML schema for the **Fourier improper potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Improper coefficient for atoms [i,j,k,l]	$K_{i,ijkl}$	Ki
Real coefficient for cosine term #0 [i,j,k,l]	$C_{0,ijkl}$	C0
Real coefficient for cosine term #1 [i,j,k,l]	$C_{1,ijkl}$	C1
Real coefficient for cosine term #2 [i,j,k,l]	$C_{2,ijkl}$	C2

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	Fourier
formula	Fixed	Ki*[C0+C1*cos(w)+C2*cos(2*w)]
convention	Optional	Enumerations specified in schema
Ki-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

16.5.3 References

1. LAMMPS Fourier Improper Potential.
2. Liquid XML Studio.

16.6 Harmonic Improper

16.6.1 Functional Form

The **harmonic improper potential** has the functional form:

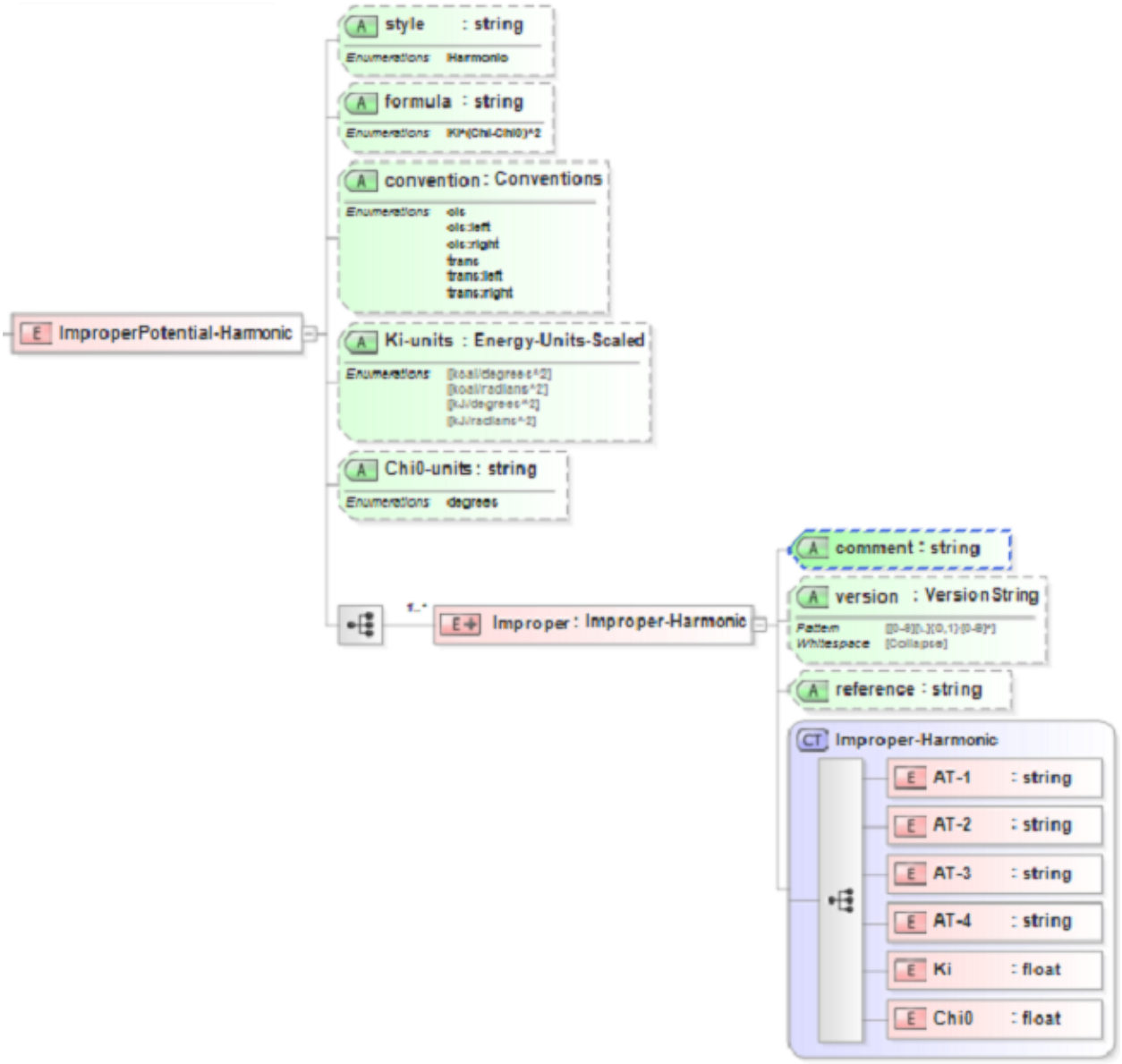
$E = K_{i,ijkl} \cdot (\chi_{ijkl} - \chi_{0,ijkl})^2$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$K_{i,ijkl}$	Improper coefficient for atoms [i,j,k,l]	energy/degrees^2
$\chi_{0,ijkl}$	Equilibrium improper angle for atoms [i,j,k,l]	degrees

16.6.2 XML Schema

The XML schema for the **harmonic improper potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Improper coefficient for atoms [i,j,k,l]	$K_{i,ijkl}$	Ki
Equilibrium improper angle for atoms [i,j,k,l]	$\chi_{0,ijkl}$	Chi0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	Harmonic
formula	Fixed	Ki*(Chi-Chi0)^2
convention	Optional	Enumerations specified in schema
Ki-units	Required	Enumerations specified in schema
Chi0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

16.6.3 References

1. LAMMPS Harmonic Improper Potential.
2. GROMACS Harmonic Improper Potential page 77.
3. Liquid XML Studio.

16.7 Umbrella Improper

16.7.1 Functional Form

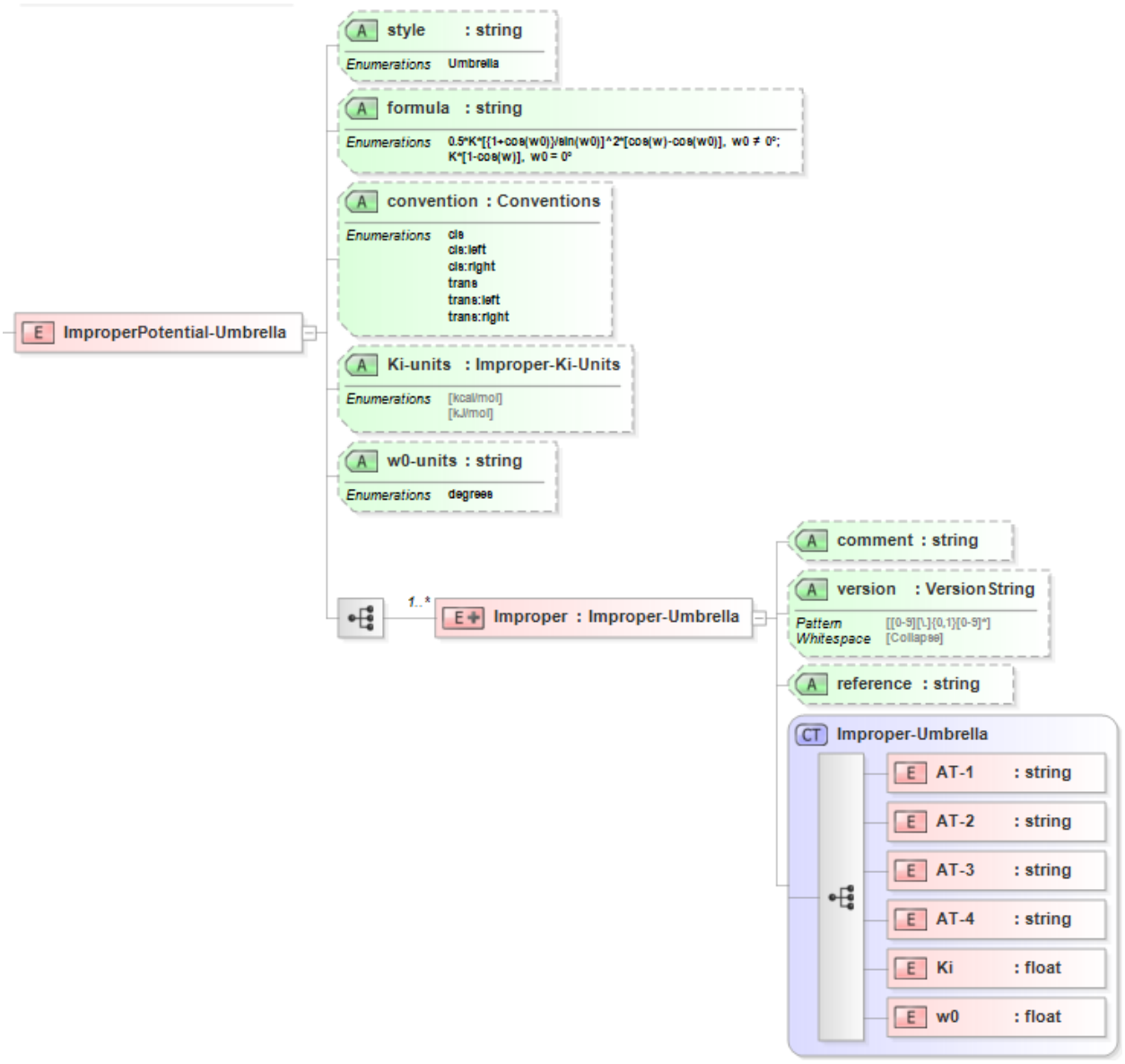
The **umbrella improper potential** has the functional form:

$E = \{$

The force-field parameters for this potential and units are given by:

16.7.2 XML Schema

The XML schema for the **umbrella improper potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Improper coefficient for atoms [i,j,k,l]	$K_{i,ijkl}$	Ki
Equilibrium improper angle for atoms [i,j,k,l]	$\omega_{0,ijkl}$	w0

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value
style	Fixed	Umbrella
formula	Fixed	0.5*K*[{1+cos(w0)}/sin(w0)]^2*[cos(w)-cos(w0)], w0 0°; K*[1-cos(w)], w0 = 0°
convention	Optional	Enumerations specified in schema
Ki-units	Required	Enumerations specified in schema
w0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

16.7.3 References

1. LAMMPS Umbrella Improper Potential.
2. Liquid XML Studio.

CHAPTER 17

Cross Potentials

17.1 Cross: Bond-Bond

17.1.1 Functional Form

The **Bond-Bond Cross Potential** has the functional form:

$E = M\left(R_{ij} - R_{1,ij}\right)\left(R_{jk} - R_{2,jk}\right)$

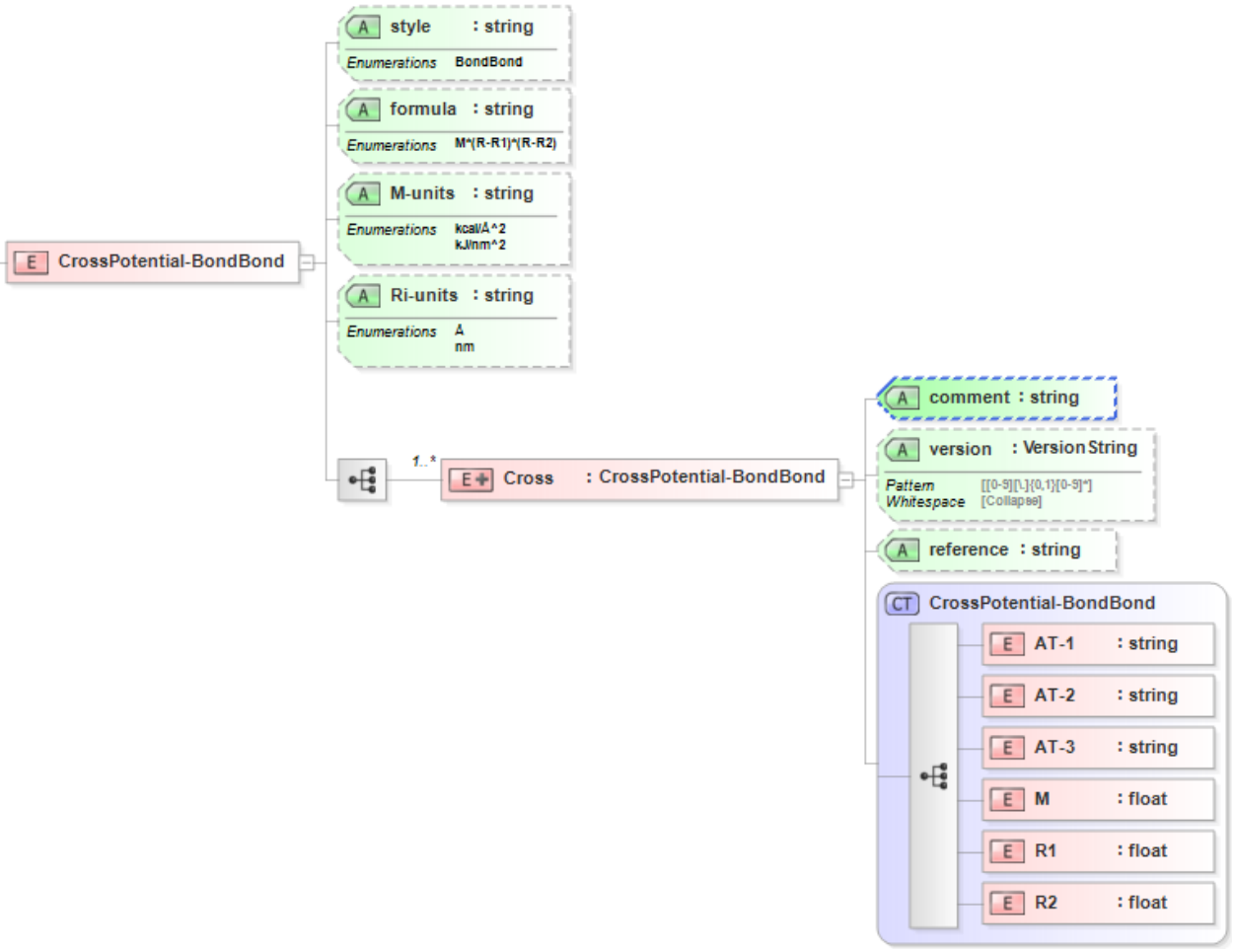
This term is part of the Class2 Angle Potential style.

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
M	Cross potential bond coefficient for atoms [i,j,k]	energy
$R_{1,ij}$	Equilibrium bond length for atoms [i,j]	length
$R_{2,jk}$	Equilibrium bond length for atoms [j,k]	length

17.1.2 XML Schema

The XML schema for the **Bond-Bond Cross Potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Bond coefficient for atoms [i,j,k]	M	M
Equilibrium bond length for atoms [i,j]	$R_{1,ij}$	R1
Equilibrium bond length for atoms [j,k]	$R_{2,jk}$	R2

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	BondBond
formula	Fixed	M*(Rij-R1)*(Rjk-R2)
M-units	Required	Enumerations specified in schema
Ri-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

17.1.3 References

1. LAMMPS Class2 Angle Potential w/ Bond-Bond Cross term.
2. SklogWiki COMPASS Force-Field.
3. Liquid XML Studio.

17.2 Cross: Bond-Bond-13

17.2.1 Functional Form

The **Bond-Bond-13 Cross Potential** has the functional form:

$E = N\left(R_{ij} - R_{1,ij}\right)\left(R_{kl} - R_{3,kl}\right)$

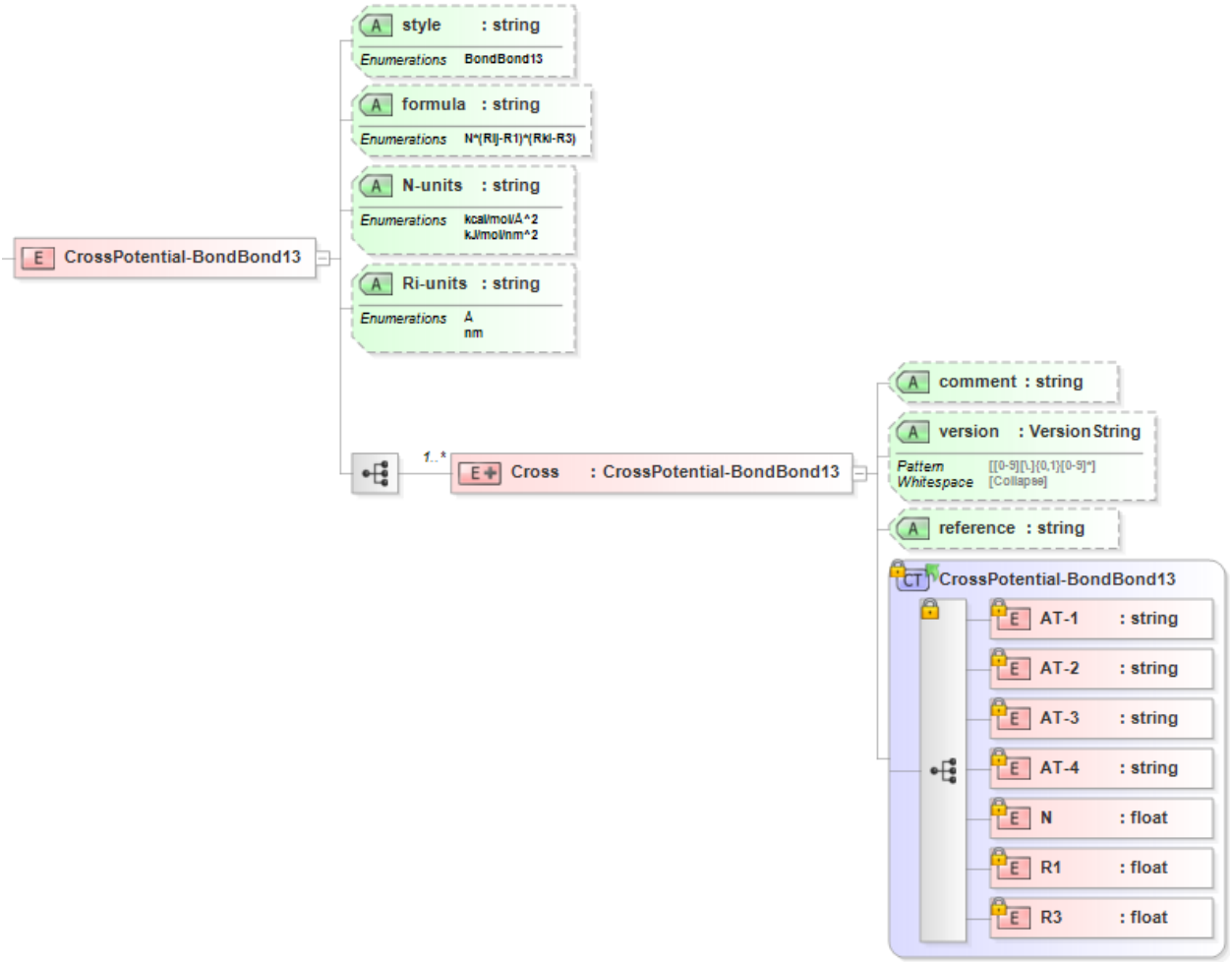
This term is part of the Class2 Dihedral Potential style.

