CHAPTER

EIGHT

IMPROPER STYLES

8.1 improper_style amoeba command

8.1.1 Syntax

```
improper_style amoeba
```

8.1.2 Examples

```
improper_style amoeba
improper_coeff 1 49.6
```

8.1.3 Description

The *amoeba* improper style uses the potential

$$E = K(\chi)^2$$

where χ is the improper angle and K is a prefactor. Note that the usual 1/2 factor is included in K.

This formula seems like a simplified version of the formula for the *improper_style harmonic* command with $\chi_0 = 0.0$. However the computation of the angle χ is done differently to match how the Tinker MD code computes its out-of-plane improper for the AMOEBA and HIPPO force fields. See the *Howto amoeba* doc page for more information about the implementation of AMOEBA and HIPPO in LAMMPS.

If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command are ordered I,J,K,L then atoms I,K,L are considered to lie in a plane and atom J is out-of-place. The angle χ_0 is computed as the Allinger angle which is defined as the angle between the plane of I,K,L, and the vector from atom I to atom J.

The following coefficient must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)

Note that the angle χ is computed in radians; hence K is effectively energy per radian^2.

8.1.4 Restrictions

This improper style can only be used if LAMMPS was built with the AMOEBA package. See the *Build package* doc page for more info.

8.1.5 Related commands

improper_coeff, *improper_harmonic*

8.1.6 Default

none

8.2 improper_style class2 command

Accelerator Variants: *class2/omp*, *class2/kk*

8.2.1 Syntax

```
improper_style class2
```

8.2.2 Examples

```
improper_style class2
improper_coeff 1 100.0 0
improper_coeff * aa 0.0 0.0 0.0 115.06 130.01 115.06
```

8.2.3 Description

The *class2* improper style uses the potential

$$
\begin{aligned}
E =& E_i + E_{aa} \\
E_i =& K[\frac{\chi_{ijkl} + \chi_{kjli} + \chi_{ljik}}{3} - \chi_0]^2 \\
E_{aa} =& M_1(\theta_{ijk} - \theta_1)(\theta_{kjl} - \theta_3) + \\
& M_2(\theta_{ijk} - \theta_1)(\theta_{ijl} - \theta_2) + \\
& M_3(\theta_{ijl} - \theta_2)(\theta_{kjl} - \theta_3)
\end{aligned}
$$

where E_i is the improper term and E_{aa} is an angle-angle term. The 3 χ terms in E_i are an average over 3 out-of-plane angles.

The 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L. χ_{ijkl} refers to the angle between the plane of I,J,K and the plane of J,K,L, and the bond JK lies in both planes. Similarly for χ_{kjli} and χ_{ljik}. Note that atom J appears in the common bonds (JI, JK, JL) of all 3 X terms. Thus J (the second atom in the quadruplet) is the atom of symmetry in the 3 χ angles.

The subscripts on the various θs refer to different combinations of three atoms (I,J,K,L) used to form a particular angle. E.g. θ_{ijl} is the angle formed by atoms I,J,L with J in the middle. θ_1, θ_2, θ_3 are the equilibrium positions of those angles. Again, atom J (the second atom in the quadruplet) is the atom of symmetry in the theta angles, since it is always the center atom.

Since atom J is the atom of symmetry, normally the bonds J-I, J-K, J-L would exist for an improper to be defined between the 4 atoms, but this is not required.

See *(Sun)* for a description of the COMPASS class2 force field.

Coefficients for the E_i and E_{aa} formulas must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands.

These are the 2 coefficients for the E_i formula:

- K (energy)
- χ_0 (degrees)

χ_0 is specified in degrees, but LAMMPS converts it to radians internally; hence K is effectively energy per radian^2.

For the E_{aa} formula, each line in a *improper_coeff* command in the input script lists 7 coefficients, the first of which is *aa* to indicate they are AngleAngle coefficients. In a data file, these coefficients should be listed under a *AngleAngle Coeffs* heading and you must leave out the *aa*, i.e. only list 6 coefficients after the improper type.

