|  |  |
| --- | --- |
| **1.** | **Contents of Common Block Variables** |

The Fortran common blocks found in the TINKER package are listed below along with a brief description of the contents of each variable in each common block. Each individual common block is present as a separate ".i" file in the /source subdirectory. A source code listing containing each of the source code modules and each of the common blocks can be produced by running the "listing.make" script found in the distribution.

**ACTION total number of each energy term computed**

neb number of bond stretch energy terms computed

nea number of angle bend energy terms computed

neba number of stretch-bend energy terms computed

neub number of Urey-Bradley energy terms computed

neaa number of angle-angle energy terms computed

neopb number of out-of-plane bend energy terms computed

neopd number of out-of-plane distance energy terms computed

neid number of improper dihedral energy terms computed

neit number of improper torsion energy terms computed

net number of torsional energy terms computed

nept number of pi-orbital torsion energy terms computed

nebt number of stretch-torsion energy terms computed

nett number of torsion-torsion energy terms computed

nev number of van der Waals energy terms computed

nec number of charge-charge energy terms computed

necd number of charge-dipole energy terms computed

ned number of dipole-dipole energy terms computed

nem number of multipole energy terms computed

nep number of polarization energy terms computed

new number of Ewald summation energy terms computed

ner number of reaction field energy terms computed

nes number of solvation energy terms computed

nelf number of metal ligand field energy terms computed

neg number of geometric restraint energy terms computed

nex number of extra energy terms computed

**ALIGN information for superposition of structures**

wfit weights assigned to atom pairs during superposition

nfit number of atoms to use in superimposing two structures

ifit atom numbers of pairs of atoms to be superimposed

**ANALYZ energy components partitioned over atoms**

aesum total potential energy partitioned over atoms

aeb bond stretch energy partitioned over atoms

aea angle bend energy partitioned over atoms

aeba stretch-bend energy partitioned over atoms

aeub Urey-Bradley energy partitioned over atoms

aeaa angle-angle energy partitioned over atoms

aeopb out-of-plane bend energy partitioned over atoms

aeopd out-of-plane distance energy partitioned over atoms

aeid improper dihedral energy partitioned over atoms

aeit improper torsion energy partitioned over atoms

aet torsional energy partitioned over atoms

aept pi-orbital torsion energy partitioned over atoms

aebt stretch-torsion energy partitioned over atoms

aett torsion-torsion energy partitioned over atoms

aev van der Waals energy partitioned over atoms

aec charge-charge energy partitioned over atoms

aecd charge-dipole energy partitioned over atoms

aed dipole-dipole energy partitioned over atoms

aem multipole energy partitioned over atoms

aep polarization energy partitioned over atoms

aer reaction field energy partitioned over atoms

aes solvation energy partitioned over atoms

aelf metal ligand field energy partitioned over atoms

aeg geometric restraint energy partitioned over atoms

aex extra energy term partitioned over atoms

**ANGANG angle-angle terms in current structure**

kaa force constant for angle-angle cross terms

nangang total number of angle-angle interactions

iaa angle numbers used in each angle-angle term

**ANGLE bond angles within the current structure**

ak harmonic angle force constant (kcal/mole/rad\*\*2)

anat ideal bond angle or phase shift angle (degrees)

afld periodicity for Fourier bond angle term

nangle total number of bond angles in the system

iang numbers of the atoms in each bond angle

angtyp potential energy function type for each bond angle

**ANGPOT specifics of bond angle functional forms**

cang cubic coefficient in angle bending potential

qang quartic coefficient in angle bending potential

pang quintic coefficient in angle bending potential

sang sextic coefficient in angle bending potential

angunit convert angle bending energy to kcal/mole

stbnunit convert stretch-bend energy to kcal/mole

aaunit convert angle-angle energy to kcal/mole

opbunit convert out-of-plane bend energy to kcal/mole

opdunit convert out-of-plane distance energy to kcal/mole

mm2stbn logical flag governing use of MM2-style stretch-bend

**ARGUE command line arguments at program startup**

maxarg maximum number of command line arguments

narg number of command line arguments to the program

listarg flag to mark available command line arguments

arg strings containing the command line arguments

**ATMLST local geometry terms involving each atom**

bndlist list of the bond numbers involving each atom

anglist list of the angle numbers centered on each atom

**ATMTYP atomic properties for each current atom**

mass atomic weight for each atom in the system

tag integer atom labels from input coordinates file

class atom class number for each atom in the system

atomic atomic number for each atom in the system

valence valence number for each atom in the system

name atom name for each atom in the system

story descriptive type for each atom in system

**ATOMS number, position and type of current atoms**

x current x-coordinate for each atom in the system

y current y-coordinate for each atom in the system

z current z-coordinate for each atom in the system

n total number of atoms in the current system

type atom type number for each atom in the system

**BATH temperature and pressure control parameters**

maxnose maximum length of the Nose-Hoover chain

kelvin0 target value for the system temperature (K)

kelvin variable target temperature for thermostat (K)

atmsph target value for the system pressure (atm)

tautemp time constant for Berendsen thermostat (psec)

taupres time constant for Berendsen barostat (psec)

compress isothermal compressibility of medium (atm-1)