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
N	Cross potential bond coefficient for atoms [i,j,k,l]	energy
$R_{1,ij}$	Equilibrium bond length for atoms [i,j]	length
$R_{3,kl}$	Equilibrium bond length for atoms [k,l]	length

17.2.2 XML Schema

The XML schema for the **Bond-Bond-13 Cross Potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Bond coefficient for atoms [i,j,k,l]	N	N
Equilibrium bond length for atoms [i,j]	$R_{1,ij}$	R1
Equilibrium bond length for atoms [k,l]	$R_{3,kl}$	R3

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	BondBond13
formula	Fixed	N*(Rij-R1)*(Rkl-R3)
N-units	Required	Enumerations specified in schema
Ri-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

17.2.3 References

1. LAMMPS Class2 Dihedral Potential w/ Bond-Bond-13 Cross term.
2. SklogWiki COMPASS Force-Field.
3. Liquid XML Studio.

17.3 Cross: Angle-Angle

17.3.1 Functional Form

The **Angle-Angle Cross Potential** has the functional form:

$$E = M_{1,ijkl}\left(\theta_{ijk} - \theta_{1,ijk}\right)\left(\theta_{kjl} - \theta_{1,kjl}\right) + M_{2,ijkl}\left(\theta_{ijk} - \theta_{1,ijk}\right)\left(\theta_{ijl} - \theta_{2,ijl}\right) + M_{3,ijkl}\left(\theta_{ijl} - \theta_{2,ijl}\right)\left(\theta_{kjl} - \theta_{1,kjl}\right)$$

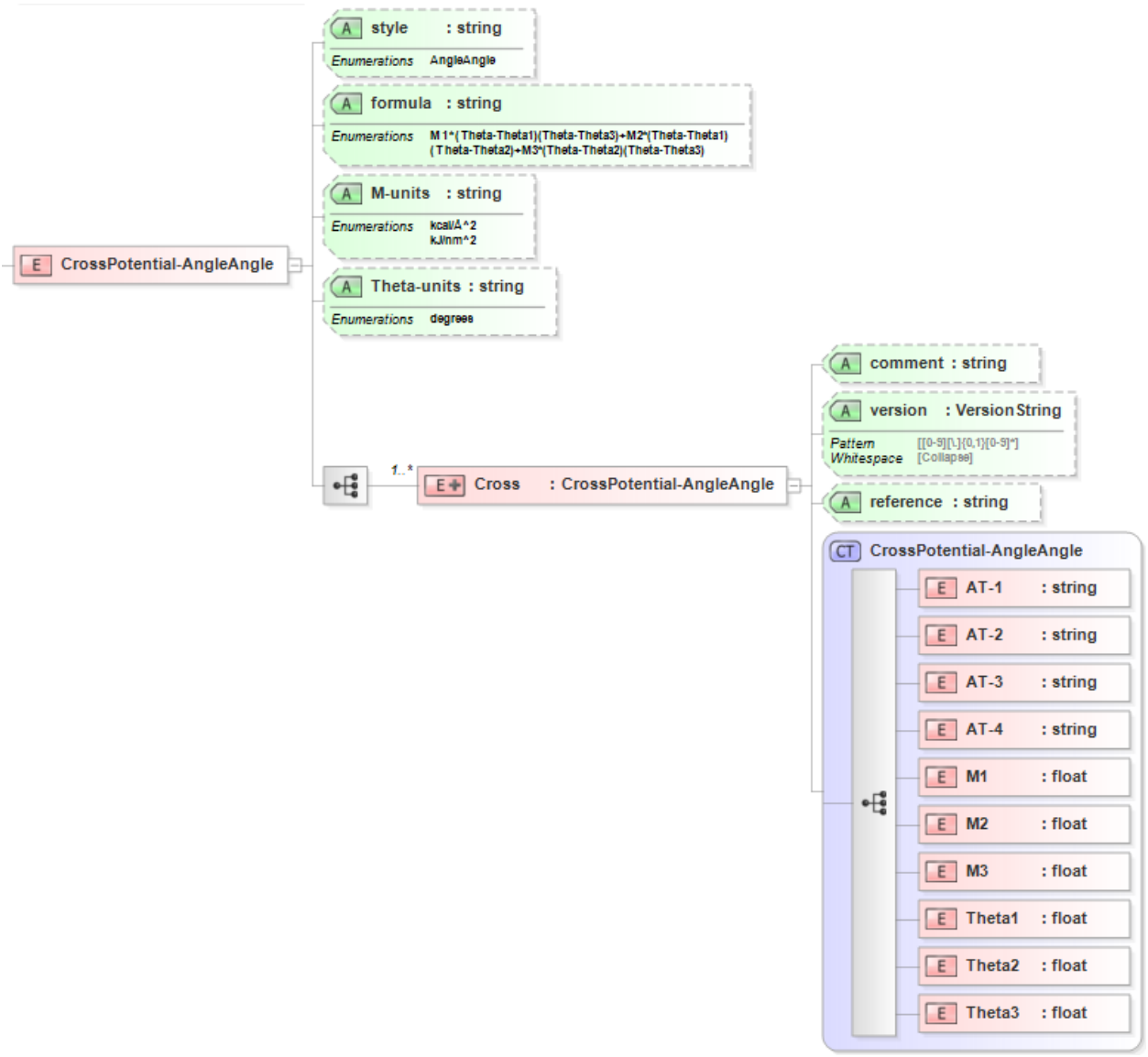
This term is part of the Class2 Improper Potential style.

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$M_{1,ijkl}$	Cross potential angle coefficient for atoms [i,j,k,l]	energy
$M_{2,ijkl}$	Cross potential angle coefficient for atoms [i,j,k,l]	energy
$M_{3,ijkl}$	Cross potential angle coefficient for atoms [i,j,k,l]	energy
$\theta_{1,ijk}$	Equilibrium angle for atoms [i,j,k]	degrees
$\theta_{2,ijl}$	Equilibrium angle for atoms [i,j,l]	degrees
$\theta_{3,kjl}$	Equilibrium angle for atoms [k,j,l]	degrees

17.3.2 XML Schema

The XML schema for the **Angle-Angle Cross Potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Cross potential angle coefficient for atoms [i,j,k,l]	$M_{1,ijkl}$	M1
Cross potential angle coefficient for atoms [i,j,k,l]	$M_{2,ijkl}$	M2
Cross potential angle coefficient for atoms [i,j,k,l]	$M_{3,ijkl}$	M3
Equilibrium angle for atoms [i,j,k]	$\theta_{1,ijk}$	Theta1
Equilibrium angle for atoms [i,j,l]	$\theta_{2,ijl}$	Theta2
Equilibrium angle for atoms [k,j,l]	$\theta_{3,kjl}$	Theta3

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	AngleAngle
formula	Fixed	M1*(Theta-Theta1)(Theta-Theta3)+M2*(Theta-Theta1)(Theta-Theta2)+M3*(Theta-Theta2)(Theta-Theta3)
M-units	Required	Enumerations specified in schema
Theta-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

17.3.3 References

1. LAMMPS Class2 Improper Potential w/ Angle-Angle Cross term.
2. SklogWiki COMPASS Force-Field.
3. Liquid XML Studio.

17.4 Cross: Bond-Angle

17.4.1 Functional Form

The **Bond-Angle Cross Potential** has the functional form:

$E = N_{1,ijk}\left(R_{ij} - R_{1,ij}\right)\left(\theta_{ijk} - \theta_{0,ijk}\right) + N_{2,ijk}\left(R_{jk} - R_{2,jk}\right)\left(\theta_{ijk} - \theta_{0,ijk}\right)$

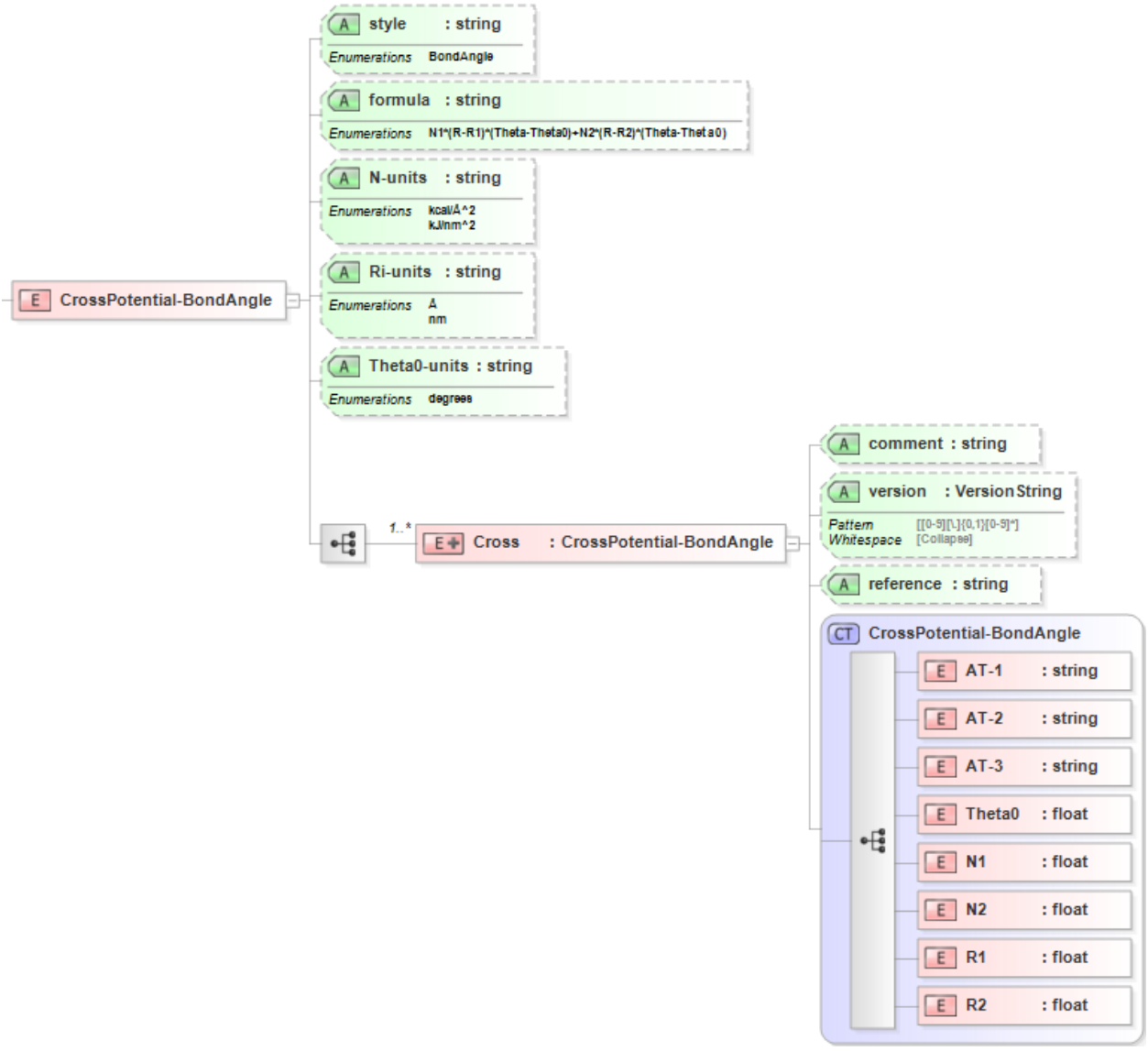
This term is part of the Class2 Angle Potential style.

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$N_{1,ijk}$	Cross potential bond-angle coefficient for atoms [i,j,k]	energy/length/degrees
$N_{2,ijk}$	Cross potential bond-angle coefficient for atoms [i,j,k]	energy/length/degrees
$R_{1,ij}$	Equilibrium bond length for atoms [i,j]	length
$R_{2,jk}$	Equilibrium bond length for atoms [j,k]	length
$\theta_{0,ijk}$	Equilibrium angle for atoms [i,j,k]	degrees

17.4.2 XML Schema

The XML schema for the **Bond-Angle Cross Potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Equilibrium angle for atoms [i,j,k]	$\theta_{0,ijk}$	Theta0
Cross potential bond-angle coefficient for atoms [i,j,k]	$N_{1,ijk}$	N1
Cross potential bond-angle coefficient for atoms [i,j,k]	$N_{2,ijk}$	N2
Equilibrium bond length for atoms [i,j]	$R_{1,ij}$	R1
Equilibrium bond length for atoms [j,k]	$R_{2,jk}$	R2

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	BondAngle
formula	Fixed	N1*(R-R1)*(Theta-Theta0)+N2*(R-R2)*(Theta-Theta0)
N-units	Required	Enumerations specified in schema
Ri-units	Required	Enumerations specified in schema
Theta0-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

17.4.3 References

1. LAMMPS Class2 Angle Potential w/ Bond-Angle Cross term.
2. SklogWiki COMPASS Force-Field.
3. Liquid XML Studio.

17.5 Cross: Middle-Bond-Torsion

17.5.1 Functional Form

The **Middle-Bond-Torsion Cross Potential** has the functional form:

$E = (R_{jk} - R_{2,jk}) \left[A_{1,ijkl} \cos(\phi_{ijkl}) + A_{2,ijkl} \cos(2\phi_{ijkl}) + A_{3,ijkl} \cos(3\phi_{ijkl})\right]$

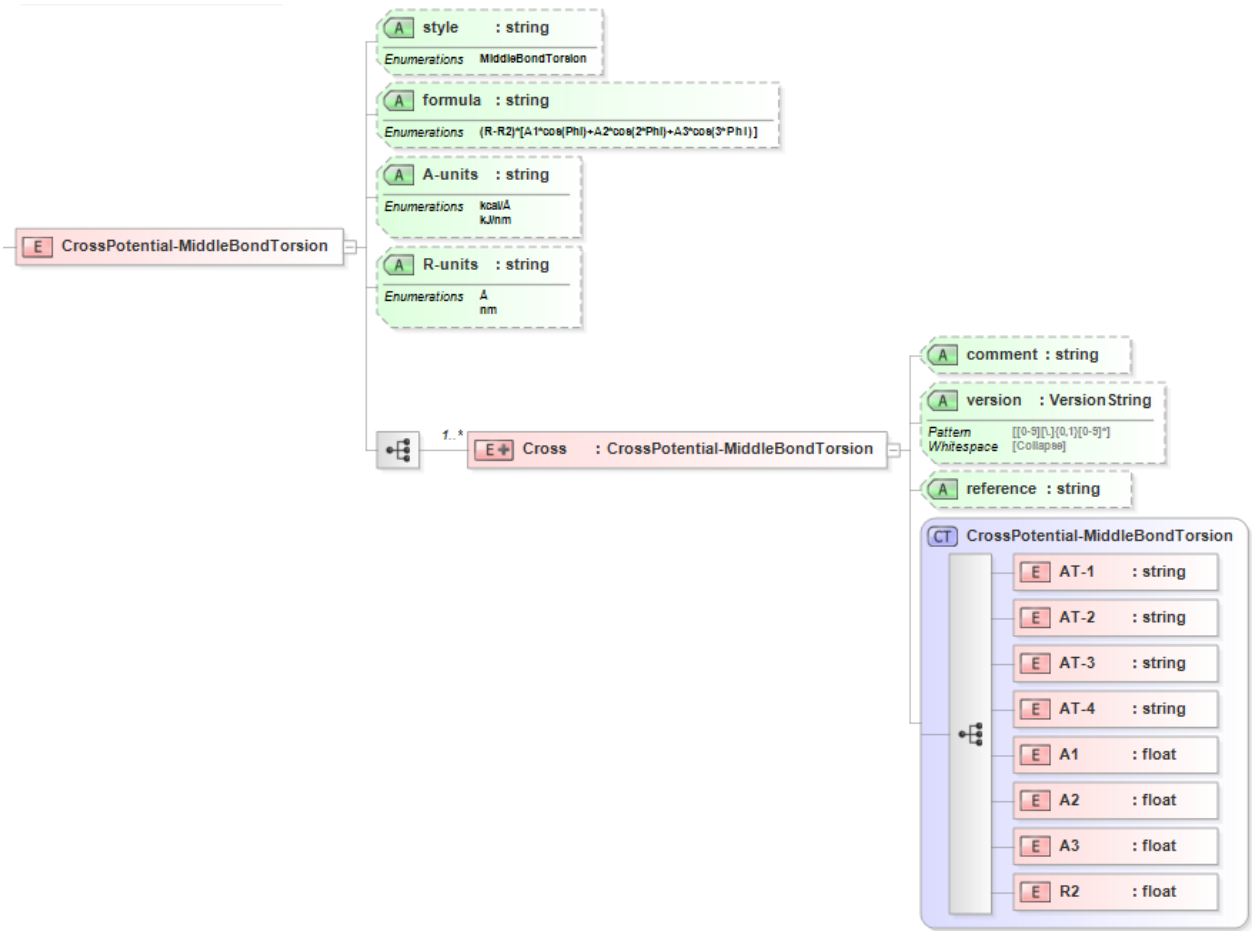
This term is part of the Class2 Dihedral Potential style.

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$A_{1,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/length
$A_{2,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/length
$A_{3,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/length
$R_{2,jk}$	Equilibrium bond length for atoms [j,k]	length

17.5.2 XML Schema

The XML schema for the **Middle-Bond-Torsion Cross Potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Cosine term coefficient for atoms [i,j,k,l]	$A_{1,ijkl}$	A1
Cosine term coefficient for atoms [i,j,k,l]	$A_{2,ijkl}$	A2
Cosine term coefficient for atoms [i,j,k,l]	$A_{3,ijkl}$	A3
Equilibrium bond length for atoms [j,k]	$R_{2,jk}$	R2

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	MiddleBondTorsion
formula	Fixed	(R-R2)*[A1*cos(Phi)+A2*cos(2*Phi)+A3*cos(3*Phi)]
A-units	Required	Enumerations specified in schema
R-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

17.5.3 References

1. LAMMPS Class2 Dihedral Potential w/ Middle-Bond-Torsion Cross term.
2. SklogWiki COMPASS Force-Field.
3. Liquid XML Studio.