- *aa*
- M_1 (energy)
- M_2 (energy)
- M_3 (energy)
- θ_1 (degrees)
- θ_2 (degrees)
- θ_3 (degrees)

The θ values are specified in degrees, but LAMMPS converts them to radians internally; hence the hence the various M are effectively energy per radian^2.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Accelerator packages* page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, INTEL, KOKKOS, OPENMP, and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Accelerator packages* page for more instructions on how to use the accelerated styles effectively.

8.2.4 Restrictions

This improper style can only be used if LAMMPS was built with the CLASS2 package. See the *Build package* doc page for more info.

8.2.5 Related commands

improper_coeff

8.2.6 Default

none

(Sun) Sun, J Phys Chem B 102, 7338-7364 (1998).

8.3 improper_style cossq command

Accelerator Variants: *cossq/omp*

8.3.1 Syntax

```
improper_style cossq
```

8.3.2 Examples

```
improper_style cossq
improper_coeff 1 4.0 0.0
```

8.3.3 Description

The *cossq* improper style uses the potential

$$E = \frac{1}{2} K \cos^2 \left(\chi - \chi_0 \right)$$

where χ is the improper angle, χ_0 is its equilibrium value, and K is a prefactor.

If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then χ is the angle between the plane of I,J,K and the plane of J,K,L. Alternatively, you can think of atoms J,K,L as being in a plane, and atom I above the plane, and χ as a measure of how far out-of-plane I is with respect to the other 3 atoms.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- χ_0 (degrees)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Accelerator packages* page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, INTEL, KOKKOS, OPENMP, and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Accelerator packages* page for more instructions on how to use the accelerated styles effectively.

8.3.4 Restrictions

This improper style can only be used if LAMMPS was built with the EXTRA-MOLECULE package. See the *Build package* doc page for more info.

8.3.5 Related commands

improper_coeff

8.3.6 Default

none

8.4 improper_style cvff command

Accelerator Variants: *cvff/intel*, *cvff/omp*

8.4.1 Syntax

```
improper_style cvff
```

8.4.2 Examples

```
improper_style cvff
improper_coeff 1 80.0 -1 4
```

8.4.3 Description

The *cvff* improper style uses the potential

$$E = K[1 + d\cos(n\phi)]$$

where phi is the improper dihedral angle.

If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then the improper dihedral angle is between the plane of I,J,K and the plane of J,K,L. Note that because this is effectively a dihedral angle, the formula for this improper style is the same as for *dihedral_style harmonic*.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- d (+1 or -1)
- n (0,1,2,3,4,6)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Accelerator packages* page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, INTEL, KOKKOS, OPENMP, and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Accelerator packages* page for more instructions on how to use the accelerated styles effectively.