collide collision frequency for Andersen thermostat

xnh position of each chained Nose-Hoover thermostat

vnh velocity of each chained Nose-Hoover thermostat

qnh mass for each chained Nose-Hoover thermostat

gnh coupling between chained Nose-Hoover thermostats

isothermal logical flag governing use of temperature control

isobaric logical flag governing use of pressure control

tempvary logical flag to enable variable target thermostat

thermostat choice of temperature control method to be used

barostat choice of pressure control method to be used

**BITOR bitorsions within the current structure**

nbitor total number of bitorsions in the system

ibitor numbers of the atoms in each bitorsion

**BNDPOT specifics of bond stretch functional forms**

cbnd cubic coefficient in bond stretch potential

qbnd quartic coefficient in bond stretch potential

bndunit convert bond stretch energy to kcal/mole

bndtyp type of bond stretch potential energy function

**BOND covalent bonds in the current structure**

bk bond stretch force constants (kcal/mole/Ang\*\*2)

bl ideal bond length values in Angstroms

nbond total number of bond stretches in the system

ibnd numbers of the atoms in each bond stretch

**BORDER bond orders for a conjugated pisystem**

pbpl pi-bond orders for bonds in "planar" pisystem

pnpl pi-bond orders for bonds in "nonplanar" pisystem

**BOUND control of periodic boundary conditions**

polycut cutoff distance for infinite polymer nonbonds

polycut2 square of infinite polymer nonbond cutoff

use\_bounds flag to use periodic boundary conditions

use\_image flag to use images for periodic system

use\_replica flag to use replicates for periodic system

use\_polymer flag to mark presence of infinite polymer

**BOXES parameters for periodic boundary conditions**

xbox length in Angs of a-axis of periodic box

ybox length in Angs of b-axis of periodic box

zbox length in Angs of c-axis of periodic box

alpha angle in degrees between b- and c-axes of box

beta angle in degrees between a- and c-axes of box

gamma angle in degrees between a- and b-axes of box

xbox2 half of the a-axis length of periodic box

ybox2 half of the b-axis length of periodic box

zbox2 half of the c-axis length of periodic box

box34 three-fourths axis length of truncated octahedron

recip reciprocal lattice vectors as matrix columns

volbox volume in Ang\*\*3 of the periodic box

beta\_sin sine of the beta periodic box angle

beta\_cos cosine of the beta periodic box angle

gamma\_sin sine of the gamma periodic box angle

gamma\_cos cosine of the gamma periodic box angle

beta\_term term used in generating triclinic box

gamma\_term term used in generating triclinic box

orthogonal flag to mark periodic box as orthogonal

monoclinic flag to mark periodic box as monoclinic

triclinic flag to mark periodic box as triclinic

octahedron flag to mark box as truncated octahedron

spacegrp space group symbol for the unitcell type

**CELL periodic boundaries using replicated cells**

xcell length of the a-axis of the complete replicated cell

ycell length of the b-axis of the complete replicated cell

zcell length of the c-axis of the complete replicated cell

xcell2 half the length of the a-axis of the replicated cell

ycell2 half the length of the b-axis of the replicated cell

zcell2 half the length of the c-axis of the replicated cell

ncell total number of cell replicates for periodic boundaries

icell offset along axes for each replicate periodic cell

**CHARGE partial charges for the current structure**

pchg magnitude of the partial charges (e-)

nion total number of partial charges in system

iion number of the atom site for each partial charge

jion neighbor generation site for each partial charge

kion cutoff switching site for each partial charge

chglist partial charge site for each atom (0=no charge)