17.6 Cross: End-Bond-Torsion

17.6.1 Functional Form

The **End-Bond-Torsion Cross Potential** has the functional form:

$$E = (R_{jk} - R_{1,jk}) \left[B_{1,ijkl} \cos(\phi_{ijkl}) + B_{2,ijkl} \cos(2\phi_{ijkl}) + B_{3,ijkl} \cos(3\phi_{ijkl})\right] + (R_{kl} - R_{3,kl}) \left[C_{1,ijkl} \cos(\phi_{ijkl}) + C_{2,ijkl} \cos(2\phi_{ijkl}) + C_{3,ijkl} \cos(3\phi_{ijkl})\right]$$

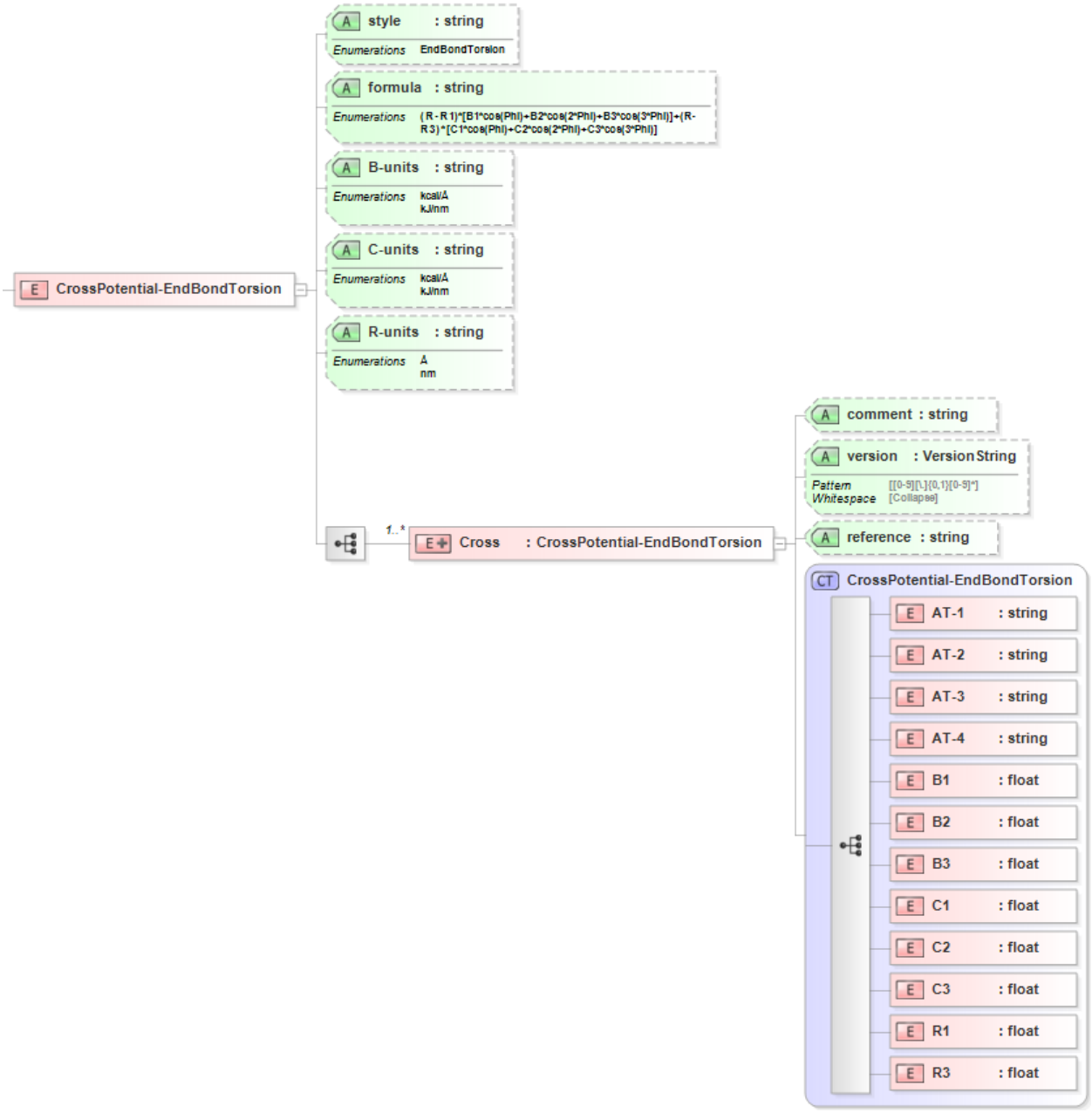
This term is part of the Class2 Dihedral Potential style.

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$B_{1,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/length
$B_{2,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/length
$B_{3,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/length
$C_{1,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/length
$C_{2,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/length
$C_{3,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/length
$R_{1,jk}$	Equilibrium bond length for atoms [i,j]	length
$R_{3,kl}$	Equilibrium bond length for atoms [k,l]	length

17.6.2 XML Schema

The XML schema for the **End-Bond-Torsion Cross Potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Cosine term coefficient for atoms [i,j,k,l]	$B_{1,ijkl}$	B1
Cosine term coefficient for atoms [i,j,k,l]	$B_{2,ijkl}$	B2
Cosine term coefficient for atoms [i,j,k,l]	$B_{3,ijkl}$	B3
Cosine term coefficient for atoms [i,j,k,l]	$C_{1,ijkl}$	C1
Cosine term coefficient for atoms [i,j,k,l]	$C_{2,ijkl}$	C2
Cosine term coefficient for atoms [i,j,k,l]	$C_{3,ijkl}$	C3
Equilibrium bond length for atoms [i,j]	$R_{1,ij}$	R1
Equilibrium bond length for atoms [k,l]	$R_{3,kl}$	R3

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	EndBondTorsion
formula	Fixed	(R-R1)*[B1*cos(Phi)+B2*cos(2*Phi)+B3*cos(3*Phi)]+(R-R3)*[C1*cos(Phi)+C2*cos(2*Phi)+C3*cos(3*Phi)]
B-units	Required	Enumerations specified in schema
C-units	Required	Enumerations specified in schema
R-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

17.6.3 References

1. LAMMPS Class2 Dihedral Potential w/ End-Bond-Torsion Cross term.
2. SklogWiki COMPASS Force-Field.
3. Liquid XML Studio.

17.7 Cross: Angle-Torsion

17.7.1 Functional Form

The **Angle-Torsion Cross Potential** has the functional form:

$$E = (\theta_{ijk} - \theta_{1,ijk}) \left[D_{1,ijkl} \cos(\phi_{ijkl}) + D_{2,ijkl} \cos(2\phi_{ijkl}) + D_{3,ijkl} \cos(3\phi_{ijkl})\right] + (\theta_{jkl} - \theta_{2,jkl}) \left[E_{1,ijkl} \cos(\phi_{ijkl}) + E_{2,ijkl} \cos(2\phi_{ijkl}) + E_{3,ijkl} \cos(3\phi_{ijkl})\right]$$

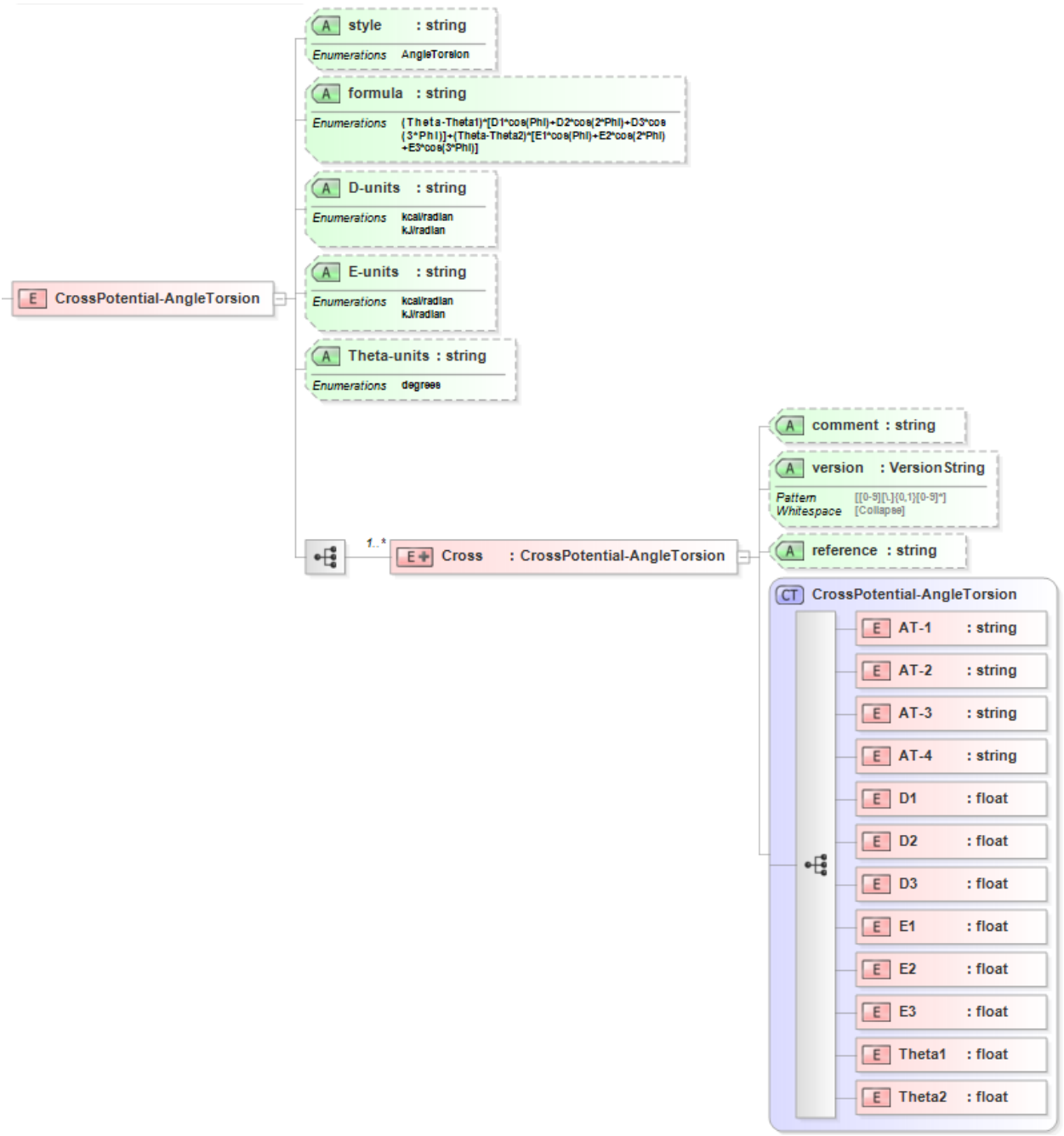
This term is part of the Class2 Dihedral Potential style.

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
$D_{1,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/degrees
$D_{2,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/degrees
$D_{3,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/degrees
$E_{1,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/degrees
$E_{2,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/degrees
$E_{3,ijkl}$	Cosine term coefficient for atoms [i,j,k,l]	energy/degrees
$\theta_{1,ijk}$	Equilibrium bond length for atoms [i,j]	degrees
$\theta_{2,jkl}$	Equilibrium bond length for atoms [k,l]	degrees

17.7.2 XML Schema

The XML schema for the **Angle-Torsion Cross Potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Cosine term coefficient for atoms [i,j,k,l]	$D_{1,ijkl}$	D1
Cosine term coefficient for atoms [i,j,k,l]	$D_{2,ijkl}$	D2
Cosine term coefficient for atoms [i,j,k,l]	$D_{3,ijkl}$	D3
Cosine term coefficient for atoms [i,j,k,l]	$E_{1,ijkl}$	E1
Cosine term coefficient for atoms [i,j,k,l]	$E_{2,ijkl}$	E2
Cosine term coefficient for atoms [i,j,k,l]	$E_{3,ijkl}$	E3
Equilibrium bond length for atoms [i,j]	$\theta_{1,ijk}$	Theta1
Equilibrium bond length for atoms [k,l]	$\theta_{2,jkl}$	Theta2

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	AngleTorsion
formula	Fixed	(Theta-Theta1)*[D1*cos(Phi)+D2*cos(2*Phi)+D3*cos(3*Phi)]+(Theta-Theta2)*[E1*cos(Phi)+E2*cos(2*Phi)+E3*cos(3*Phi)]
D-units	Required	Enumerations specified in schema
E-units	Required	Enumerations specified in schema
Theta-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

17.7.3 References

1. LAMMPS Class2 Dihedral Potential w/ Angle-Torsion Cross term.
2. SklogWiki COMPASS Force-Field.
3. Liquid XML Studio.

17.8 Cross: Angle-Angle-Torsion

17.8.1 Functional Form

The **Angle-Angle-Torsion Cross Potential** has the functional form:

$$E = M_{ijkl} \left(\theta_{ijk} - \theta_{1,ijk}\right) \left(\theta_{jkl} - \theta_{2,jkl}\right) \cos\left(\phi_{ijkl}\right)$$

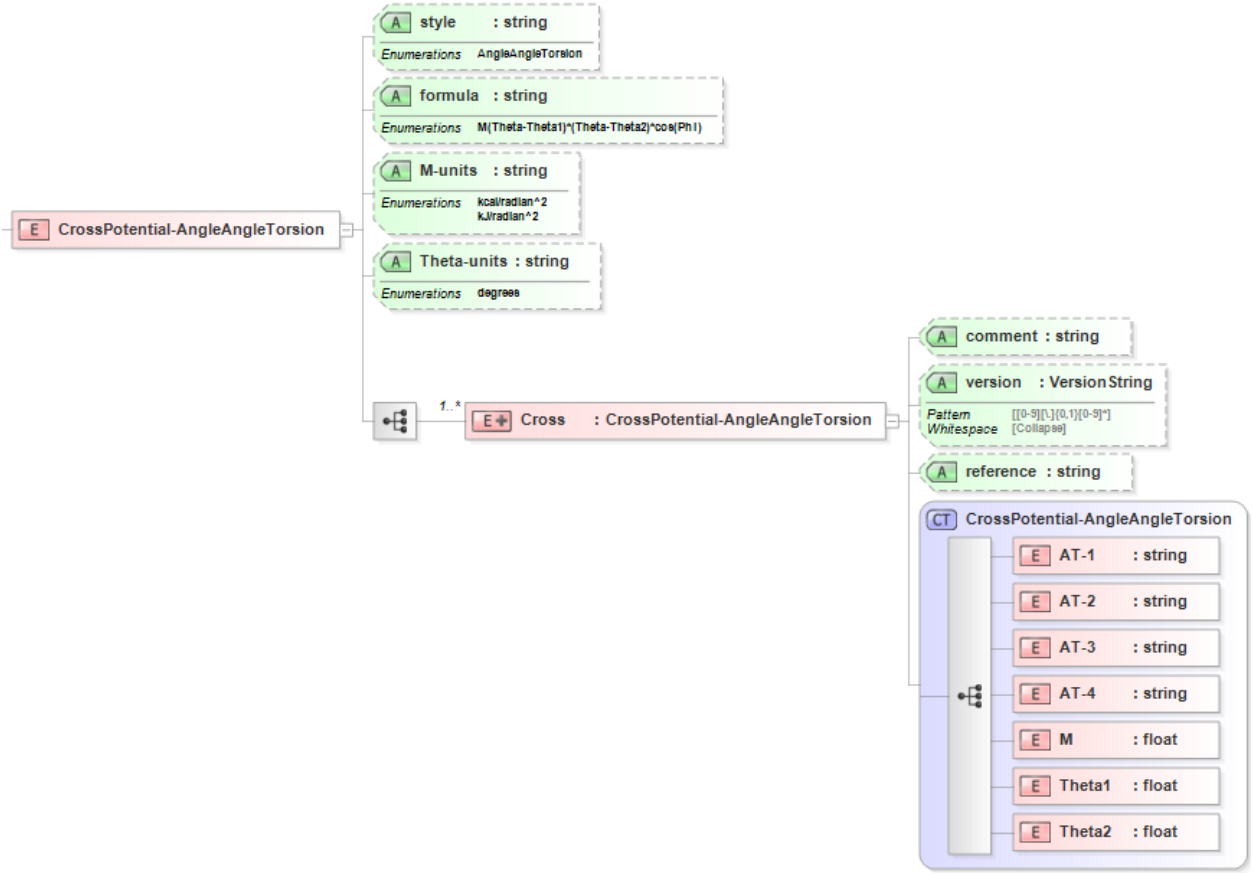
This term is part of the Class2 Dihedral Potential style.

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
M_{ijkl}	Bond coefficient for atoms [i,j,k,l]	energy
$\theta_{1,ijk}$	Equilibrium angle for atoms [i,j,k]	degrees
$\theta_{2,jkl}$	Equilibrium angle for atoms [j,k,l]	degrees

17.8.2 XML Schema

The XML schema for the **Angle-Angle-Torsion Cross Potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Atom type of atom [k]	k	AT-3
Atom type of atom [l]	l	AT-4
Bond coefficient for atoms [i,j,k,l]	M_{ijkl}	M
Equilibrium angle for atoms [i,j,k]	$\theta_{1,ijk}$	Theta1
Equilibrium angle for atoms [j,k,l]	$\theta_{2,jkl}$	Theta2

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	AngleAngleTorsion
formula	Fixed	M(Theta-Theta1)*(Theta-Theta2)*cos(Phi)
M-units	Required	Enumerations specified in schema
Theta-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

17.8.3 References

1. LAMMPS Class2 Dihedral Potential w/ Angle-Angle-Torsion Cross term.
2. SklogWiki COMPASS Force-Field.
3. Liquid XML Studio.

CHAPTER 18

Non-Bond Potentials

18.1 Non-Bond Lennard-Jones Potential

18.1.1 Functional Form

The **non-bond Lennard-Jones potential** has the functional form:

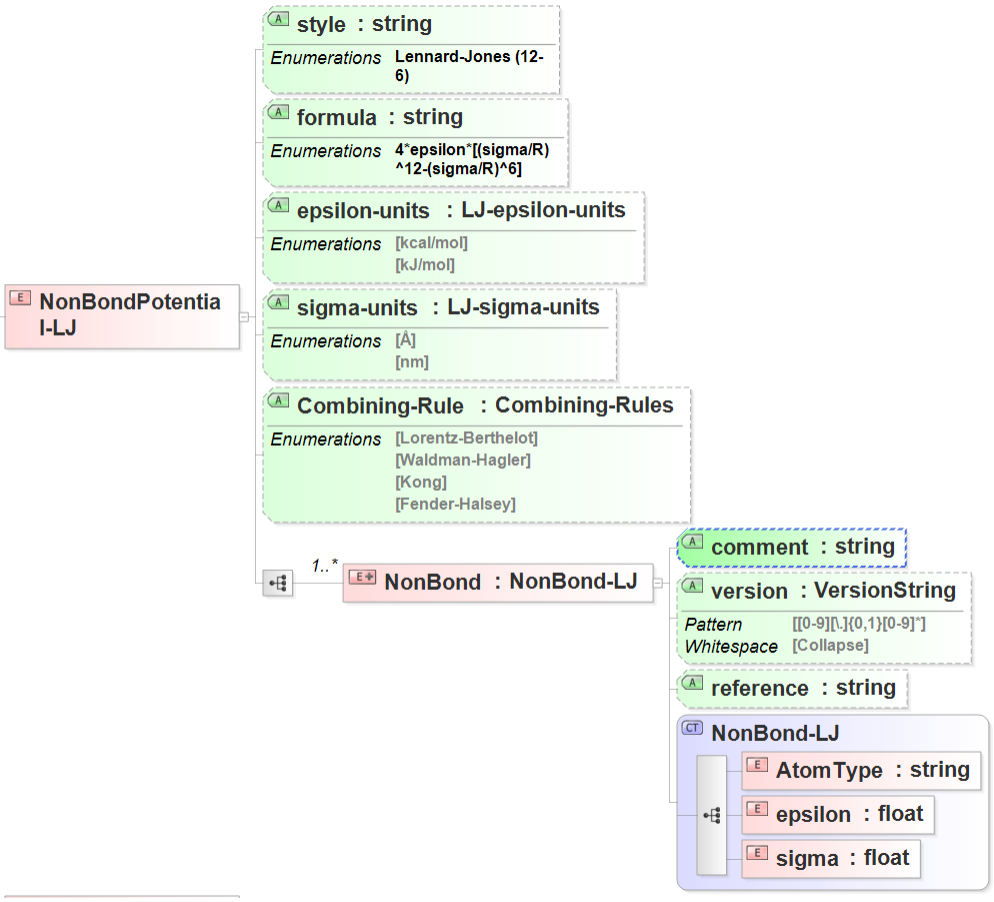
$$E = 4 \cdot \epsilon \cdot \left[\left(\frac{\sigma}{R_{ij}} \right)^{12} - \left(\frac{\sigma}{R_{ij}} \right)^{6} \right]$$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
ϵ	Potential well depth for atom [i]	energy/mol
σ	Interatomic cut-off distance for atom [i]	length

