Out-of-plane potential, improper torsion definition

This section supplies the parameters used for the potential when the out-of-plane coordinate is defined according to an improper torsion. An out-of-plane potential is usually applied to planar groups containing an sp^2 central atom bonded to three other atoms. Examples are amide nitrogens, amide carbons, and the carbon atoms in a benzene ring. The out-of-plane potential acts to keep the central atom in the plane defined by the other three atoms. The functional form is:

$$E = V[1 + \cos(n\chi - \chi_0)] \qquad \text{Eq. 36}$$

where V is the force constant with units of kcal mol^{-1}; n is the (dimensionless) periodicity of the improper torsion (always 2); χ is the current improper-torsion angle in degrees; and χ_0 the reference improper-torsion angle (always 180°).

The format of the out-of-plane potential (improper torsion definition) section is:

#improper_torsion *section_label*
version reference i j k l n χ_0 *V*
…
#

where *i*, *j*, *k*, and *l* are the atom types of the four atoms involved in the out-of-plane term, *j* being the central atom. This term is asymmetric with respect to the three outer atoms *i*, *k*, and *l*. For example:

```
#improper_torsion    cvff

> E = V * [ 1 + cos( n * chi - chi0) ]

!Ver Ref    I    J    K    L       n      Chi0      V
!--- ---   ---  ---  ---  ---      -      ----    ----
 2.50 1     c    c'   n    o'       2      180.0   10.0
 2.50 1     c'   n    c    hn       2      180.0    0.05
…
#
```

Out-of-plane, Wilson definition

This section supplies the parameters used for the potential when the out-of-plane coordinate is defined according to the angle between one bond from the central atom and the plane defined by the other two bonds. An out-of-plane potential is usually applied to planar groups containing an sp^2 central atom bonded to three

other atoms. Examples are amide nitrogens, amide carbons, and the carbon atoms in a benzene ring. The out-of-plane potential acts to keep the central atom in the plane defined by the other three atoms. The functional form is:

$$E = V\chi^2 \qquad \text{Eq. 37}$$

where V is the force constant in kcal mol^{-1} rad^{-2}; and χ is the current Wilson out-of-plane angle in degrees. The program automatically converts the angle to radians before carrying out the calculation.

The format of the out-of-plane potential (Wilson definition) section is:

#wilson_out_of_plane *section_label*
version reference i j k l χ_0 *V*
…
#

where *i*, *j*, *k*, and *l* are the atom types of the four atoms involved in the out-of-plane term, *j* being the central atom; and χ_0 the reference angle in degrees. This term is asymmetric with respect to the outer atoms *i*, *k*, and *l*, but is made symmetric by summing over the three different out-of-planes defined by a trigonal center. For example:

```
#wilson_out_of_plane     cff91

> E = K * (Chi - Chi0)^2

!Ver  Ref     I     J     K     L          K      Chi0
!---- ---    ----  ----  ----  ----      -------   ----
 1.0   1     c     c=    c=    h          2.0765    0.0
 1.0   1     c=    c=    h     h          2.8561    0.0
…
#
```

Out-of-plane interaction potential using improper torsion definition

This section supplies the parameters used for the interaction potential between two out-of-plane coordinates defined according to improper torsions. The central atom of one out-of-plane must be bonded to the central atom of the other. The functional form is:

$$E = V[1 - \cos 2\chi]^{1/2}[1 - \cos 2\chi']^{1/2} \qquad \text{Eq. 38}$$