**CHGPOT specifics of charge-charge functional form**

dielec dielectric constant for electrostatic interactions

c2scale factor by which 1-2 charge interactions are scaled

c3scale factor by which 1-3 charge interactions are scaled

c4scale factor by which 1-4 charge interactions are scaled

c5scale factor by which 1-5 charge interactions are scaled

neutnbr logical flag governing use of neutral group neighbors

neutcut logical flag governing use of neutral group cutoffs

**CHRONO timing statistics for the current program**

cputim elapsed cpu time in seconds since start of program

**COUPLE near-neighbor atom connectivity lists**

maxn13 maximum number of atoms 1-3 connected to an atom

maxn14 maximum number of atoms 1-4 connected to an atom

maxn15 maximum number of atoms 1-5 connected to an atom

n12 number of atoms directly bonded to each atom

i12 atom numbers of atoms 1-2 connected to each atom

n13 number of atoms in a 1-3 relation to each atom

i13 atom numbers of atoms 1-3 connected to each atom

n14 number of atoms in a 1-4 relation to each atom

i14 atom numbers of atoms 1-4 connected to each atom

n15 number of atoms in a 1-5 relation to each atom

i15 atom numbers of atoms 1-5 connected to each atom

**CUTOFF cutoff distances for energy interactions**

vdwcut cutoff distance for van der Waals interactions

chgcut cutoff distance for charge-charge interactions

dplcut cutoff distance for dipole-dipole interactions

mpolecut cutoff distance for atomic multipole interactions

vdwtaper distance at which van der Waals switching begins

chgtaper distance at which charge-charge switching begins

dpltaper distance at which dipole-dipole switching begins

mpoletaper distance at which atomic multipole switching begins

ewaldcut cutoff distance for direct space Ewald summation

use\_ewald logical flag governing use of Ewald summation term

use\_lights logical flag to use method of lights neighbors

**DERIV Cartesian coordinate derivative components**

desum total energy Cartesian coordinate derivatives

deb bond stretch Cartesian coordinate derivatives

dea angle bend Cartesian coordinate derivatives

deba stretch-bend Cartesian coordinate derivatives

deub Urey-Bradley Cartesian coordinate derivatives

deaa angle-angle Cartesian coordinate derivatives

deopb out-of-plane bend Cartesian coordinate derivatives

deopd out-of-plane distance Cartesian coordinate derivatives

deid improper dihedral Cartesian coordinate derivatives

deit improper torsion Cartesian coordinate derivatives

det torsional Cartesian coordinate derivatives

dept pi-orbital torsion Cartesian coordinate derivatives

debt stretch-torsion Cartesian coordinate derivatives

dett torsion-torsion Cartesian coordinate derivatives

dev van der Waals Cartesian coordinate derivatives

dec charge-charge Cartesian coordinate derivatives

decd charge-dipole Cartesian coordinate derivatives

ded dipole-dipole Cartesian coordinate derivatives

dem multipole Cartesian coordinate derivatives

dep polarization Cartesian coordinate derivatives

der reaction field Cartesian coordinate derivatives

des solvation Cartesian coordinate derivatives

delf metal ligand field Cartesian coordinate derivatives

deg geometric restraint Cartesian coordinate derivatives

dex extra energy term Cartesian coordinate derivatives

**DIPOLE atom & bond dipoles for current structure**

bdpl magnitude of each of the dipoles (Debyes)

sdpl position of each dipole between defining atoms

ndipole total number of dipoles in the system

idpl numbers of atoms that define each dipole

**DISGEO distance geometry bounds and parameters**

bnd distance geometry upper and lower bounds matrix

vdwrad hard sphere radii for distance geometry atoms

vdwmax maximum value of hard sphere sum for an atom pair

compact index of local distance compaction on embedding

pathmax maximum value of upper bound after smoothing

use\_invert flag to use enantiomer closest to input structure

use\_anneal flag to use simulated annealing refinement

**DOMEGA derivative components over torsions**

tesum total energy derivatives over torsions

teb bond stretch derivatives over torsions

tea angle bend derivatives over torsions

teba stretch-bend derivatives over torsions

teub Urey-Bradley derivatives over torsions

teaa angle-angle derivatives over torsions

teopb out-of-plane bend derivatives over torsions

teopd out-of-plane distance derivatives over torsions

teid improper dihedral derivatives over torsions

teit improper torsion derivatives over torsions

tet torsional derivatives over torsions

tept pi-orbital torsion derivatives over torsions

tebt stretch-torsion derivatives over torsions

tett torsion-torsion derivatives over torsions

tev van der Waals derivatives over torsions

tec charge-charge derivatives over torsions

tecd charge-dipole derivatives over torsions

ted dipole-dipole derivatives over torsions

tem atomic multipole derivatives over torsions

tep polarization derivatives over torsions

ter reaction field derivatives over torsions

tes solvation derivatives over torsions

telf metal ligand field derivatives over torsions

teg geometric restraint derivatives over torsions

tex extra energy term derivatives over torsions

**ENERGI individual potential energy components**

esum total potential energy of the system

eb bond stretch potential energy of the system

ea angle bend potential energy of the system

eba stretch-bend potential energy of the system

eub Urey-Bradley potential energy of the system

eaa angle-angle potential energy of the system

eopb out-of-plane bend potential energy of the system

eopd out-of-plane distance potential energy of the system

eid improper dihedral potential energy of the system

eit improper torsion potential energy of the system

et torsional potential energy of the system

ept pi-orbital torsion potential energy of the system

ebt stretch-torsion potential energy of the system

ett torsion-torsion potential energy of the system

ev van der Waals potential energy of the system

ec charge-charge potential energy of the system

ecd charge-dipole potential energy of the system

ed dipole-dipole potential energy of the system

em atomic multipole potential energy of the system

ep polarization potential energy of the system

er reaction field potential energy of the system

es solvation potential energy of the system

elf metal ligand field potential energy of the system

eg geometric restraint potential energy of the system

ex extra term potential energy of the system

**EWALD parameters for regular or PM Ewald summation**

aewald Ewald convergence coefficient value (Ang-1)