18.1.2 XML Schema

The XML schema for the **non-bond Lennard-Jones potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AtomType
Potential well depth for atom [i]	ϵ	epsilon
Interatomic cut-off distance for atom [i]	σ	sigma

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Lennard-Jones (12-6)
formula	Fixed	4*epsilon*[(sigma/R)^12-(sigma/R)^6]
epsilon-units	Required	Enumerations specified in schema
sigma-units	Required	Enumerations specified in schema
Combining-Rule	Required	Combining rule for mixed atom types

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.1.3 References

1. LAMMPS Lennard-Jones Pair Potential.
2. **'GROMACS Lennard-Jones Pair Potential'_** page 66.
3. Liquid XML Studio.

18.2 Non-Bond Lennard-Jones Potential

18.2.1 Functional Form

The **non-bond Lennard-Jones potential** has the functional form:

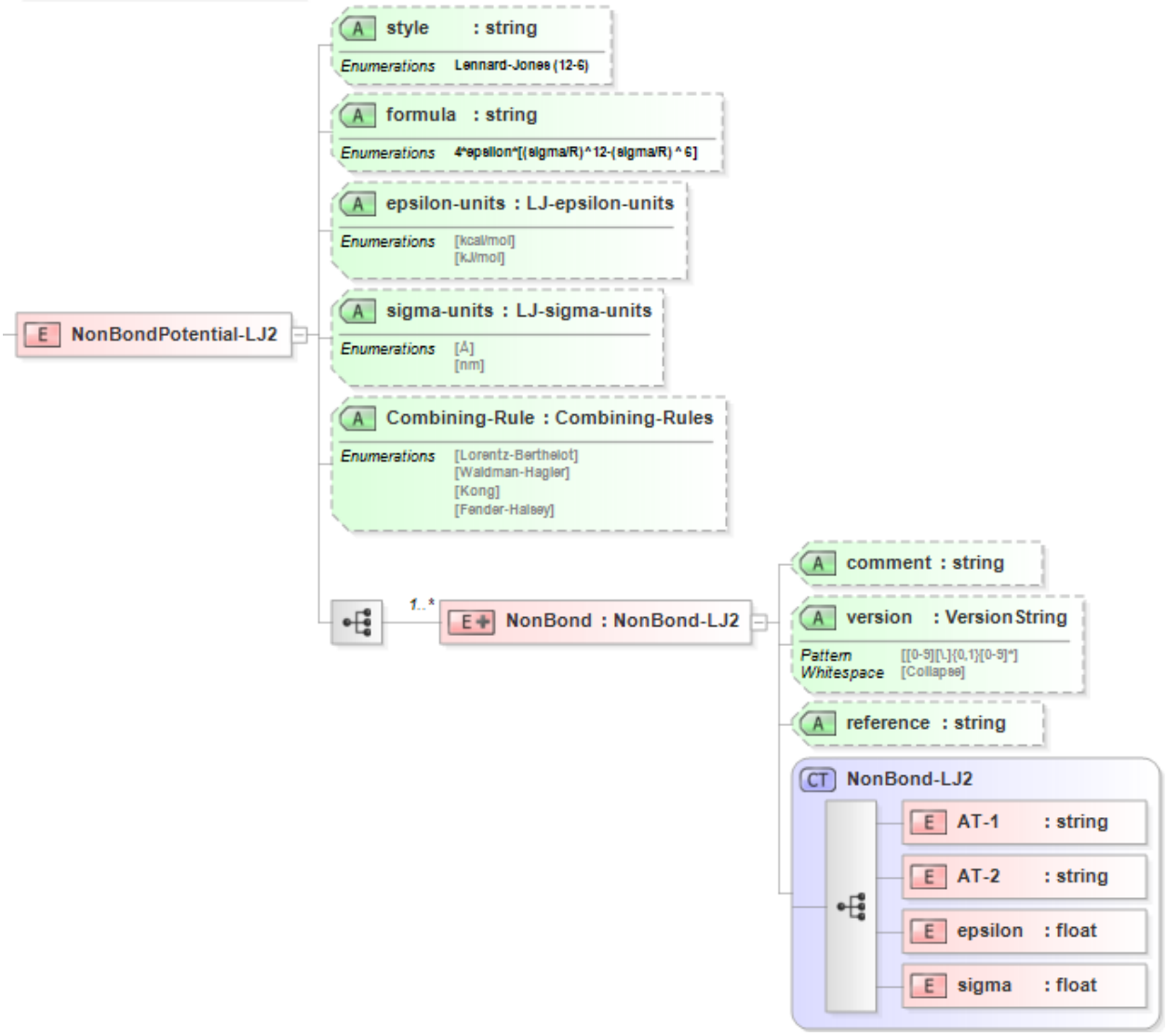
$$E = 4 \cdot \epsilon \cdot \left[\left(\frac{\sigma}{R_{ij}} \right)^{12} - \left(\frac{\sigma}{R_{ij}} \right)^{6} \right]$$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
ϵ	Potential well depth for atom [i]	energy/mol
σ	Interatomic cut-off distance for atom [i]	length

18.2.2 XML Schema

The XML schema for the **non-bond Lennard-Jones potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AT-1
Atom type of atom [j]	(implicit)	AT-2
Potential well depth for atom [i]	ϵ	epsilon
Interatomic cut-off distance for atom [i]	σ	sigma

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Lennard-Jones (12-6)
formula	Fixed	4*epsilon*[(sigma/R)^12-(sigma/R)^6]
epsilon-units	Required	Enumerations specified in schema
sigma-units	Required	Enumerations specified in schema
Combining-Rule	Required	Combining rule for mixed atom types

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.2.3 References

1. **'LAMMPS Lennard-Jones Pair Potential'_**.
2. **'GROMACS Lennard-Jones Pair Potential'_** page 66.
3. Liquid XML Studio.

18.3 Non-Bond Lennard-Jones (9-6 Form) Potential

18.3.1 Functional Form

The **non-bond Lennard-Jones (9-6 Form) potential** has the functional form:

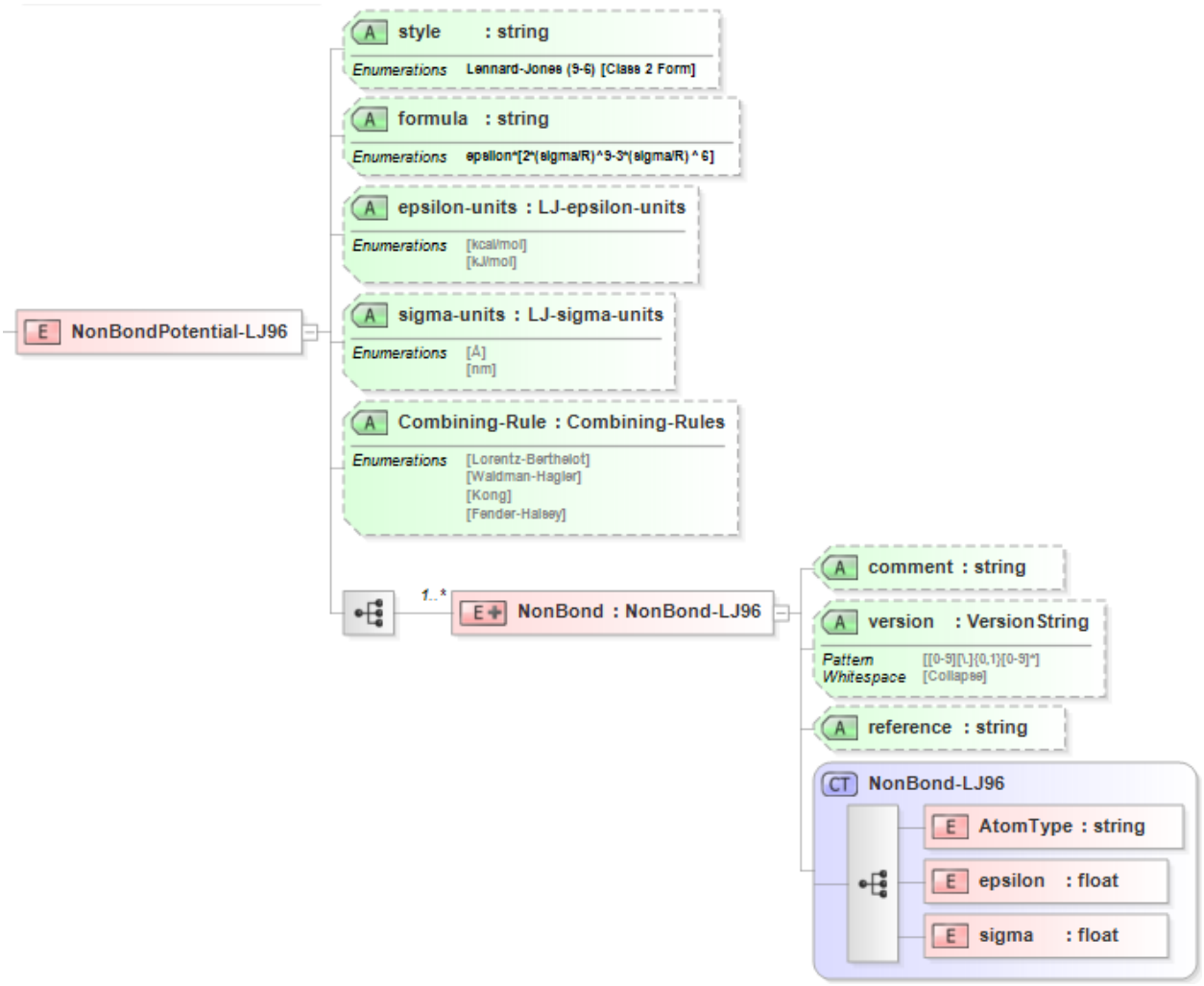
$$E = \epsilon \left[2\left(\frac{\sigma}{R_{ij}}\right)^9 - 3\left(\frac{\sigma}{R_{ij}}\right)^6 \right]$$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
ϵ	Potential well depth for atom [i]	energy/mol
σ	Interatomic cut-off distance for atom [i]	length

18.3.2 XML Schema

The XML schema for the **non-bond Lennard-Jones (9-6 Form) potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AtomType
Potential well depth for atom [i]	ϵ	epsilon
Interatomic cut-off distance for atom [i]	σ	sigma

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Lennard-Jones (9-6) [Class 2 Form]
formula	Fixed	epsilon*[2*(sigma/R)^9-3*(sigma/R)^6]
epsilon-units	Required	Enumerations specified in schema
sigma-units	Required	Enumerations specified in schema
Combining-Rule	Required	Combining rule for mixed atom types

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.3.3 References

1. LAMMPS Lennard-Jones Pair Potential Class 2.
2. Liquid XML Studio.

18.4 Non-Bond Lennard-Jones Potential - AB Form

18.4.1 Functional Form

The **non-bond Lennard-Jones (AB Form) potential** has the functional form:

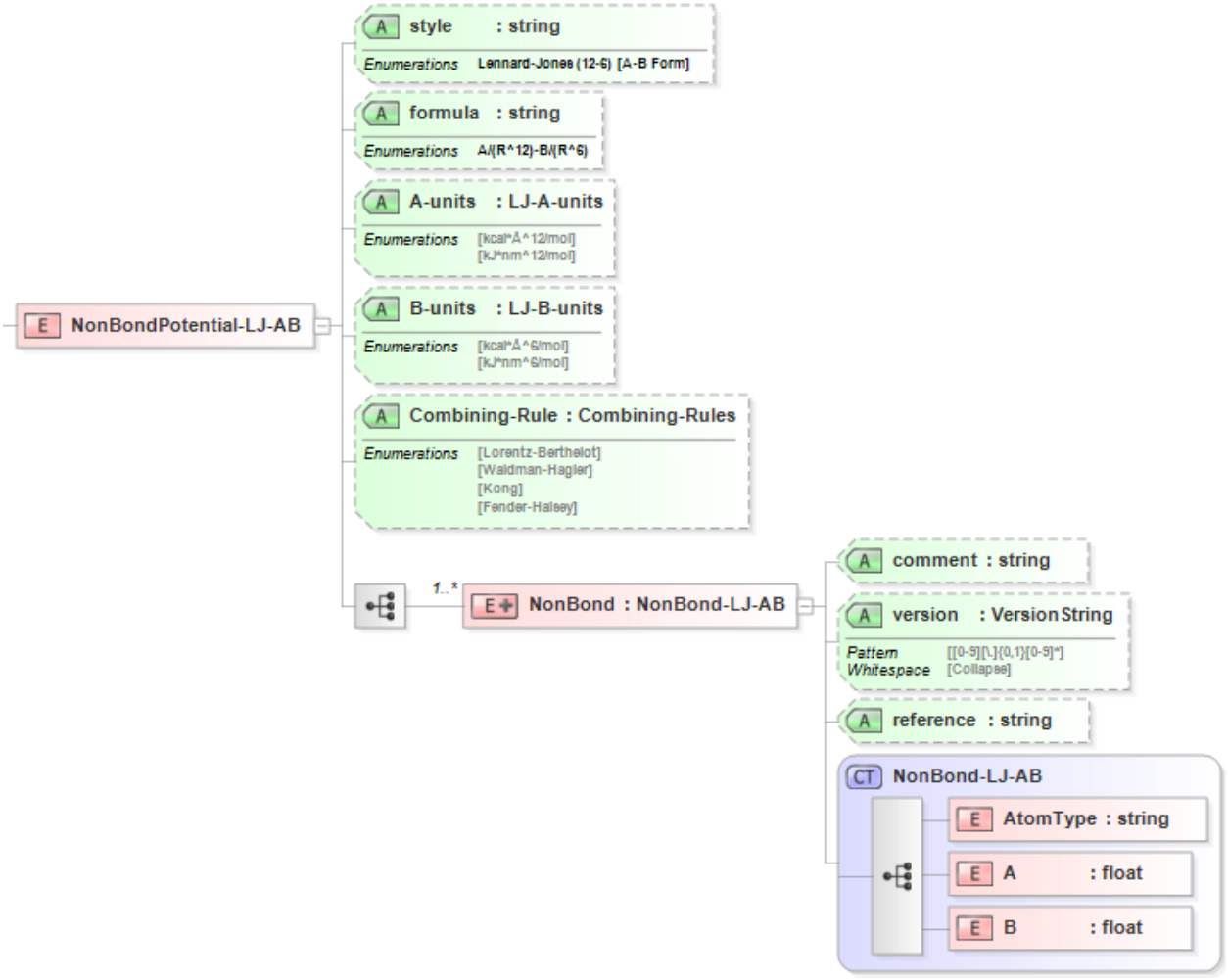
$E = \frac{A_{ij}}{R_{ij}^{12}} - \frac{B_{ij}}{R_{ij}^{6}}$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
A_{ij}	General 12th power Lennard-Jones coefficient [i]	energy*length^12/mol
B_{ij}	General 6th power Lennard-Jones coefficient [i]	energy*length^6/mol

18.4.2 XML Schema

The XML schema for the **non-bond Lennard-Jones (AB Form) potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AtomType
General 12th power Lennard-Jones coefficient [i]	A_{ij}	A
General 6th power Lennard-Jones coefficient [i]	B_{ij}	B

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Lennard-Jones (12-6) [A-B Form]
formula	Fixed	A/(R^12)-B/(R^6)
A–units	Required	Enumerations specified in schema
B-units	Required	Enumerations specified in schema
Combining-Rule	Required	Combining rule for mixed atom types

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.4.3 References

1. Amber 2017 Reference Manual page 248.
2. Wikipedia AMBER (Force-Fields).
3. Wikipedia Lennard-Jones Potential.

18.5 Non-Bond Lennard-Jones Potential - AB Form (Two atom types)

18.5.1 Functional Form

The **non-bond Lennard-Jones (AB Form) potential** has the functional form:

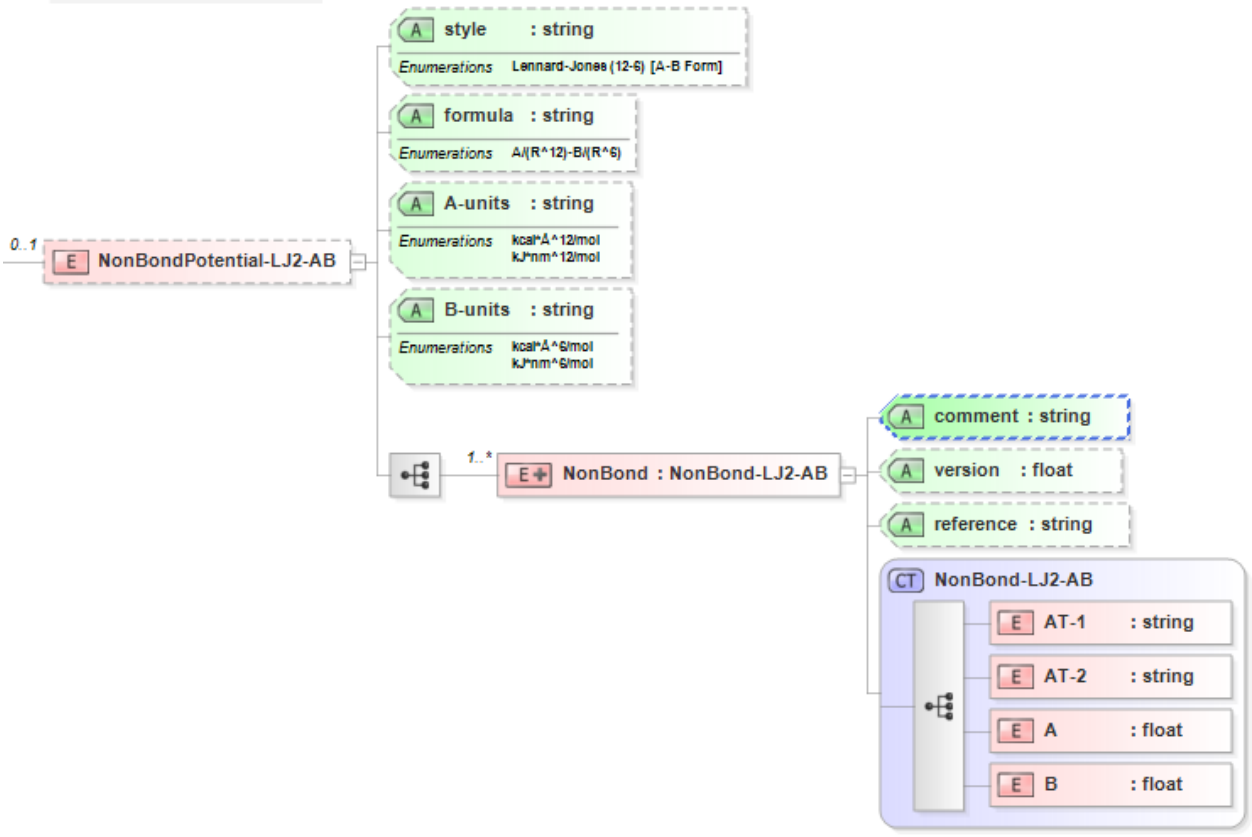
$E = \frac{A_{ij}}{R_{ij}^{12}} - \frac{B_{ij}}{R_{ij}^{6}}$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
A_{ij}	General 12th power Lennard-Jones coefficient [i]	energy*length^12/mol
B_{ij}	General 6th power Lennard-Jones coefficient [i]	energy*length^6/mol