8.4.4 Restrictions

This improper style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

8.4.5 Related commands

improper_coeff

8.4.6 Default

none

8.5 improper_style distance command

8.5.1 Syntax

```
improper_style distance
```

8.5.2 Examples

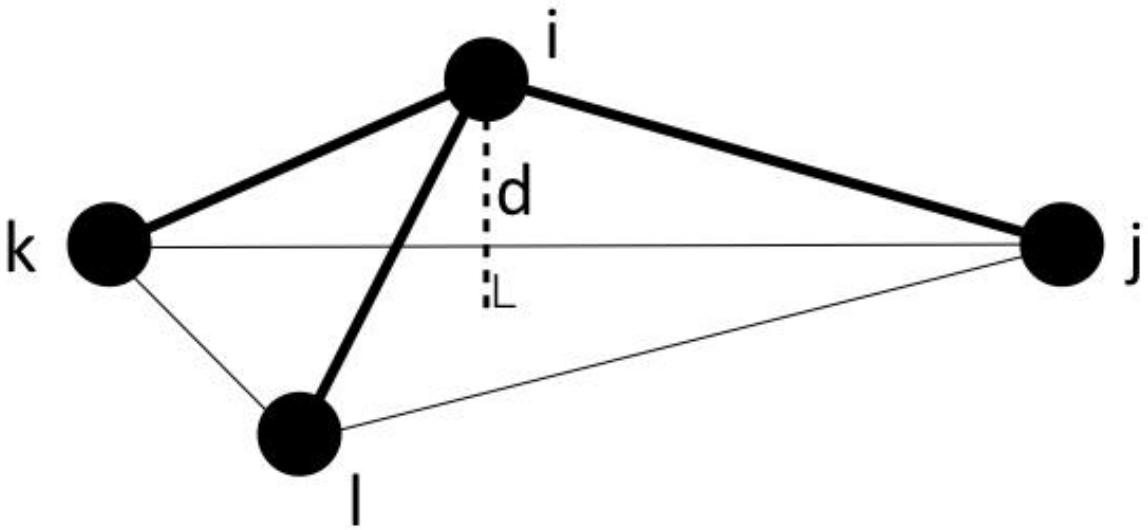
```
improper_style distance
improper_coeff 1 80.0 100.0
```

8.5.3 Description

The *distance* improper style uses the potential

$$E = K_2 d^2 + K_4 d^4$$

where d is the distance between the central atom and the plane formed by the other three atoms. If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then the I-atom is assumed to be the central atom.



Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K_2 (energy/distance^2)
- K_4 (energy/distance^4)

8.5.4 Restrictions

This improper style can only be used if LAMMPS was built with the EXTRA-MOLECULE package. See the *Build package* doc page for more info.

8.5.5 Related commands

improper_coeff

8.5.6 Default

none

8.6 improper_style distharm command

8.6.1 Syntax

```
improper_style distharm
```

8.6.2 Examples

```
improper_style distharm
improper_coeff 1 25.0 0.5
```

8.6.3 Description

The *distharm* improper style uses the potential

$$E = K(d - d_0)^2$$

where d is the oriented distance between the central atom and the plane formed by the other three atoms. If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then the L-atom is assumed to be the central atom. Note that this is different from the convention used in the improper_style distance. The distance d is oriented and can take on negative values. This may lead to unwanted behavior if d_0 is not equal to zero.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/distance^2)

- d_0 (distance)

8.6.4 Restrictions

This improper style can only be used if LAMMPS was built with the YAFF package. See the *Build package* doc page for more info.

8.6.5 Related commands

improper_coeff

8.6.6 Default

none

8.7 improper_style fourier command

Accelerator Variants: *fourier/omp*

8.7.1 Syntax

```
improper_style fourier
```

8.7.2 Examples

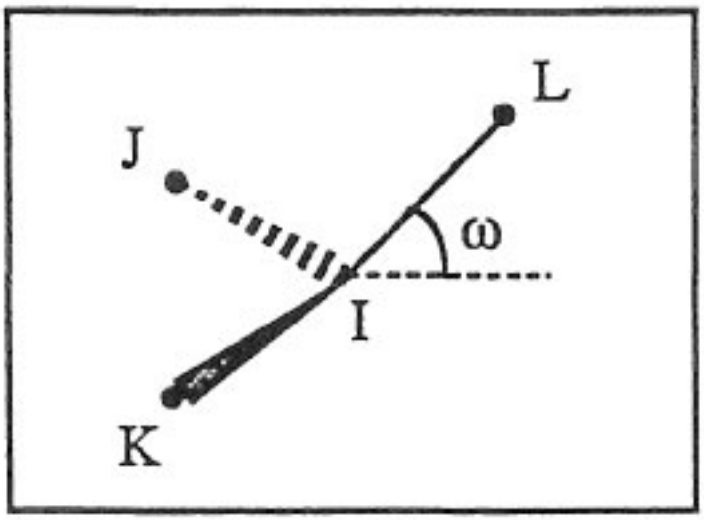
```
improper_style fourier
improper_coeff 1 100.0 0.0 1.0 0.5 1
```