frecip fractional cutoff value for reciprocal sphere

tinfoil flag governing use of tinfoil boundary conditions

**EWREG exponential factors for regular Ewald sum**

maxvec maximum number of k-vectors per reciprocal axis

ejc exponental factors for cosine along the j-axis

ejs exponental factors for sine along the j-axis

ekc exponental factors for cosine along the k-axis

eks exponental factors for sine along the k-axis

elc exponental factors for cosine along the l-axis

els exponental factors for sine along the l-axis

**FACES variables for Connolly area and volume**

maxnbr maximum number of neighboring atom pairs

maxtt maximum number of temporary tori

maxt maximum number of total tori

maxp maximum number of probe positions

maxv maximum number of vertices

maxen maximum number of concave edges

maxfn maximum number of concave faces

maxc maximum number of circles

maxep maximum number of convex edges

maxfs maximum number of saddle faces

maxcy maximum number of cycles

mxcyep maximum number of cycle convex edges

maxfp maximum number of convex faces

mxfpcy maximum number of convex face cycles

**FIELDS molecular mechanics force field description**

biotyp force field atom type of each biopolymer type

forcefield string used to describe the current forcefield

**FILES name and number of current structure files**

nprior number of previously existing cycle files

ldir length in characters of the directory name

leng length in characters of the base filename

filename base filename used by default for all files

outfile output filename used for intermediate results

**FRACS atom distances to molecular center of mass**

xfrac fractional coordinate along a-axis of center of mass

yfrac fractional coordinate along b-axis of center of mass

zfrac fractional coordinate along c-axis of center of mass

**GROUP partitioning of system into atom groups**

grpmass total mass of all the atoms in each group

wgrp weight for each set of group-group interactions

ngrp total number of atom groups in the system

kgrp contiguous list of the atoms in each group

igrp first and last atom of each group in the list

grplist number of the group to which each atom belongs

use\_group flag to use partitioning of system into groups

use\_intra flag to include only intragroup interactions

use\_inter flag to include only intergroup interactions

**HESCUT cutoff value for Hessian matrix elements**

hesscut magnitude of smallest allowed Hessian element

**HESSN Cartesian Hessian elements for a single atom**

hessx Hessian elements for x-component of current atom

hessy Hessian elements for y-component of current atom

hessz Hessian elements for z-component of current atom

**IMPROP improper dihedrals in the current structure**

kprop force constant values for improper dihedral angles

vprop ideal improper dihedral angle value in degrees

niprop total number of improper dihedral angles in the system

iiprop numbers of the atoms in each improper dihedral angle

**IMPTOR improper torsions in the current structure**

itors1 1-fold amplitude and phase for each improper torsion

itors2 2-fold amplitude and phase for each improper torsion

itors3 3-fold amplitude and phase for each improper torsion

nitors total number of improper torsional angles in the system

iitors numbers of the atoms in each improper torsional angle

**INFORM control values for I/O and program flow**

digits decimal places output for energy and coordinates

iprint steps between status printing (0=no printing)

iwrite steps between coordinate dumps (0=no dumps)

isend steps between socket communication (0=no sockets)

verbose logical flag to turn on extra information

debug logical flag to turn on full debug printing

holdup logical flag to wait for carriage return on exit

abort logical flag to stop execution at next chance

**INTER sum of intermolecular energy components**

einter total intermolecular potential energy

**IOUNIT Fortran input/output (I/O) unit numbers**

iout Fortran I/O unit for major output (default=6)

input Fortran I/O unit for major input (default=5)