18.5.2 XML Schema

The XML schema for the **non-bond Lennard-Jones (AB Form) potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AT-1
Atom type of atom [j]	(implicit)	AT-2
General 12th power Lennard-Jones coefficient [i]	A_{ij}	A
General 6th power Lennard-Jones coefficient [i]	B_{ij}	B

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Lennard-Jones (12-6) [A-B Form]
formula	Fixed	A/(R^12)-B/(R^6)
A–units	Required	Enumerations specified in schema
B-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.5.3 References

1. Amber 2017 Reference Manual page 248.
2. Wikipedia AMBER (Force-Fields).
3. Wikipedia Lennard-Jones Potential.

18.6 Non-Bond Lennard-Jones (Rmin Form) Potential

18.6.1 Functional Form

The **non-bond Lennard-Jones (Rmin Form) potential** has the functional form:

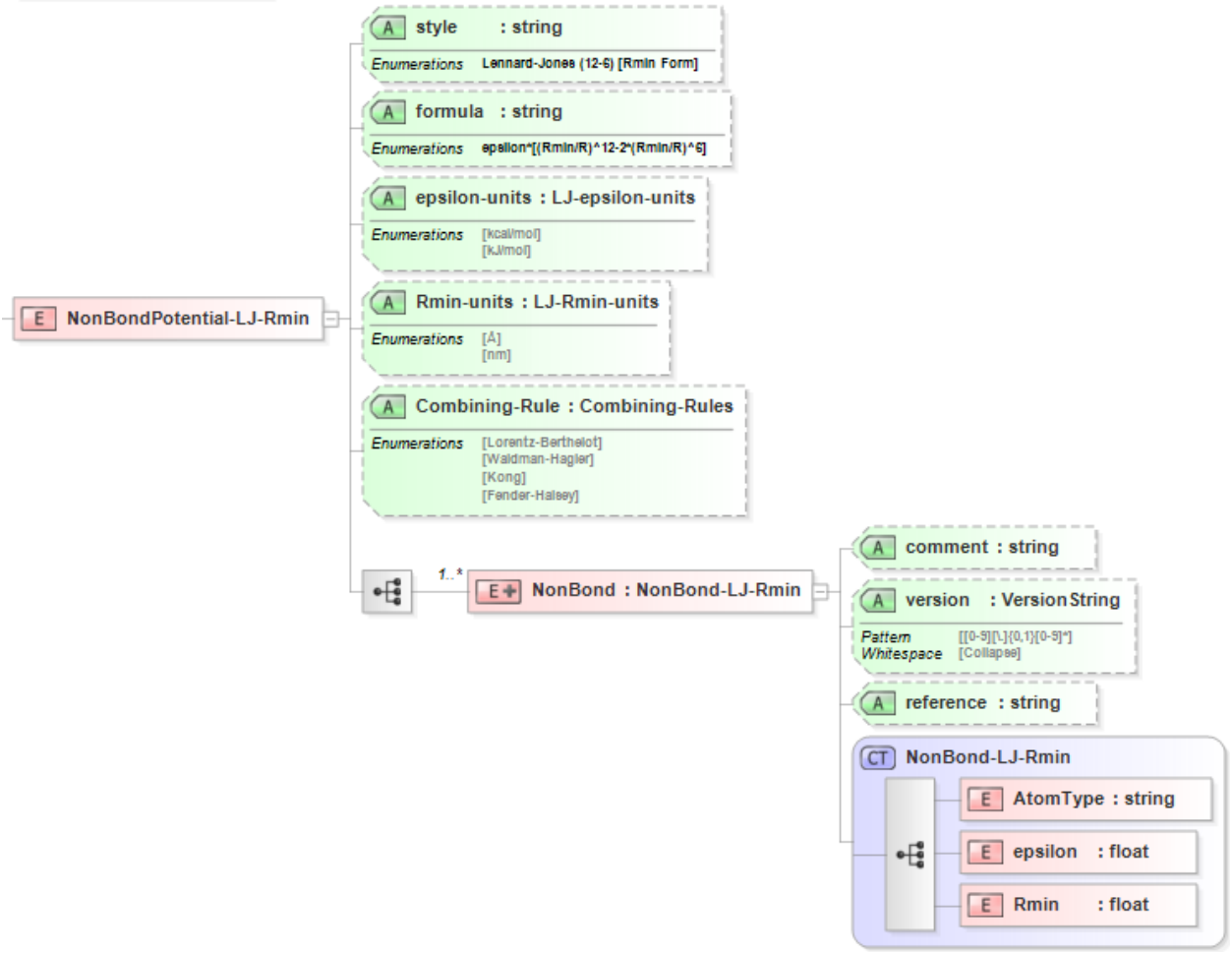
$$E = \epsilon \left[\left(\frac{R_{\min,ij}}{R_{ij}} \right)^{12} - 2 \left(\frac{R_{\min,ij}}{R_{ij}} \right)^{6} \right]$$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
ϵ	Potential well depth for atom [i]	energy/mol
$R_{min,ij}$	Interatomic cut-off distance for atom [i]	length

18.6.2 XML Schema

The XML schema for the **non-bond Lennard-Jones (Rmin Form) potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AtomType
Potential well depth for atom [i]	ϵ	epsilon
Distance at the Lennard-Jones minimum [i]	$R_{min,ij}$	Rmin

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Lennard-Jones (12-6) [Rmin Form]
formula	Fixed	epsilon*[(Rmin/R)^12-2*(Rmin/R)^6]
epsilon-units	Required	Enumerations specified in schema
Rmin-units	Required	Enumerations specified in schema
Combining-Rule	Required	Combining rule for mixed atom types

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.6.3 References

1. Amber 2017 Reference Manual page 248.
2. Wikipedia AMBER (Force-Fields).
3. Wikipedia Lennard-Jones Potential.

18.7 Non-Bond Lennard-Jones GROMACS Potential

18.7.1 Functional Form

The **non-bond Lennard-Jones GROMACS potential** has the functional form:

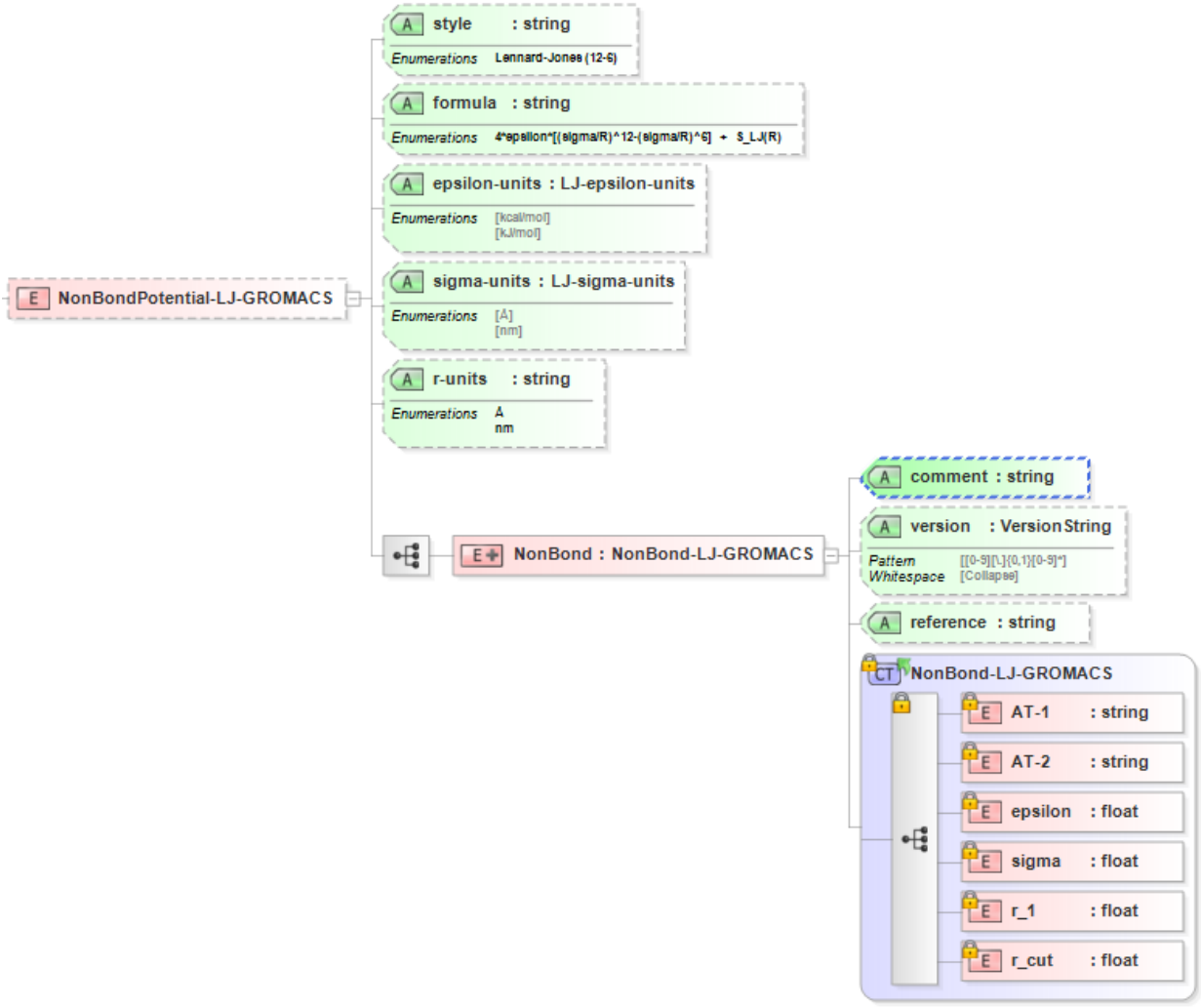
$$E = 4 \cdot \epsilon \cdot \left[\left(\frac{\sigma}{R_{ij}} \right)^{12} - \left(\frac{\sigma}{R_{ij}} \right)^{6} \right] + S_{LJ} \left(R_{ij} \right)$$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
ϵ	Potential well depth for atom [i]	energy/mol
σ	Interatomic cut-off distance for atom [i]	length

18.7.2 XML Schema

The XML schema for the **non-bond Lennard-Jones GROMACS potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AtomType
Potential well depth for atom [i]	ϵ	epsilon
Interatomic cut-off distance for atom [i]	σ	sigma
Inner cut-off distance for atom [i]		r_1
Outer cut-off distance for atom [i]		r_cut

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Lennard-Jones (12-6)
formula	Fixed	4*epsilon*[(sigma/R)^12-(sigma/R)^6] + S_LJ(R)
epsilon-units	Required	Enumerations specified in schema
sigma-units	Required	Enumerations specified in schema
r-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.7.3 References

1. **'LAMMPS Lennard-Jones GROMACS Potential'_**.
2. **'GROMACS Lennard-Jones Pair Potential (Modified non-bonded interactions)'_** page 69.
3. Liquid XML Studio.

18.8 Non-Bond Lennard-Jones (Class 2 Form) Potential

18.8.1 Functional Form

The **non-bond Lennard-Jones (Class 2 Form) potential** has the functional form:

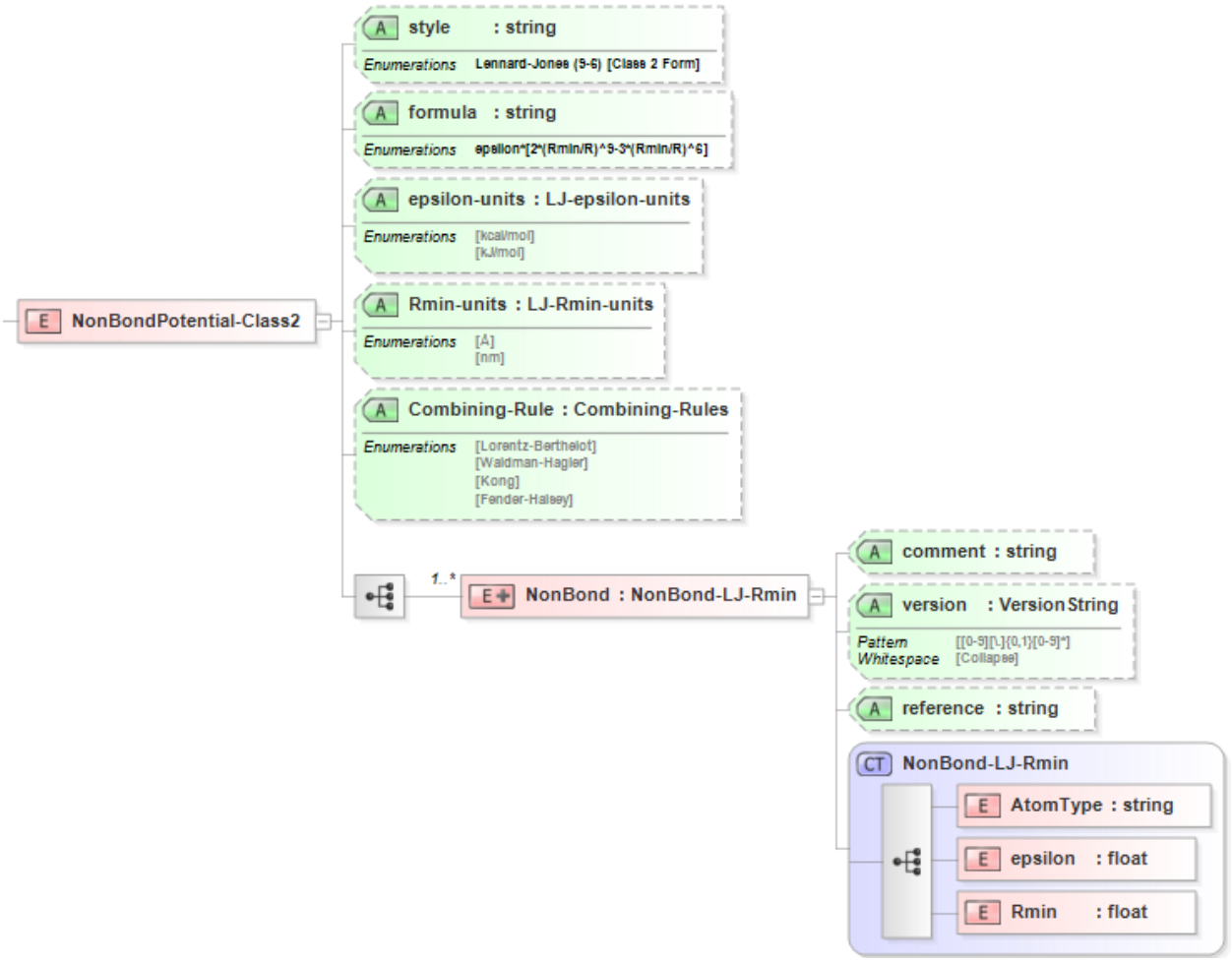
$$E = \epsilon \left[2\left(\frac{R_{min}}{R_{ij}}\right)^9 - 3\left(\frac{R_{min}}{R_{ij}}\right)^6 \right]$$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
ϵ	Potential well depth for atom [i]	energy/mol
R_{min}	Interatomic cut-off distance for atom [i]	length

18.8.2 XML Schema

The XML schema for the **non-bond Lennard-Jones (9-6 Form) potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AtomType
Potential well depth for atom [i]	ϵ	epsilon
Interatomic cut-off distance for atom [i]	σ	sigma

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Lennard-Jones (9-6) [Class 2 Form]
formula	Fixed	epsilon*[2*(Rmin/R)^9-3*(Rmin/R)^6]
epsilon-units	Required	Enumerations specified in schema
sigma-units	Required	Enumerations specified in schema
Combining-Rule	Required	Combining rule for mixed atom types

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.8.3 References

1. LAMMPS Lennard-Jones Pair Potential Class 2.
2. Liquid XML Studio.

18.9 Non-Bond Energy Renormalization Potential

18.9.1 Functional Form

The **non-bond Energy Renormalization potential** has the functional form:

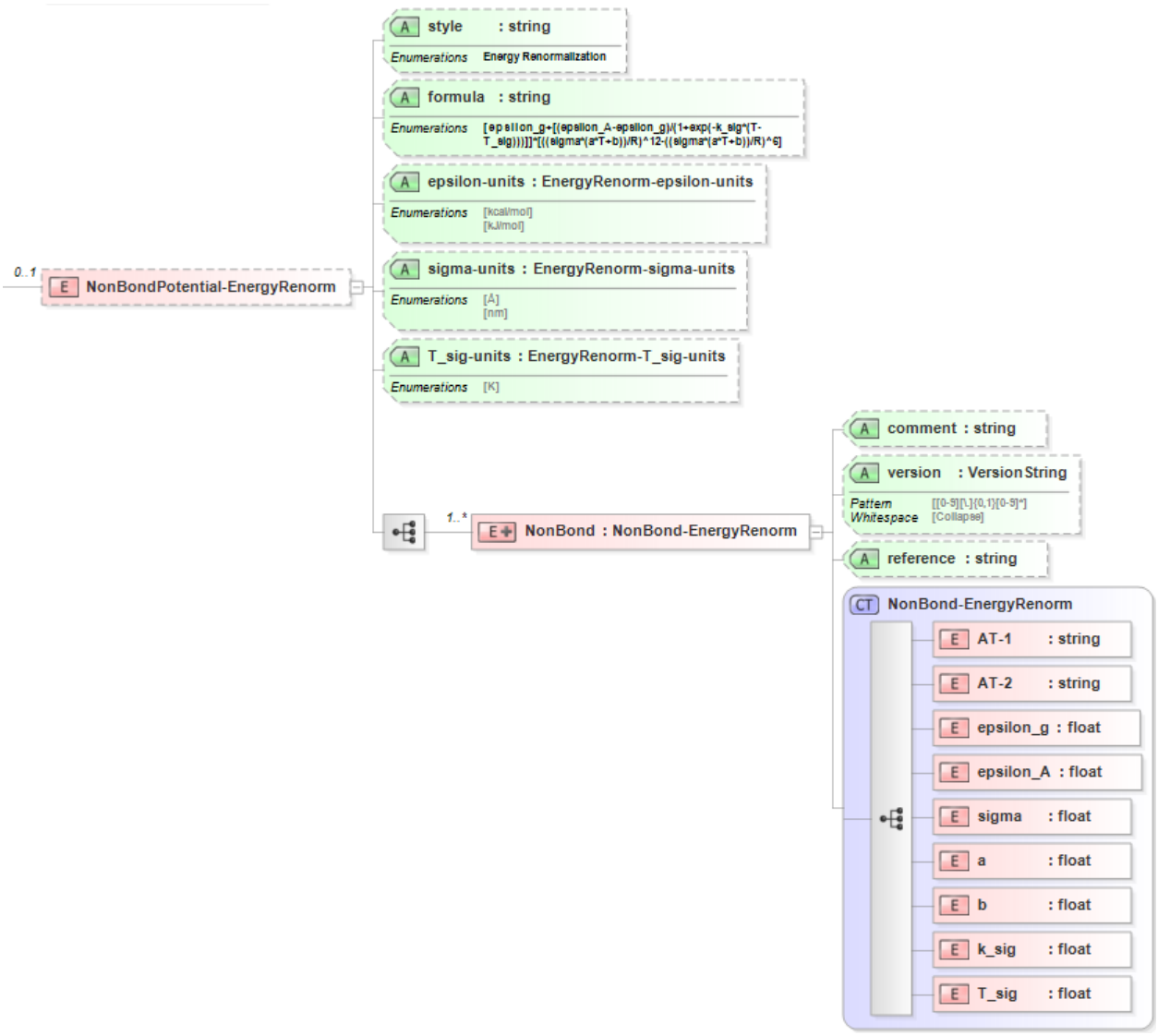
$E = (\epsilon_A - \epsilon_g)\left[\frac{1}{1+e^{-k(T-T_T)}}\right] + \epsilon_g$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
ϵ_A	Epsilon value in Arrhenius regime	energy/mol
ϵ_g	Epsilon value in glassy regime	energy/mol
k	Temperature breadth of the transition	N/A
T_T	Crossover point of sigmoidal function	temperature