8.7.3 Description

The *fourier* improper style uses the following potential:

$$E = K[C_0 + C_1 \cos(\omega) + C_2 \cos(2\omega)]$$

where K is the force constant, C0, C1, C2 are dimensionless coefficients, and omega is the angle between the IL axis and the IJK plane:



If all parameter (see below) is not zero, the all the three possible angles will taken in account.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- C_0 (unitless)
- C_1 (unitless)
- C_2 (unitless)
- all (0 or 1, optional)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Accelerator packages* page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, INTEL, KOKKOS, OPENMP, and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Accelerator packages* page for more instructions on how to use the accelerated styles effectively.

8.7.4 Restrictions

This angle style can only be used if LAMMPS was built with the EXTRA-MOLECULE package. See the *Build package* doc page for more info.

8.7.5 Related commands

improper_coeff

8.7.6 Default

none

8.8 improper_style harmonic command

Accelerator Variants: *harmonic/intel*, *harmonic/kk*, *harmonic/omp*

8.8.1 Syntax

```
improper_style harmonic
```

8.8.2 Examples

```
improper_style harmonic
improper_coeff 1 100.0 0
```

8.8.3 Description

The *harmonic* improper style uses the potential

$$E = K(\chi - \chi_0)^2$$

where χ is the improper angle, χ_0 is its equilibrium value, and K is a prefactor. Note that the usual 1/2 factor is included in K.

If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then χ is the angle between the plane of I,J,K and the plane of J,K,L. Alternatively, you can think of atoms J,K,L as being in a plane, and atom I above the plane, and χ as a measure of how far out-of-plane I is with respect to the other 3 atoms.

Note that defining 4 atoms to interact in this way, does not mean that bonds necessarily exist between I-J, J-K, or K-L, as they would in a linear dihedral. Normally, the bonds I-J, I-K, I-L would exist for an improper to be defined between the 4 atoms.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)

- χ_0 (degrees)

χ_0 is specified in degrees, but LAMMPS converts it to radians internally; hence K is effectively energy per radian^2.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Accelerator packages* page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, INTEL, KOKKOS, OPENMP, and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Accelerator packages* page for more instructions on how to use the accelerated styles effectively.

8.8.4 Restrictions

This improper style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

8.8.5 Related commands

improper_coeff

8.8.6 Default

none

8.9 improper_style hybrid command

Accelerator Variants: *hybrid/kk*

8.9.1 Syntax

```
improper_style hybrid style1 style2 ...
```

- style1,style2 = list of one or more improper styles

8.9.2 Examples

```
improper_style hybrid harmonic cvff
improper_coeff 1 harmonic 120.0 30
improper_coeff 2 cvff 20.0 -1 2
```

8.9.3 Description

The *hybrid* style enables the use of multiple improper styles in one simulation. An improper style is assigned to each improper type. For example, impropers in a polymer flow (of improper type 1) could be computed with a *harmonic* potential and impropers in the wall boundary (of improper type 2) could be computed with a *cvff* potential. The assignment of improper type to style is made via the *improper_coeff* command or in the data file.

In the improper_coeff command, the first coefficient sets the improper style and the remaining coefficients are those appropriate to that style. In the example above, the 2 improper_coeff commands would set impropers of improper type 1 to be computed with a *harmonic* potential with coefficients 120.0, 30 for K, χ_0. Improper type 2 would be computed with a *cvff* potential with coefficients 20.0, -1, 2 for K, d, and n, respectively.