**KANANG forcefield parameters for angle-angle terms**

anan angle-angle cross term parameters for each atom class

**KANGS forcefield parameters for bond angle bending**

maxna maximum number of harmonic angle bend parameter entries

maxna5 maximum number of 5-membered ring angle bend entries

maxna4 maximum number of 4-membered ring angle bend entries

maxna3 maximum number of 3-membered ring angle bend entries

maxnaf maximum number of Fourier angle bend parameter entries

acon force constant parameters for harmonic angle bends

acon5 force constant parameters for 5-ring angle bends

acon4 force constant parameters for 4-ring angle bends

acon3 force constant parameters for 3-ring angle bends

aconf force constant parameters for Fourier angle bends

ang bond angle parameters for harmonic angle bends

ang5 bond angle parameters for 5-ring angle bends

ang4 bond angle parameters for 4-ring angle bends

ang3 bond angle parameters for 3-ring angle bends

angf phase shift angle and periodicity for Fourier bends

ka string of atom classes for harmonic angle bends

ka5 string of atom classes for 5-ring angle bends

ka4 string of atom classes for 4-ring angle bends

ka3 string of atom classes for 3-ring angle bends

kaf string of atom classes for Fourier angle bends

**KATOMS forcefield parameters for the atom types**

weight average atomic mass of each atom type

atmcls atom class number for each of the atom types

atmnum atomic number for each of the atom types

ligand number of atoms to be attached to each atom type

symbol modified atomic symbol for each atom type

describe string identifing each of the atom types

**KBONDS forcefield parameters for bond stretching**

maxnb maximum number of bond stretch parameter entries

maxnb5 maximum number of 5-membered ring bond stretch entries

maxnb4 maximum number of 4-membered ring bond stretch entries

maxnb3 maximum number of 3-membered ring bond stretch entries

maxnel maximum number of electronegativity bond corrections

bcon force constant parameters for harmonic bond stretch

bcon5 force constant parameters for 5-ring bond stretch

bcon4 force constant parameters for 4-ring bond stretch

bcon3 force constant parameters for 3-ring bond stretch

blen bond length parameters for harmonic bond stretch

blen5 bond length parameters for 5-ring bond stretch

blen4 bond length parameters for 4-ring bond stretch

blen3 bond length parameters for 3-ring bond stretch

dlen electronegativity bond length correction parameters

kb string of atom classes for harmonic bond stretch

kb5 string of atom classes for 5-ring bond stretch

kb4 string of atom classes for 4-ring bond stretch

kb3 string of atom classes for 3-ring bond stretch

kel string of atom classes for electronegativity corrections

**KCHRGE forcefield parameters for partial charges**

chg partial charge parameters for each atom type

**KDIPOL forcefield parameters for bond dipoles**

maxnd maximum number of bond dipole parameter entries

maxnd5 maximum number of 5-membered ring dipole entries

maxnd4 maximum number of 4-membered ring dipole entries

maxnd3 maximum number of 3-membered ring dipole entries

dpl dipole moment parameters for bond dipoles

dpl5 dipole moment parameters for 5-ring dipoles

dpl4 dipole moment parameters for 4-ring dipoles

dpl3 dipole moment parameters for 3-ring dipoles

pos dipole position parameters for bond dipoles

pos5 dipole position parameters for 5-ring dipoles

pos4 dipole position parameters for 4-ring dipoles

pos3 dipole position parameters for 3-ring dipoles

kd string of atom classes for bond dipoles

kd5 string of atom classes for 5-ring dipoles

kd4 string of atom classes for 4-ring dipoles

kd3 string of atom classes for 3-ring dipoles

**KEYS contents of current keyword parameter file**

nkey number of nonblank lines in the keyword file

keyline contents of each individual keyword file line

**KGEOMS parameters for the geometrical restraints**

xpfix x-coordinate target for each restrained position

ypfix y-coordinate target for each restrained position

zpfix z-coordinate target for each restrained position

pfix force constant and flat-well range for each position

dfix force constant and target range for each distance

afix force constant and target range for each angle

tfix force constant and target range for each torsion

gfix force constant and target range for each group distance

chir force constant and target range for chiral centers

depth depth of shallow Gaussian basin restraint

width exponential width coefficient of Gaussian basin

rwall radius of spherical droplet boundary restraint

npfix number of position restraints to be applied

ipfix atom number involved in each position restraint

kpfix flags to use x-, y-, z-coordinate position restraints

ndfix number of distance restraints to be applied

idfix atom numbers defining each distance restraint

nafix number of angle restraints to be applied

iafix atom numbers defining each angle restraint

ntfix number of torsional restraints to be applied

itfix atom numbers defining each torsional restraint

ngfix number of group distance restraints to be applied

igfix group numbers defining each group distance restraint

nchir number of chirality restraints to be applied

ichir atom numbers defining each chirality restraint

use\_basin logical flag governing use of Gaussian basin

use\_wall logical flag governing use of droplet boundary

**KHBOND forcefield parameters for H-bonding terms**

maxnhb maximum number of hydrogen bonding pair entries

radhb radius parameter for hydrogen bonding pairs

epshb well depth parameter for hydrogen bonding pairs

khb string of atom types for hydrogen bonding pairs

**KIPROP forcefield parameters for improper dihedral**

maxndi maximum number of improper dihedral parameter entries

dcon force constant parameters for improper dihedrals

tdi ideal dihedral angle values for improper dihedrals

kdi string of atom classes for improper dihedral angles

**KITORS forcefield parameters for improper torsions**

maxnti maximum number of improper torsion parameter entries

ti1 torsional parameters for improper 1-fold rotation

ti2 torsional parameters for improper 2-fold rotation

ti3 torsional parameters for improper 3-fold rotation

kti string of atom classes for improper torsional parameters

**KMULTI forcefield parameters for atomic multipoles**

maxnmp maximum number of atomic multipole parameter entries

multip atomic monopole, dipole and quadrupole values

mpaxis type of local axis definition for atomic multipoles

kmp string of atom types for atomic multipoles

**KOPBND forcefield parameters for out-of-plane bend**

maxnopb maximum number of out-of-plane bending entries

copb force constant parameters for out-of-plane bending

kaopb string of atom classes for out-of-plane bending

**KOPDST forcefield parameters for out-plane distance**

maxnopb maximum number of out-of-plane distance entries

copb force constant parameters for out-of-plane distance

kaopb string of atom classes for out-of-plane distance

**KORBS forcefield parameters for pisystem orbitals**

maxnpi maximum number of pisystem bond parameter entries

electron number of pi-electrons for each atom class

ionize ionization potential for each atom class

repulse repulsion integral value for each atom class

sslope slope for bond stretch vs. pi-bond order

tslope slope for 2-fold torsion vs. pi-bond order

kpi string of atom classes for pisystem bonds

**KPITOR forcefield parameters for pi-orbit torsions**

maxnpt maximum number of pi-orbital torsion parameter entries

ptcon force constant parameters for pi-orbital torsions