18.9.2 XML Schema

The XML schema for the **non-bond Energy Renormalization potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AT1
Atom type of atom [j]	(implicit)	AT2
Epsilon value in Arrhenius regime	ϵ_A	epsilon_A
Epsilon value in glassy regime	ϵ_g	epsilon_g
Temperature breadth of the transition	k	k_sig
Exponent of attractive term	γ_{att}	n_att

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Mie
formula	Fixed	C*epsilon*[(sigma/R)^m_rep-(sigma/R)^n_att]
a_ij-units	Required	Enumerations specified in schema
r_c-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.9.3 References

1. LAMMPS Mie Pair Potential.
2. Liquid XML Studio.
3. Wenjie Xia, Jake Song, Cheol Jeong, David D. Hsu, Frederick R. Phelan Jr., Jack F. Douglas, Sinan Keten, "Energy-Renormalization for Achieving Temperature Transferable Coarse-Graining of Polymer Dynamics," Macromolecules, 50 (21), pp. 8787–8796, (2017). DOI: 10.1021/acs.macromol.7b01717
4. Wenjie Xia, Jake Song, Nitin H. Krishnamurthy, Frederick R. Phelan Jr., Sinan Keten, Jack F. Douglas, "Energy Renormalization for Coarse-Graining the Dynamics of a Model Glass-Forming Liquid," Journal of Physical Chemistry B, 122 (6), pp. 2040-2045, (2018). DOI: 10.1021/acs.jpcb.8b00321
5. Jake Song, David D. Hsu, Kenneth R. Shull, Frederick R. Phelan Jr., Jack F. Douglas, Wenjie Xia, Sinan Keten, "Energy Renormalization Method for the Coarse-Graining of Polymer Viscoelasticity," Macromolecules, 51(10), pp. 3818–3827, (2018). DOI: 10.1021/acs.macromol.7b02560
6. Wenjie Xia, Nitin K. Hansoge, Wen-Sheng Xu, Frederick R. Phelan Jr., Sinan Keten, and Jack F. Douglas, "Energy renormalization for coarse-graining polymers having different segmental structures," Science Advances 5(4), eaav4683, (19 Apr 2019). DOI: 10.1126/sciadv.aav4683

18.10 Non-Bond Mie Potential

18.10.1 Functional Form

The **non-bond Mie potential** has the functional form:

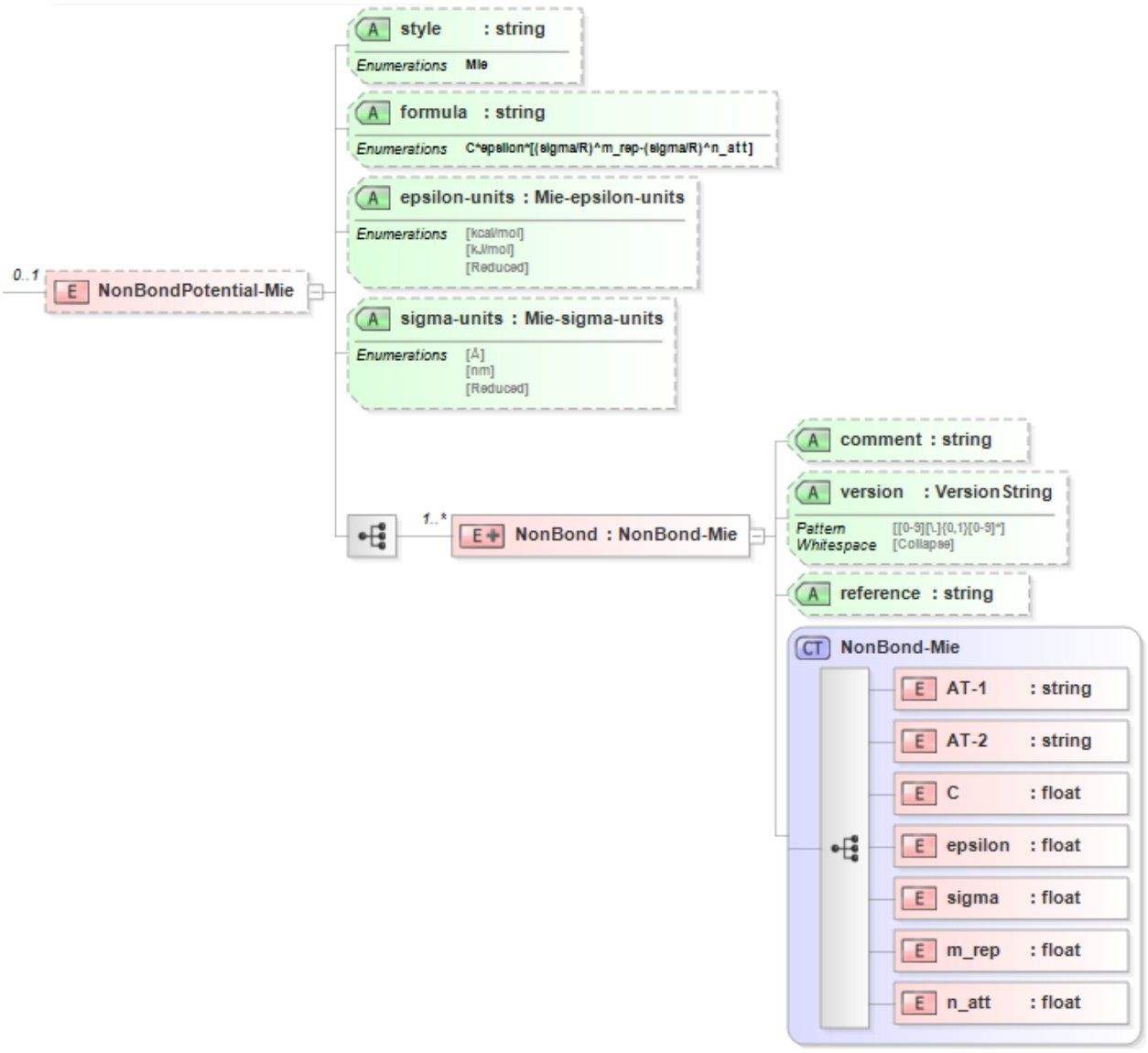
$$E = C\epsilon \left[\left(\frac{\sigma_{ij}}{R_{ij}} \right)^{\gamma_{rep}} - \left(\frac{\sigma_{ij}}{R_{ij}} \right)^{\gamma_{att}} \right]$$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
ϵ	Potential well depth for atom [i]	energy/mol
σ	Interatomic cut-off distance for atom [i]	length
γ_{rep}	Exponent of repulsive term	N/A
γ_{att}	Exponent of attractive term	N/A

18.10.2 XML Schema

The XML schema for the **non-bond Mie potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AT1
Atom type of atom [j]	(implicit)	AT2
Potential well depth for atom [i]	ϵ	epsilon
Interatomic cut-off distance for atom [i]	σ	sigma
Exponent of repulsive term	γ_{rep}	m_rep
Exponent of attractive term	γ_{att}	n_att

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Mie
formula	Fixed	C*epsilon*[(sigma/R)^m_rep-(sigma/R)^n_att]
a_ij-units	Required	Enumerations specified in schema
r_c-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.10.3 References

1. LAMMPS Mie Pair Potential.
2. Liquid XML Studio.

18.11 Non-Bond Soft Potential

18.11.1 Functional Form

The **non-bond Soft potential** has the functional form:

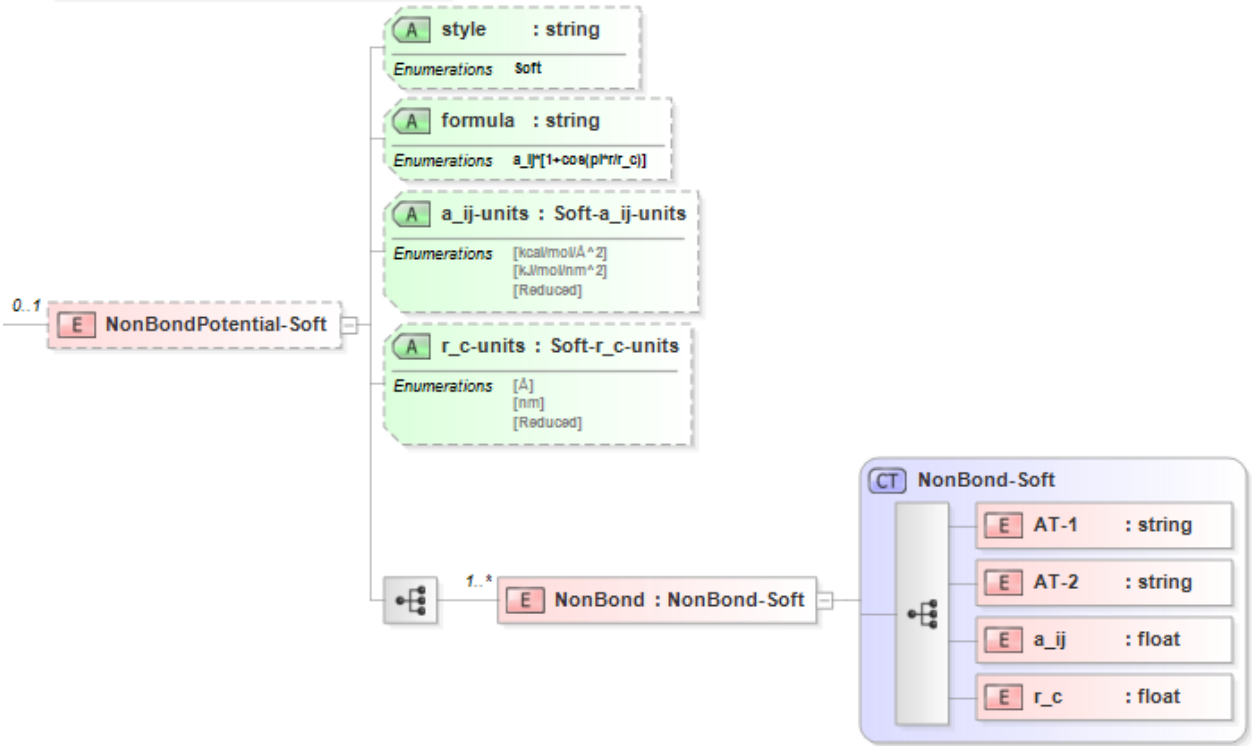
$E = A_{ij}\left[1 + \cos\left(\frac{\pi R}{R_c}\right)\right]$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
A_{ij}	Coefficient for atom [i]	energy/mol
R_c	Interatomic cut-off distance for atom [i]	length

18.11.2 XML Schema

The XML schema for the **non-bond Soft potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AT1
Atom type of atom [j]	(implicit)	AT2
Coefficient for atom [i]	A_{ij}	a_ij
Interatomic cut-off distance for atom [i]	R_c	r_c

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Soft
formula	Fixed	a_ij*[1+cos(pi*r/r_c)]
a_ij-units	Required	Enumerations specified in schema
r_c-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.11.3 References

1. LAMMPS Soft Pair Potential.
2. Liquid XML Studio.

18.12 Tabular Non-Bond

18.12.1 Tabular Form

The **tabular non-bond potential** has the parameters:

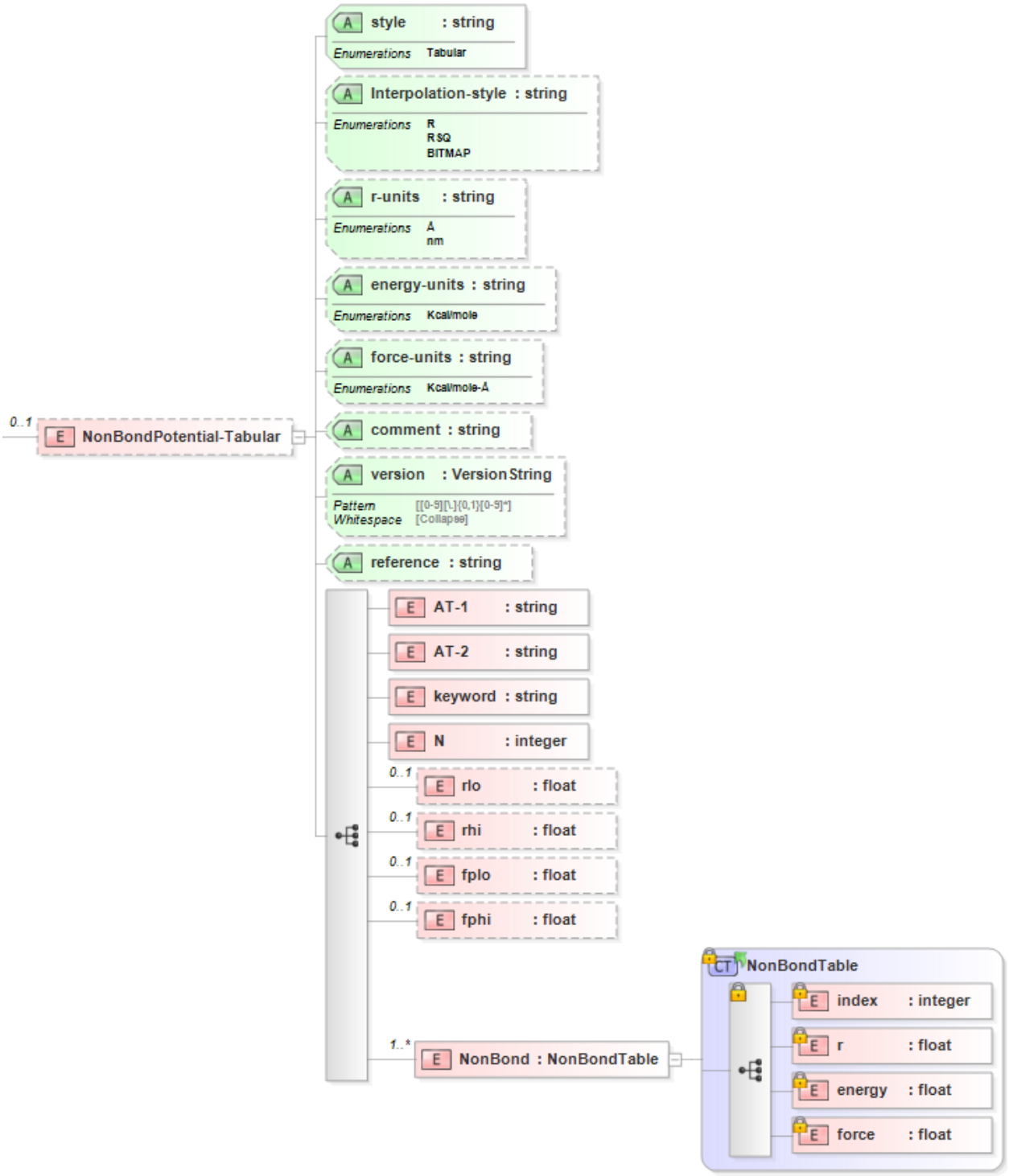
Parameter	Parameter Definition	Units
N	Number of tabulated values	N/A
R	Interatomic distance (least: rlo, greatest: rhi)	length
RSQ	Interatomic distance squared (least: rlo, greatest: rhi)	length^2
BITMAP	Determines ordering of tabulated values (least: rlo, greatest: rhi)	length
FPRIME	Derivatives of the force at the innermost (fplo) and outermost (fphi) bond lengths	force/length length^2

The **tabular non-bond potential** has the tabulated values:

index	r	energy	force
i_1	r_1	e_1	f_1
...	...	...	...
i_N	r_N	e_n	f_N

18.12.2 XML Schema

The XML schema for the **tabular non-ond potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the parameters/symbols and XML schema notations are given by:

Parameter Definition	Parameter/Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Section identifying keyword	N/A	keyword
Number of tabulated values	N	N
Interatomic distance (least)	R	rlo
Interatomic distance (greatest)	R	rhi
Interatomic distance squared (least)	RSQ	rlo
Interatomic distance squared (greatest)	RSQ	rhi
Determines ordering of tabulated values (least)	BITMAP	rlo
Determines ordering of tabulated values (greatest)	BITMAP	rhi
Derivative of the force at the innermost	FPRIME	fplo
Derivative of the force at the outermost	FPRIME	fphi
Index	index	index
Interatomic distance	r	r
Energy	energy	energy
Force	force	force

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Tabular
Interpolation-style	Required	Enumerations specified in schema
r-units	Required	Enumerations specified in schema
energy-units	Required	Enumerations specified in schema
force-units	Required	Enumerations specified in schema
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.12.3 References

1. LAMMPS Tabular Pair Potential.
2. Liquid XML Studio.

18.13 Non-Bond Weeks-Chandler-Anderson Potential

18.13.1 Functional Form

The **non-bond Weeks-Chandler-Anderson potential** has the functional form:

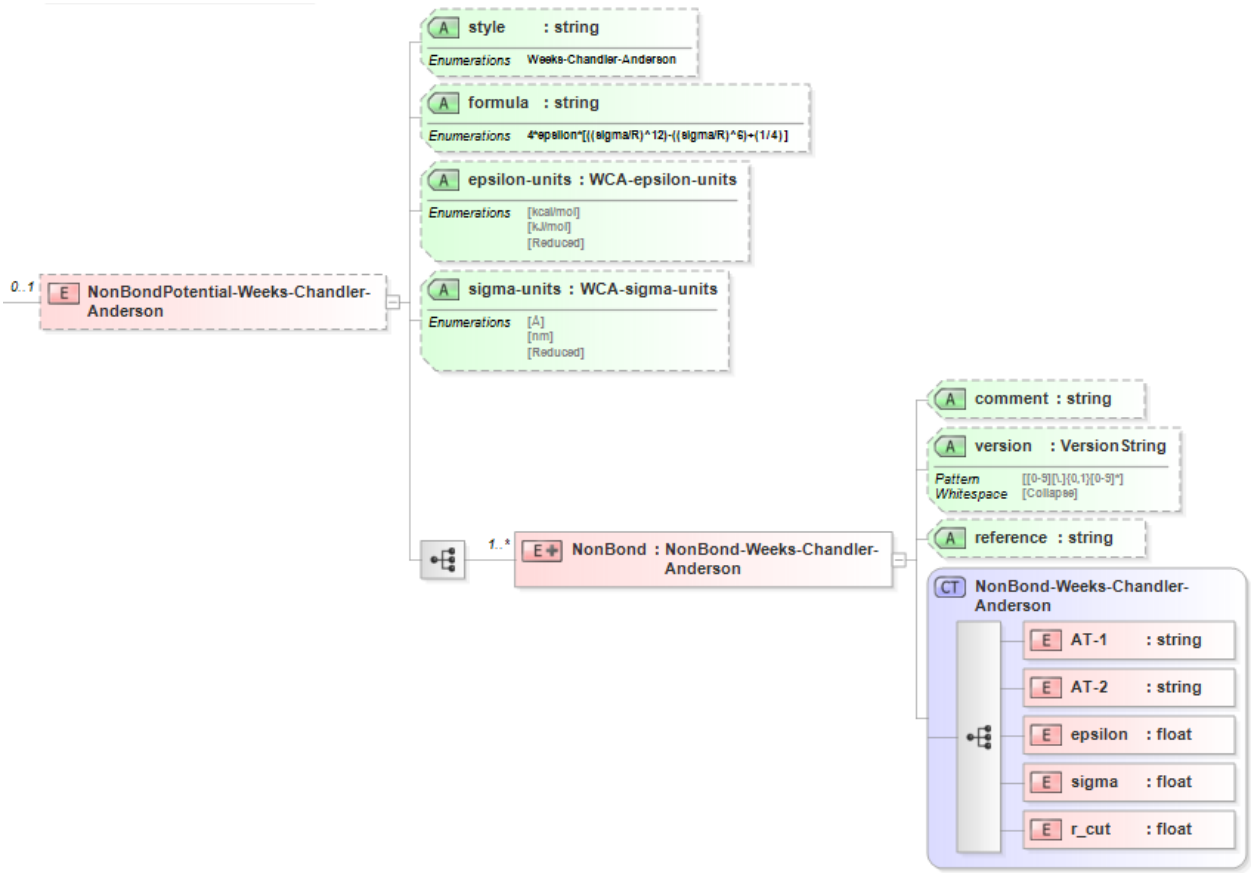
$$E = 4\epsilon \left[\left(\frac{\sigma_{ij}}{R_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{R_{ij}} \right)^{12} + \frac{1}{4} \right]$$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
ϵ	Potential well depth for atom [i]	energy/mol
σ	Interatomic cut-off distance for atom [i]	length