If improper coefficients are specified in the data file read via the *read_data* command, then the same rule applies. E.g. "harmonic" or "cvff", must be added after the improper type, for each line in the "Improper Coeffs" section, e.g.

```
Improper Coeffs

1 harmonic 120.0 30
2 cvff 20.0 -1 2
...
```

If *class2* is one of the improper hybrid styles, the same rule holds for specifying additional AngleAngle coefficients either via the input script or in the data file. I.e. *class2* must be added to each line after the improper type. For lines in the AngleAngle Coeffs section of the data file for dihedral types that are not *class2*, you must use an improper style of *skip* as a placeholder, e.g.

```
AngleAngle Coeffs

1 skip
2 class2 0.0 0.0 0.0 115.06 130.01 115.06
...
```

Note that it is not necessary to use the improper style *skip* in the input script, since AngleAngle coefficients need not be specified at all for improper types that are not *class2*.

An improper style of *none* can be specified as the second argument to the improper_coeff command, if you desire to turn off certain improper types.

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Accelerator packages* page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, INTEL, KOKKOS, OPENMP, and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Accelerator packages* page for more instructions on how to use the accelerated styles effectively.

8.9.4 Restrictions

This improper style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

Unlike other improper styles, the hybrid improper style does not store improper coefficient info for individual sub-styles in *binary restart files* or *data files*. Thus when restarting a simulation, you need to re-specify the improper_coeff commands.

8.9.5 Related commands

improper_coeff

8.9.6 Default

none

8.10 improper_style inversion/harmonic command

8.10.1 Syntax

```
improper_style inversion/harmonic
```

8.10.2 Examples

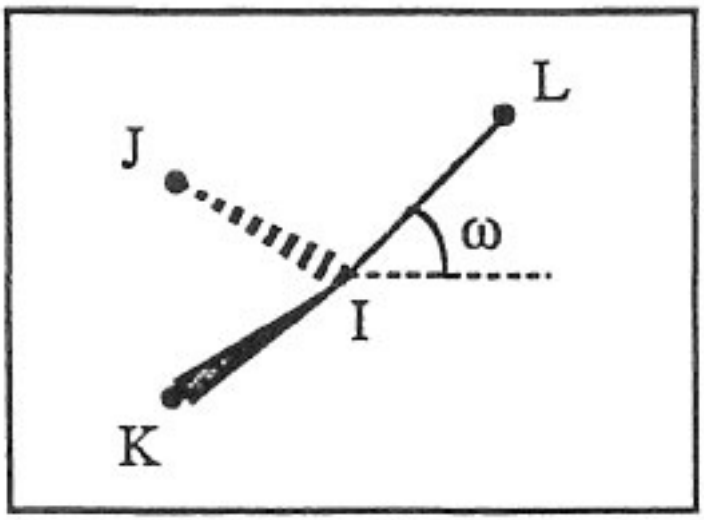
```
improper_style inversion/harmonic
improper_coeff 1 18.776340 0.000000
```

8.10.3 Description

The *inversion/harmonic* improper style follows the Wilson-Decius out-of-plane angle definition and uses an harmonic potential:

$$E = K\left(\omega - \omega_0\right)^2$$

where K is the force constant and ω is the angle evaluated for all three axis-plane combinations centered around the atom I. For the IL axis and the IJK plane ω looks as follows:



Note that the *inversion/harmonic* angle term evaluation differs to the *improper_umbrella* due to the cyclic evaluation of all possible angles ω.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- ω_0 (degrees)

If ω_0 = 0 the potential term has a single minimum for the planar structure. Otherwise it has two minima at +/- ω_0, with a barrier in between.

8.10.4 Restrictions

This improper style can only be used if LAMMPS was built with the MOFFF package. See the *Build package* doc page for more info.

8.10.5 Related commands

improper_coeff

8.10.6 Default

none

8.11 improper_style none command

8.11.1 Syntax

```
improper_style none
```

8.11.2 Examples

```
improper_style none
```

8.11.3 Description

Using an improper style of none means improper forces and energies are not computed, even if quadruplets of improper atoms were listed in the data file read by the *read_data* command.