kpt string of atom classes for pi-orbital torsion terms

**KPOLR forcefield parameters for polarizability**

polr dipole polarizability parameters for each atom type

pgrp connected types in polarization group of each atom type

**KSTBND forcefield parameters for stretch-bending**

stbn stretch-bending parameters for each atom class

**KSTTOR forcefield parameters for stretch-torsions**

maxnbt maximum number of stretch-torsion parameter entries

btcon force constant parameters for stretch-torsion

kbt string of atom classes for bonds in stretch-torsion

**KTORSN forcefield parameters for torsional angles**

maxnt maximum number of torsional angle parameter entries

maxnt5 maximum number of 5-membered ring torsion entries

maxnt4 maximum number of 4-membered ring torsion entries

t1 torsional parameters for standard 1-fold rotation

t2 torsional parameters for standard 2-fold rotation

t3 torsional parameters for standard 3-fold rotation

t4 torsional parameters for standard 4-fold rotation

t5 torsional parameters for standard 5-fold rotation

t6 torsional parameters for standard 6-fold rotation

t15 torsional parameters for 1-fold rotation in 5-ring

t25 torsional parameters for 2-fold rotation in 5-ring

t35 torsional parameters for 3-fold rotation in 5-ring

t45 torsional parameters for 4-fold rotation in 5-ring

t55 torsional parameters for 5-fold rotation in 5-ring

t65 torsional parameters for 6-fold rotation in 5-ring

t14 torsional parameters for 1-fold rotation in 4-ring

t24 torsional parameters for 2-fold rotation in 4-ring

t34 torsional parameters for 3-fold rotation in 4-ring

t44 torsional parameters for 4-fold rotation in 4-ring

t54 torsional parameters for 5-fold rotation in 4-ring

t64 torsional parameters for 6-fold rotation in 4-ring

kt string of atom classes for torsional angles

kt5 string of atom classes for 5-ring torsions

kt4 string of atom classes for 4-ring torsions

**KTRTOR forcefield parameters for torsion-torsions**

maxntt maximum number of torsion-torsion parameter entries

maxtgrd maximum dimension of torsion-torsion spline grid

maxtgrd2 maximum number of torsion-torsion spline grid points

ttx angle values for first torsion of spline grid

tty angle values for second torsion of spline grid

tbf function values at points on spline grid

tbx gradient over first torsion of spline grid

tby gradient over second torsion of spline grid

tbxy Hessian cross components over spline grid

tnx number of columns in torsion-torsion spline grid

tny number of rows in torsion-torsion spline grid

ktt string of torsion-torsion atom classes

**KURYBR forcefield parameters for Urey-Bradley terms**

maxnu maximum number of Urey-Bradley parameter entries

ucon force constant parameters for Urey-Bradley terms

dst13 ideal 1-3 distance parameters for Urey-Bradley terms

ku string of atom classes for Urey-Bradley terms

**KVDWPR forcefield parameters for special vdw terms**

maxnvp maximum number of special van der Waals pair entries

radpr radius parameter for special van der Waals pairs

epspr well depth parameter for special van der Waals pairs

kvpr string of atom classes for special van der Waals pairs

**KVDWS forcefield parameters for van der Waals terms**

rad van der Waals radius parameter for each atom class

eps van der Waals well depth parameter for each atom class

rad4 van der Waals radius parameter in 1-4 interactions

eps4 van der Waals well depth parameter in 1-4 interactions

reduct van der Waals reduction factor for each atom class

**LIGHT indices for method of lights pair neighbors**

nlight total number of sites for method of lights calculation

kbx low index of neighbors of each site in the x-sorted list

kby low index of neighbors of each site in the y-sorted list

kbz low index of neighbors of each site in the z-sorted list

kex high index of neighbors of each site in the x-sorted list

key high index of neighbors of each site in the y-sorted list

kez high index of neighbors of each site in the z-sorted list

locx pointer from x-sorted list into original interaction list

locy pointer from y-sorted list into original interaction list

locz pointer from z-sorted list into original interaction list

rgx pointer from original interaction list into x-sorted list

rgy pointer from original interaction list into y-sorted list

rgz pointer from original interaction list into z-sorted list

**LINMIN parameters for line search minimization**

stpmin minimum step length in current line search direction

stpmax maximum step length in current line search direction

cappa stringency of line search (0=tight < cappa < 1=loose)

slpmax projected gradient above which stepsize is reduced

angmax maximum angle between search direction and -gradient

intmax maximum number of interpolations during line search

**MATH mathematical and geometrical constants**

radian conversion factor from radians to degrees

pi numerical value of the geometric constant

sqrtpi numerical value of the square root of Pi

logten numerical value of the natural log of ten

sqrttwo numerical value of the square root of two

twosix numerical value of the sixth root of two

**MDSTUF control of molecular dynamics trajectory**

nfree total number of degrees of freedom for a system

velsave flag to save velocity vector components to a file

frcsave flag to save force vector components to a file

uindsave flag to save induced atomic dipoles to a file

integrate type of molecular dynamics integration algorithm

**MINIMA general parameters for minimizations**

fctmin value below which function is deemed optimized

hguess initial value for the H-matrix diagonal elements

maxiter maximum number of iterations during optimization

nextiter iteration number to use for the first iteration

**MOLCUL individual molecules within current system**

molmass molecular weight for each molecule in the system

totmass total weight of all the molecules in the system

nmol total number of separate molecules in the system

kmol contiguous list of the atoms in each molecule

imol first and last atom of each molecule in the list

molcule number of the molecule to which each atom belongs

**MOLDYN velocity and acceleration on MD trajectory**

v current velocity of each atom along the x,y,z-axes

a current acceleration of each atom along x,y,z-axes

aold previous acceleration of each atom along x,y,z-axes

**MOMENT components of electric multipole moments**

netchg net electric charge for the total system

netdpl dipole moment magnitude for the total system

netqdp diagonal quadrupole (Qxx, Qyy, Qzz) for system

xdpl dipole vector x-component in the global frame

ydpl dipole vector y-component in the global frame

zdpl dipole vector z-component in the global frame

xxqdp quadrupole tensor xx-component in global frame

xyqdp quadrupole tensor xy-component in global frame

xzqdp quadrupole tensor xz-component in global frame

yxqdp quadrupole tensor yx-component in global frame

yyqdp quadrupole tensor yy-component in global frame

yzqdp quadrupole tensor yz-component in global frame

zxqdp quadrupole tensor zx-component in global frame

zyqdp quadrupole tensor zy-component in global frame

zzqdp quadrupole tensor zz-component in global frame

**MPLPOT specifics of atomic multipole functions**

m2scale factor by which 1-2 multipole interactions are scaled

m3scale factor by which 1-3 multipole interactions are scaled

m4scale factor by which 1-4 multipole interactions are scaled

m5scale factor by which 1-5 multipole interactions are scaled

**MPOLE multipole components for current structure**

maxpole max components (monopole=1,dipole=4,quadrupole=13)