18.13.2 XML Schema

The XML schema for the **non-bond Weeks-Chandler-Anderson potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	(implicit)	AT-1
Atom type of atom [j]	(implicit)	AT-2
Potential well depth for atom [i]	ϵ	epsilon
Interatomic cut-off distance for atom [i]	σ	sigma
Interatomic cut-off distance for atom [i]	N/A	r_cut

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Weeks-Chandler-Anderson
formula	Fixed	4*epsilon*[((sigma/R)^-12)-((sigma/R)^-6)+(1/4)]
epsilon-units	Required	Enumerations specified in schema
sigma-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

18.13.3 References

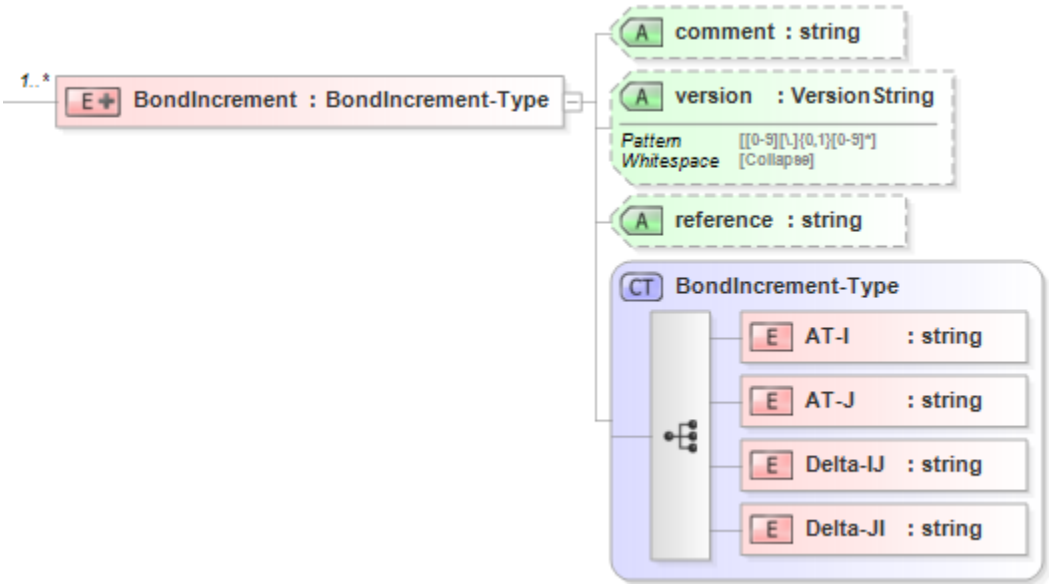
1. The Journal of Chemical Physics 54, 5237 (1971); doi 10.1063/1.1674820.
2. Liquid XML Studio.

CHAPTER 19

Table Potentials

19.1 Bond Increment Table

The XML schema for the **bond increment table** has the following representation (design mode representation using Liquid XML Studio):



The specific elements (describing each set of parameters) are given by:

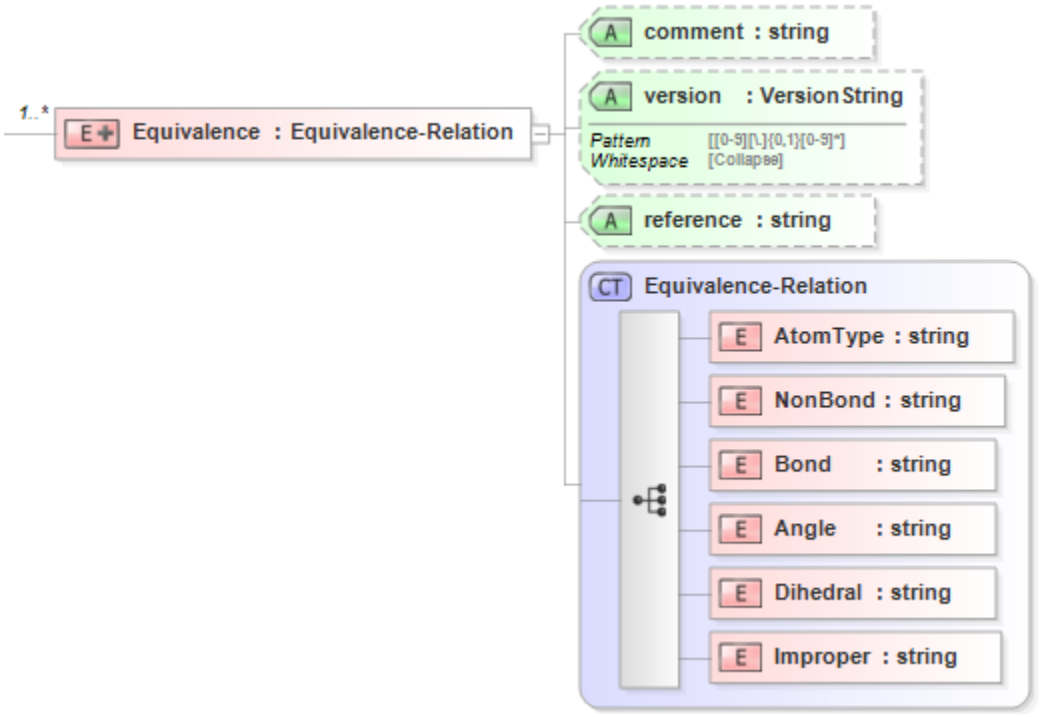
Parameter Definition	Schema Notation
Atom type of atom [i]	AT-I
Atom type of atom [j]	AT-J
Increment step size for atoms [i,j]	Delta-IJ
Increment step size for atoms [j,i]	Delta-JI

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

19.2 Equivalence Table

The XML schema for the **equivalence table** has the following representation (design mode representation using Liquid XML Studio):



The specific elements (describing each set of parameters) are given by:

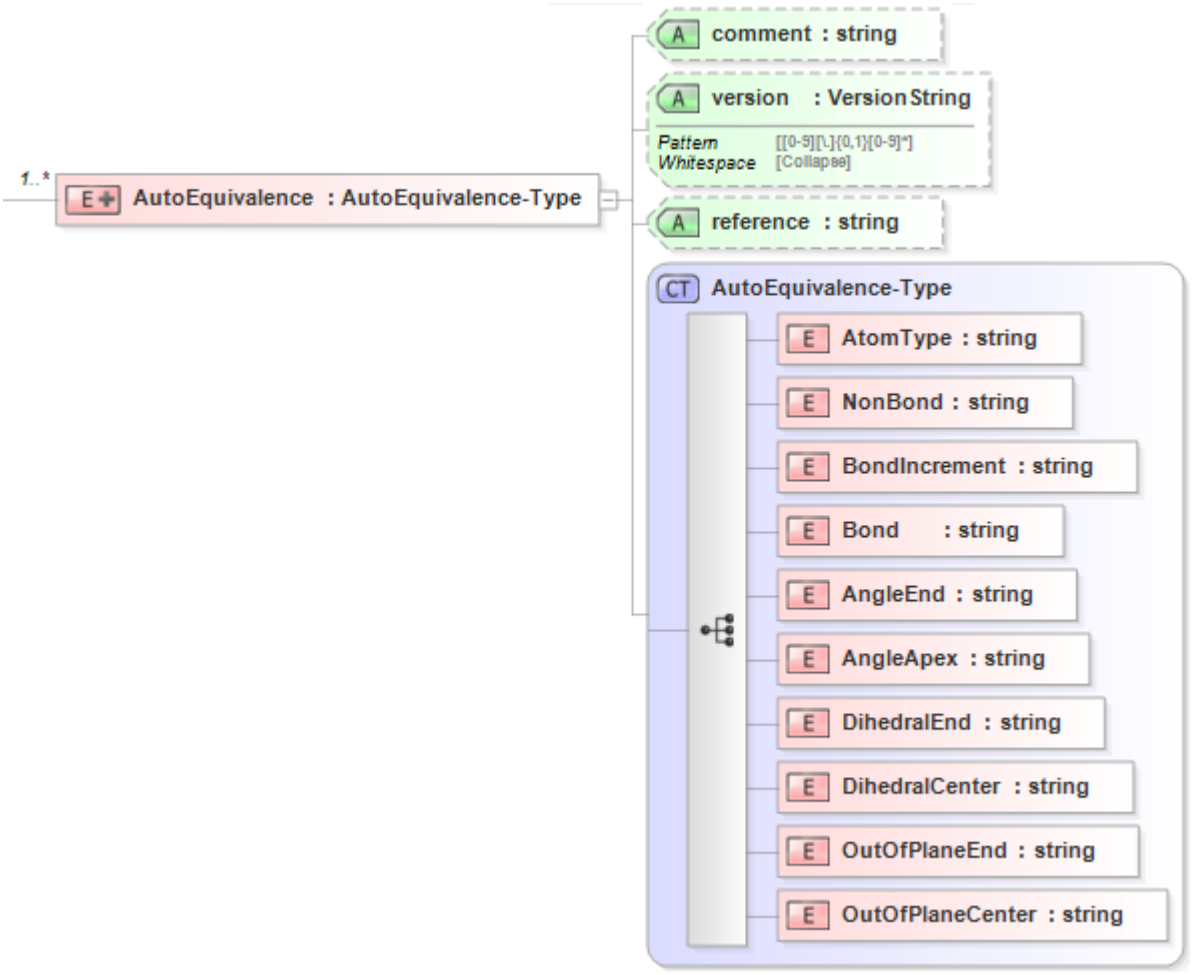
Parameter Definition	Schema Notation
Atom type of atom [i]	AtomType
	NonBond
	Bond
	Angle
	Dihedral
	Improper

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

19.3 Auto-Equivalence Table

The XML schema for the **auto-equivalence table** has the following representation (design mode representation using Liquid XML Studio):



The specific elements (describing each set of parameters) are given by:

Parameter Definition	Schema Notation
Atom type of atom [i]	AtomType
	NonBond
	BondIncrement
	Bond
	AngleEnd
	AngleApex
	DihedralEnd
	DihedralCenter
	OutOfPlaneEnd
	OutOfPlaneCenter

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

CHAPTER 20

Mesoscale Potentials

20.1 Langevin Dissipative

20.1.1 Functional Form

The **Langevin dissipative potential** has the functional form:

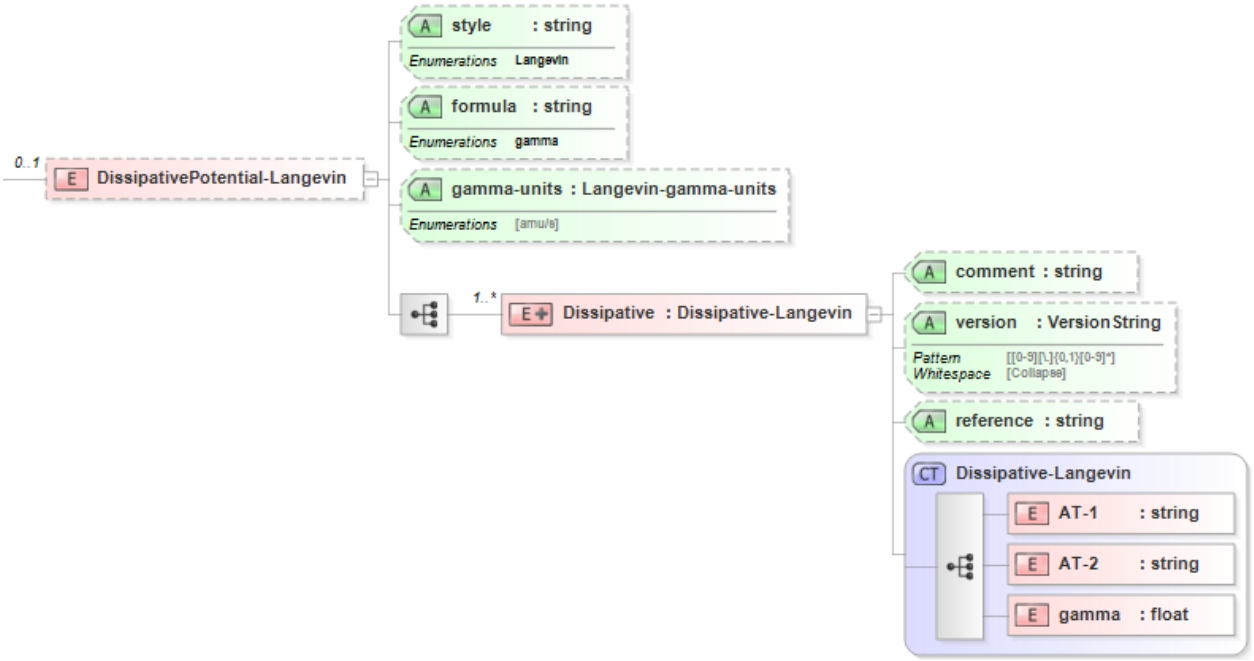
$E = \gamma$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
γ	Langevin thermostat	mass/time

20.1.2 XML Schema

The XML schema for the **Langevin dissipative potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Langevin thermostat	γ	gamma

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	Langevin
formula	Fixed	gamma
gamma-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

20.1.3 References

1. Multiscale approach to equilibrating model polymer melts.
2. Liquid XML Studio.

20.2 DPD Soft

20.2.1 Functional Form

The **DPD soft potential** has the functional form:

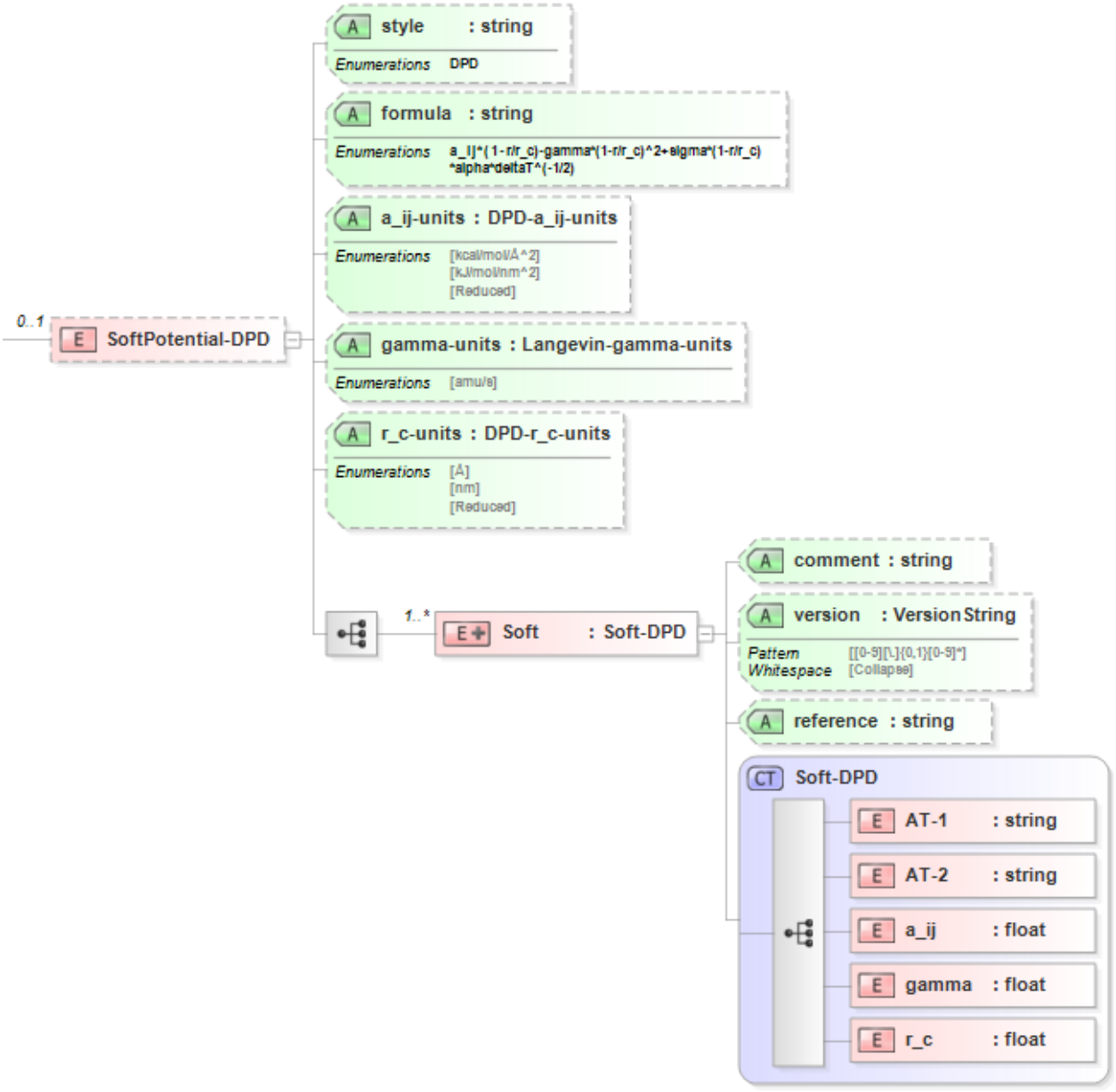
$$E = A_{ij}\left(1 - \frac{R_{ij}}{R_c}\right) - \gamma\left(1 - \frac{R_{ij}}{R_c}\right)^2 + \sigma\left(1 - \frac{R_{ij}}{R_c}\right)\alpha(\Delta T)^{-\frac{1}{2}}$$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
A_{ij}	Coefficient for conservative force	force
γ	Coefficient for dissipative force	force/velocity
R_c	Cutoff distance value	length