See the *improper_style zero* command for a way to calculate improper statistics, but compute no improper interactions.

8.11.4 Restrictions

none

8.11.5 Related commands

improper_style zero

8.11.6 Default

none

8.12 improper_style ring command

Accelerator Variants: *ring/omp*

8.12.1 Syntax

```
improper_style ring
```

8.12.2 Examples

```
improper_style ring
improper_coeff 1 8000 70.5
```

8.12.3 Description

The *ring* improper style uses the potential

$$E = \frac{1}{6}K\left(\Delta_{ijl} + \Delta_{ijk} + \Delta_{kjl}\right)^6$$
$$\Delta_{ijl} = \cos\theta_{ijl} - \cos\theta_0$$
$$\Delta_{ijk} = \cos\theta_{ijk} - \cos\theta_0$$
$$\Delta_{kjl} = \cos\theta_{kjl} - \cos\theta_0$$

where K is a prefactor, θ is the angle formed by the atoms specified by (i,j,k,l) indices and θ_0 its equilibrium value.

If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered i,j,k,l then θ_{ijl} is the angle between atoms i,j and l, θ_{ijk} is the angle between atoms i,j and k, θ_{kjl} is the angle between atoms j,k, and l.

The "ring" improper style implements the improper potential introduced by Destree et al., in Equation (9) of *(Destree)*. This potential does not affect small amplitude vibrations but is used in an ad-hoc way to prevent the onset of accidentally large amplitude fluctuations leading to the occurrence of a planar conformation of the three bonds i-j, j-k and j-l, an intermediate conformation toward the chiral inversion of a methine carbon. In the "Impropers" section of data file four atoms: i, j, k and l are specified with i,j and l lying on the backbone of the chain and k specifying the chirality of j.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- θ_0 (degrees)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Accelerator packages* page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, INTEL, KOKKOS, OPENMP, and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Accelerator packages* page for more instructions on how to use the accelerated styles effectively.

8.12.4 Restrictions

This improper style can only be used if LAMMPS was built with the EXTRA-MOLECULE package. See the *Build package* doc page for more info.

8.12.5 Related commands

improper_coeff

(Destree) M. Destree, F. Laupretre, A. Lyulin, and J.-P. Ryckaert, J Chem Phys, 112, 9632 (2000).

8.13 improper_style sqdistharm command

8.13.1 Syntax

```
improper_style sqdistharm
```

8.13.2 Examples

```
improper_style sqdistharm
improper_coeff 1 50.0 0.1
```

8.13.3 Description

The *sqdistharm* improper style uses the potential

$$E = K(d^2 - {d_0}^2)^2$$

where d is the distance between the central atom and the plane formed by the other three atoms. If the 4 atoms in an improper quadruplet (listed in the data file read by the *read_data* command) are ordered I,J,K,L then the L-atom is assumed to be the central atom. Note that this is different from the convention used in the improper_style distance.

The following coefficients must be defined for each improper type via the improper_coeff command as in the example above, or in the data file or restart files read by the read_data or read_restart commands:

- K (energy/distance^4)
- ${d_0}^2$ (distance^2)

Note that ${d_0}^2$ (in units distance^2) has be provided and not d_0.