pole multipole values for each site in the local frame

rpole multipoles rotated to the global coordinate system

npole total number of multipole sites in the system

ipole number of the atom for each multipole site

polsiz number of mutipole components at each multipole site

zaxis number of the z-axis defining atom for each site

xaxis number of the x-axis defining atom for each site

yaxis number of the y-axis defining atom for each site

polaxe local axis type for each multipole site

**MUTANT hybrid atoms for free energy perturbation**

lambda weighting of initial state in hybrid Hamiltonian

nhybrid number of atoms mutated from initial to final state

ihybrid atomic sites differing in initial and final state

type0 atom type of each atom in the initial state system

class0 atom class of each atom in the initial state system

type1 atom type of each atom in the final state system

class1 atom class of each atom in the final state system

alter true if an atom is to be mutated, false otherwise

**NUCLEO parameters for nucleic acid structure**

bkbone phosphate backbone angles for each nucleotide

glyco glycosidic torsional angle for each nucleotide

pucker sugar pucker, either 2=2'-endo or 3=3'-endo

dblhlx flag to mark system as nucleic acid double helix

deoxy flag to mark deoxyribose or ribose sugar units

hlxform helix form (A, B or Z) of polynucleotide strands

**OMEGA dihedrals for torsional space computations**

dihed current value in radians of each dihedral angle

nomega number of dihedral angles allowed to rotate

iomega numbers of two atoms defining rotation axis

zline line number in Z-matrix of each dihedral angle

**OPBEND out-of-plane bends in the current structure**

kopb force constant values for out-of-plane bending

nopbend total number of out-of-plane bends in the system

iopb bond angle numbers used in out-of-plane bending

**OPDIST out-of-plane distances in current structure**

kopd force constant values for out-of-plane distance

nopdist total number of out-of-plane distances in the system

iopb numbers of the atoms in each out-of-plane distance

**ORBITS orbital energies for conjugated pisystem**

q number of pi-electrons contributed by each atom

w ionization potential of each pisystem atom

em repulsion integral for each pisystem atom

nfill number of filled pisystem molecular orbitals

**OUTPUT control of coordinate output file format**

archive logical flag to save structures in an archive

noversion logical flag governing use of filename versions

overwrite logical flag to overwrite intermediate files inplace

cyclesave logical flag to mark use of numbered cycle files

coordtype selects Cartesian, internal, rigid body or none

**PARAMS contents of force field parameter file**

nprm number of nonblank lines in the parameter file

prmline contents of each individual parameter file line

**PATHS parameters for Elber reaction path method**

p0 reactant Cartesian coordinates as variables

p1 product Cartesian coordinates as variables

pmid midpoint between the reactant and product

pvect vector connecting the reactant and product

pstep step per cycle along reactant-product vector

pzet current projection on reactant-product vector

pnorm length of the reactant-product vector

acoeff transformation matrix 'A' from Elber paper

gc gradients of the path constraints

**PDB definition of a Protein Data Bank structure**

xpdb x-coordinate of each atom stored in PDB format

ypdb y-coordinate of each atom stored in PDB format

zpdb z-coordinate of each atom stored in PDB format

npdb number of atoms stored in Protein Data Bank format

resnum number of the residue to which each atom belongs

npdb12 number of atoms directly bonded to each CONECT atom

ipdb12 atom numbers of atoms connected to each CONECT atom

pdblist list of the Protein Data Bank atom number of each atom

pdbtyp Protein Data Bank record type assigned to each atom

atmnam Protein Data Bank atom name assigned to each atom

resnam Protein Data Bank residue name assigned to each atom

**PHIPSI phi-psi-omega-chi angles for a protein**

phi value of the phi angle for each amino acid residue

psi value of the psi angle for each amino acid residue

omega value of the omega angle for each amino acid residue

chi values of the chi angles for each amino acid residue

chiral chirality of each amino acid residue (1=L, -1=D)

disulf residue joined to each residue via a disulfide link

**PIORBS conjugated system in the current structure**

norbit total number of pisystem orbitals in the system

iorbit numbers of the atoms containing pisystem orbitals

reorbit number of evaluations between orbital updates

piperp atoms defining a normal plane to each orbital

nbpi total number of bonds affected by the pisystem

bpi bond and piatom numbers for each pisystem bond

ntpi total number of torsions affected by the pisystem

tpi torsion and pibond numbers for each pisystem torsion

listpi atom list indicating whether each atom has an orbital

**PISTUF bonds and torsions in the current pisystem**

bkpi bond stretch force constants for pi-bond order of 1.0

blpi ideal bond length values for a pi-bond order of 1.0

kslope rate of force constant decrease with bond order decrease

lslope rate of bond length increase with a bond order decrease

torsp2 2-fold torsional energy barrier for pi-bond order of 1.0

**PITORS pi-orbital torsions in the current structure**

kpit 2-fold pi-orbital torsional force constants

npitors total number of pi-orbital torsional interactions

ipit numbers of the atoms in each pi-orbital torsion

**PME parameters for particle mesh Ewald summation**

maxfft maximum number of points along each FFT direction

maxorder maximum order of the B-spline approximation

maxtable maximum size of the FFT table array

maxgrid maximum dimension of the PME charge grid array

bsmod1 B-spline moduli along the a-axis direction

bsmod2 B-spline moduli along the b-axis direction

bsmod3 B-spline moduli along the c-axis direction

table intermediate array used by the FFT calculation

nfft1 number of grid points along the a-axis direction

nfft2 number of grid points along the b-axis direction

nfft3 number of grid points along the c-axis direction

bsorder order of the PME B-spline approximation

**POLAR polarizabilities and induced dipole moments**

polarity dipole polarizability for each multipole site (Ang\*\*3)