20.2.2 XML Schema

The XML schema for the **soft DPD potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Coefficient for conservative force	A_{ij}	a_ij
Coefficient for dissipative force	γ	gamma
Cutoff distance value	R_c	r_c

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	DPD
formula	Fixed	a_ij*(1-r/r_c)-gamma*(1-r/r_c)^2+sigma*(1-r/r_c)*alpha*deltaT^(-1/2)
a_ij-units	Required	Enumerations specified in schema
gamma-units	Required	Enumerations specified in schema
r_c-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

20.2.3 References

1. LAMMPS DPD Pair Potential.
2. Liquid XML Studio.

20.3 SRP Soft

20.3.1 Functional Form

The **SRP soft potential** has the functional form:

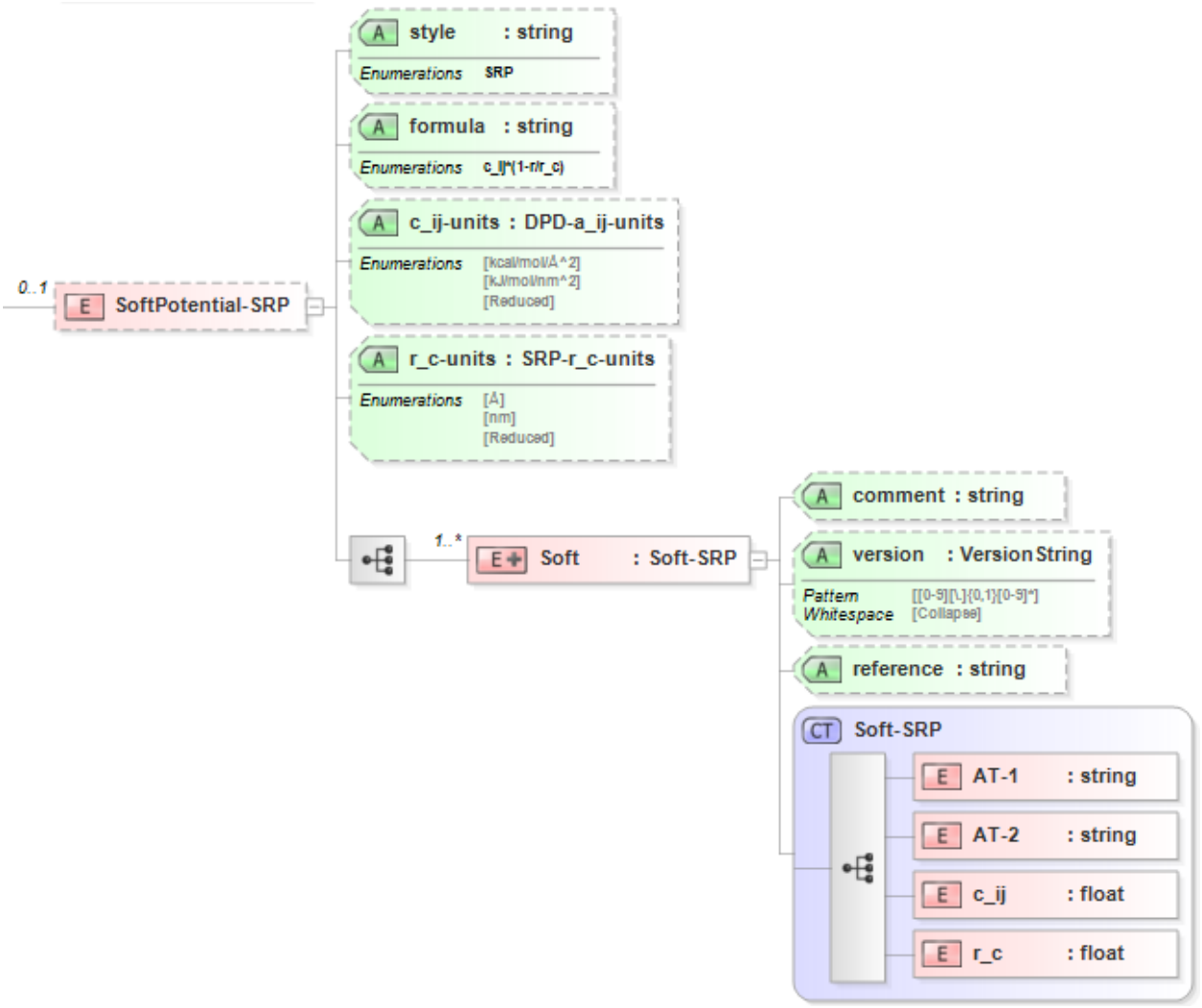
$E = C_{ij}\left(1 - \frac{R_{ij}}{R_c}\right)$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
C_{ij}	Coefficient for repulsive force	force
R_c	Cutoff distance value	length

20.3.2 XML Schema

The XML schema for the **soft SRP potential** has the following representation (design mode representation using Liquid XML Studio):



The relationship between the equation symbols and XML schema notations are given by:

Parameter Definition	Equation Symbol	Schema Notation
Atom type of atom [i]	i	AT-1
Atom type of atom [j]	j	AT-2
Coefficient for repulsive force	C_{ij}	c_ij
Cutoff distance value	R_c	r_c

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
style	Fixed	SRP
formula	Fixed	c_ij*(1-r/r_c)
c_ij-units	Required	Enumerations specified in schema
r_c-units	Required	Enumerations specified in schema

The specific attributes (attached to each set of parameters) are given by:

Specific Attributes	Cardinality	Value/Definition
comment	Optional	Comment attached to parameter set
version	Optional	Version number of parameter set
reference	Optional	Reference attached to parameter set

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

20.3.3 References

1. LAMMPS SRP Pair Potential.
2. Liquid XML Studio.

CHAPTER 21

Water Models

21.1 3Site-Rigid Water Model

21.1.1 Functional Form

The **3Site-Rigid water model** has the functional form:

$E = E_q + E_{LJ}$

or alternatively:

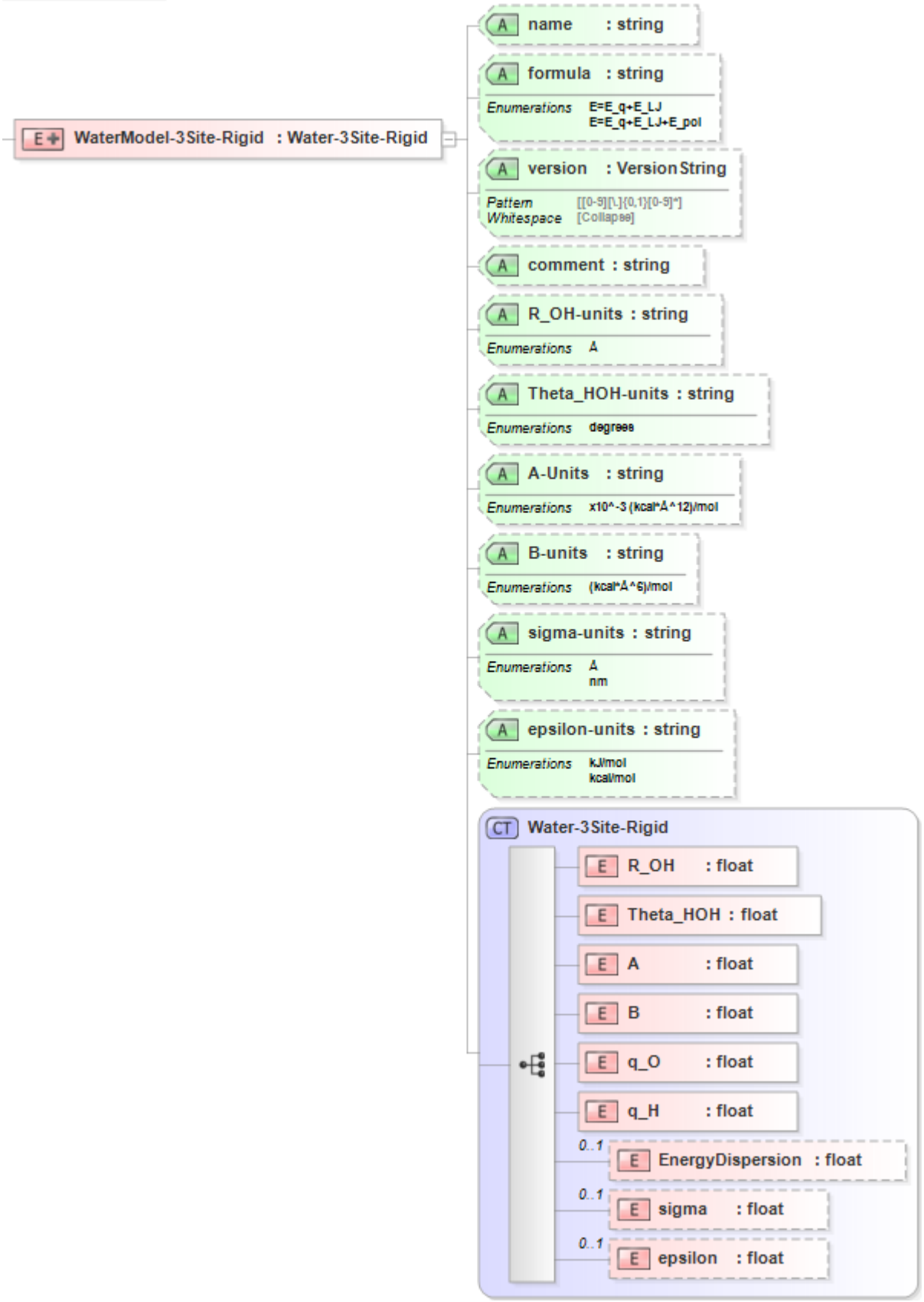
$E = E_q + E_{LJ} + E_{pol}$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
E_q	Charge potential energy	energy
E_{LJ}	Lennard-Jones potential energy	energy
E_{pol}	Average polarization correction	energy

21.1.2 XML Schema

The XML schema for the **3Site-Rigid water model** has the following representation (design mode representation using Liquid XML Studio):


WaterModel-3Site-Rigid : Water-3Site-Rigid
name : string
formula : string
Enumerations E=E_q+E_LJ
E=E_q+E_LJ+E_pol
version : VersionString
Pattern [[0-9]{1,}.]{0,1}[0-9]*]
Whitespace [Collapse]
comment : string
R_OH-units : string
Enumerations A
Theta_HOH-units : string
Enumerations degrees
A-Units : string
Enumerations x10^-3 (kcal*A^12)/mol
B-units : string
Enumerations (kcal*A^6)/mol
sigma-units : string
Enumerations A
nm
epsilon-units : string
Enumerations kJ/mol
kcal/mol
Water-3Site-Rigid
R_OH : float
Theta_HOH : float
A : float
B : float
q_O : float
q_H : float
0..1
EnergyDispersion : float
0..1
sigma : float
0..1
epsilon : float

The general sub-elements (the actual data set) are given by:

Parameter Definition	Schema Notation
Distance between O and H	R_OH
Angle between HOH	Theta_HOH
Lennard-Jones parameter	A
Lennard-Jones parameter	B
Charge of O	q_O
Charge of H	q_H
	EnergyDispersion
	sigma
	epsilon

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
name	Required	The name
formula	Fixed	E=E_q+E_LJ | E=E_q+E_LJ+E_pol
version	Optional	Version number of parameter set
comment	Optional	Comment attached to data set
R_OH-units	Required	Enumerations specified in schema
Theta_HOH-units	Required	Enumerations specified in schema
A-units	Required	Enumerations specified in schema
B-units	Required	Enumerations specified in schema
sigma-units	Required	Enumerations specified in schema
epsilon-units	Required	Enumerations specified in schema

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

21.1.3 References

1. SklogWiki page for TIP3P Water Model.
2. Wiki page for Water Model.
3. Liquid XML Studio.

21.2 4Site-Rigid Water Model

21.2.1 Functional Form

The **4Site-Rigid water model** has the functional form:

$E = E_q + E_{LJ}$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
E_q	Charge potential energy	energy
E_{LJ}	Lennard-Jones potential energy	energy

21.2.2 XML Schema

The XML schema for the **4Site-Rigid water model** has the following representation (design mode representation using Liquid XML Studio):

The general sub-elements (the actual data set) are given by:

Parameter Definition	Schema Notation
Distance between O and H	R_OH
Distance between O and M	R_OM
Angle between HOH	Theta_HOH
Lennard-Jones parameter	A
Lennard-Jones parameter	B
Charge of M	q_M
Charge of H	q_H
	sigma
	epsilon

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
name	Required	The name
formula	Fixed	E=E_q+E_LJ
version	Optional	Version number of parameter set
comment	Optional	Comment attached to data set
A-units	Required	Enumerations specified in schema
B-units	Required	Enumerations specified in schema
R-units	Required	Enumerations specified in schema
Theta_HOH-units	Required	Enumerations specified in schema
sigma-units	Required	Enumerations specified in schema
epsilon-units	Required	Enumerations specified in schema

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

21.2.3 References

1. SklogWiki page for TIP4P Water Model.
2. Wiki page for Water Model.
3. Liquid XML Studio.

21.3 5Site-Rigid Water Model

21.3.1 Functional Form

The **5Site-Rigid water model** has the functional form:

$E = E_q + E_{LJ}$

or alternatively:

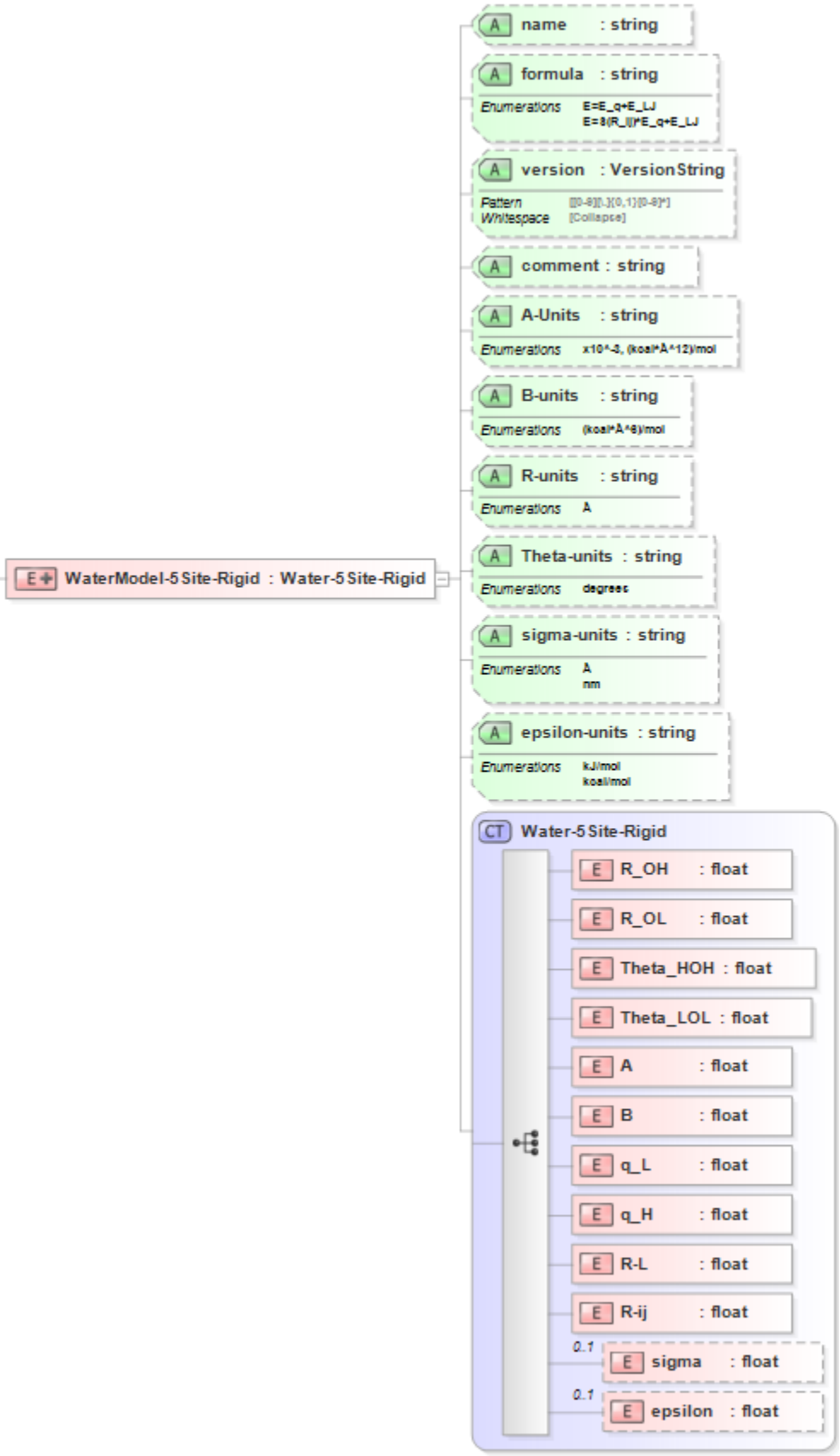
$E = S\left(R_{ij}\right) E_q + E_{LJ}$

The force-field parameters for this potential and units are given by:

Equation Symbol	Parameter Definition	Units
E_q	Charge potential energy	energy
E_{LJ}	Lennard-Jones potential energy	energy
$S\left(R_{ij}\right)$	Switching function	N/A

21.3.2 XML Schema

The XML schema for the **5Site-Rigid water model** has the following representation (design mode representation using Liquid XML Studio):


WaterModel-5 Site-Rigid : Water-5 Site-Rigid
name : string
formula : string
Enumerations E=E_q+E_LJ
E=f(R_ij)*E_q+E_LJ
version : VersionString
Pattern [[0-9][.][0,1][0-9]*]
Whitespace [Collapse]
comment : string
A-Units : string
Enumerations x10^-3, (kcal*Å^12)/mol
B-units : string
Enumerations (kcal*Å^6)/mol
R-units : string
Enumerations Å
Theta-units : string
Enumerations degrees
sigma-units : string
Enumerations Å
nm
epsilon-units : string
Enumerations kJ/mol
kcal/mol
Water-5 Site-Rigid
R_OH : float
R_OL : float
Theta_HOH : float
Theta_LOL : float
A : float
B : float
q_L : float
q_H : float
R-L : float
R-ij : float
0..1
sigma : float
0..1
epsilon : float

The general sub-elements (the actual data set) are given by:

Parameter Definition	Schema Notation
Distance between O and H	R_OH
Distance between O and M	R_OL
Angle between HOH	Theta_HOH
Angle between LOL	Theta_LOL
Lennard-Jones parameter	A
Lennard-Jones parameter	B
Charge of L	q_L
Charge of H	q_H
	R_L
	R_ij
	sigma
	epsilon

The general attributes (describing the entire data set) are given by:

General Attributes	Cardinality	Value/Definition
name	Required	The name
formula	Fixed	E=E_q+E_LJ
version	Optional	Version number of parameter set
comment	Optional	Comment attached to data set
A-units	Required	Enumerations specified in schema
B-units	Required	Enumerations specified in schema
R-units	Required	Enumerations specified in schema
Theta-units	Required	Enumerations specified in schema
sigma-units	Required	Enumerations specified in schema
epsilon-units	Required	Enumerations specified in schema

Note that an XML document will be rejected from being entered into the WebFF database if a required attribute is left unspecified.

21.3.3 References

1. SklogWiki page for TIP5P Water Model.
2. Wiki page for Water Model.
3. Liquid XML Studio.

CHAPTER 22

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