8.13.4 Restrictions

This improper style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

8.13.5 Related commands

improper_coeff

8.13.6 Default

none

8.14 improper_style umbrella command

Accelerator Variants: *umbrella/omp*

8.14.1 Syntax

```
improper_style umbrella
```

8.14.2 Examples

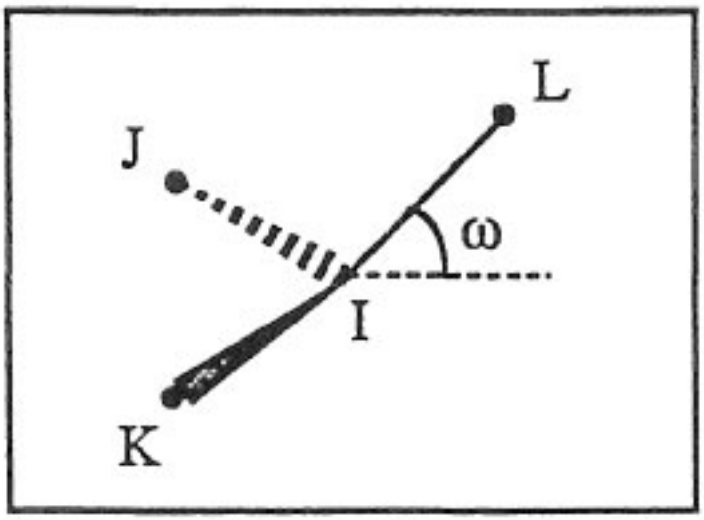
```
improper_style umbrella
improper_coeff 1 100.0 180.0
```

8.14.3 Description

The *umbrella* improper style uses the following potential, which is commonly referred to as a classic inversion and used in the *DREIDING* force field:

$$E = \frac{1}{2}K\left(\frac{1}{\sin\omega_0}\right)^2(\cos\omega - \cos\omega_0)^2 \qquad \omega_0 \neq 0^o$$
$$E = K(1 - cos\omega) \qquad \omega_0 = 0^o$$

where K is the force constant and ω is the angle between the IL axis and the IJK plane:



If $\omega_0 = 0$ the potential term has a minimum for the planar structure. Otherwise it has two minima at $\omega + / - \omega_0$, with a barrier in between.

See *(Mayo)* for a description of the DREIDING force field.

The following coefficients must be defined for each improper type via the *improper_coeff* command as in the example above, or in the data file or restart files read by the *read_data* or *read_restart* commands:

- K (energy)
- ω_0 (degrees)

Styles with a *gpu*, *intel*, *kk*, *omp*, or *opt* suffix are functionally the same as the corresponding style without the suffix. They have been optimized to run faster, depending on your available hardware, as discussed on the *Accelerator packages* page. The accelerated styles take the same arguments and should produce the same results, except for round-off and precision issues.

These accelerated styles are part of the GPU, INTEL, KOKKOS, OPENMP, and OPT packages, respectively. They are only enabled if LAMMPS was built with those packages. See the *Build package* page for more info.

You can specify the accelerated styles explicitly in your input script by including their suffix, or you can use the *-suffix command-line switch* when you invoke LAMMPS, or you can use the *suffix* command in your input script.

See the *Accelerator packages* page for more instructions on how to use the accelerated styles effectively.

8.14.4 Restrictions

This improper style can only be used if LAMMPS was built with the MOLECULE package. See the *Build package* doc page for more info.

8.14.5 Related commands

improper_coeff

8.14.6 Default

none

(Mayo) Mayo, Olfason, Goddard III, J Phys Chem, 94, 8897-8909 (1990),

8.15 improper_style zero command

8.15.1 Syntax

```
improper_style zero [nocoeff]
```

8.15.2 Examples

```
improper_style zero
improper_style zero nocoeff
improper_coeff *
```

8.15.3 Description

Using an improper style of zero means improper forces and energies are not computed, but the geometry of improper quadruplets is still accessible to other commands.

As an example, the *compute improper/local* command can be used to compute the chi values for the list of quadruplets of improper atoms listed in the data file read by the *read_data* command. If no improper style is defined, this command cannot be used.

The optional *nocoeff* flag allows to read data files with a ImproperCoeff section for any improper style. Similarly, any improper_coeff commands will only be checked for the improper type number and the rest ignored.

Note that the *improper_coeff* command must be used for all improper types, though no additional values are specified.

8.15.4 Restrictions

none

8.15.5 Related commands

none

improper_style none

8.15.6 Default

none