pdamp value of polarizability damping factor for each site

uind induced dipole components at each multipole site

uinp induced dipoles in field used for energy interactions

npolar total number of polarizable sites in the system

**POLGRP polarizable site group connectivity lists**

maxp11 maximum number of atoms in a polarization group

maxp12 maximum number of atoms in groups 1-2 to an atom

maxp13 maximum number of atoms in groups 1-3 to an atom

maxp14 maximum number of atoms in groups 1-4 to an atom

np11 number of atoms in polarization group of each atom

ip11 atom numbers of atoms in same group as each atom

np12 number of atoms in groups 1-2 to each atom

ip12 atom numbers of atoms in groups 1-2 to each atom

np13 number of atoms in groups 1-3 to each atom

ip13 atom numbers of atoms in groups 1-3 to each atom

np14 number of atoms in groups 1-4 to each atom

ip14 atom numbers of atoms in groups 1-4 to each atom

**POLPOT specifics of polarization functional form**

poleps induced dipole convergence criterion (rms Debyes/atom)

polsor induced dipole SOR convergence acceleration factor

pgamma prefactor in exponential polarization damping term

p2scale field 1-2 scale factor for energy evaluations

p3scale field 1-3 scale factor for energy evaluations

p4scale field 1-4 scale factor for energy evaluations

p5scale field 1-5 scale factor for energy evaluations

d1scale field intra-group scale factor for direct induced

d2scale field 1-2 group scale factor for direct induced

d3scale field 1-3 group scale factor for direct induced

d4scale field 1-4 group scale factor for direct induced

u1scale field intra-group scale factor for mutual induced

u2scale field 1-2 group scale factor for mutual induced

u3scale field 1-3 group scale factor for mutual induced

u4scale field 1-4 group scale factor for mutual induced

poltyp type of polarization potential (direct or mutual)

**POTENT usage of each potential energy component**

use\_bond logical flag governing use of bond stretch potential

use\_angle logical flag governing use of angle bend potential

use\_strbnd logical flag governing use of stretch-bend potential

use\_urey logical flag governing use of Urey-Bradley potential

use\_angang logical flag governing use of angle-angle cross term

use\_opbend logical flag governing use of out-of-plane bend term

use\_opdist logical flag governing use of out-of-plane distance

use\_improp logical flag governing use of improper dihedral term

use\_imptor logical flag governing use of improper torsion term

use\_tors logical flag governing use of torsional potential

use\_pitors logical flag governing use of pi-orbital torsion term

use\_strtor logical flag governing use of stretch-torsion term

use\_tortor logical flag governing use of torsion-torsion term

use\_vdw logical flag governing use of vdw der Waals potential

use\_charge logical flag governing use of charge-charge potential

use\_chgdpl logical flag governing use of charge-dipole potential

use\_dipole logical flag governing use of dipole-dipole potential

use\_mpole logical flag governing use of multipole potential

use\_polar logical flag governing use of polarization term

use\_rxnfld logical flag governing use of reaction field term

use\_solv logical flag governing use of surface area solvation

use\_gbsa logical flag governing use of GB/SA solvation term

use\_metal logical flag governing use of ligand field term

use\_geom logical flag governing use of geometric restraints

use\_extra logical flag governing use of extra potential term

use\_orbit logical flag governing use of pisystem computation

**PRECIS values of machine precision tolerances**

tiny the smallest positive floating point value

small the smallest relative floating point spacing

huge the largest relative floating point spacing

**REFER storage of reference atomic coordinate set**

xref reference x-coordinate for each atom in the system

yref reference y-coordinate for each atom in the system

zref reference z-coordinate for each atom in the system

nref total number of atoms in the reference system

reftyp atom type for each atom in the reference system

n12ref number of atoms bonded to each reference atom

i12ref atom numbers of atoms 1-2 connected to each atom

refleng length in characters of the reference filename

refltitle length in characters of the reference title string

refnam atom name for each atom in the reference system

reffile base filename for the reference structure

reftitle title used to describe the reference structure

**RESDUE standard biopolymer residue abbreviations**

amino three-letter abbreviations for amino acids types

nuclz three-letter abbreviations for nucleic acids types

amino1 one-letter abbreviations for amino acids types

nuclz1 one-letter abbreviations for nucleic acids types

**RGDDYN velocities and momenta for rigid body MD**

vcm current translational velocity of each rigid body

wcm current angular velocity of each rigid body

lm current angular momentum of each rigid body

linear logical flag to mark group as linear or nonlinear

**RIGID rigid body coordinates for atom groups**

xrb rigid body reference x-coordinate for each atom

yrb rigid body reference y-coordinate for each atom

zrb rigid body reference z-coordinate for each atom

rbc current rigid body coordinates for each group

use\_rigid flag to mark use of rigid body coordinate system

**RING number and location of small ring structures**

nring3 total number of 3-membered rings in the system

iring3 numbers of the atoms involved in each 3-ring

nring4 total number of 4-membered rings in the system

iring4 numbers of the atoms involved in each 4-ring

nring5 total number of 5-membered rings in the system

iring5 numbers of the atoms involved in each 5-ring

nring6 total number of 6-membered rings in the system

iring6 numbers of the atoms involved in each 6-ring

**ROTATE molecule partitions for rotation of a bond**

nrot total number of atoms moving when bond rotates

rot atom numbers of atoms moving when bond rotates

use\_short logical flag governing use of shortest atom list

**RXNFLD reaction field matrix elements and indices**

b1 first reaction field matrix element array

b2 second reaction field matrix element array

ijk indices into the reaction field element arrays

**RXNPOT specifics of reaction field functional form**

rfsize radius of reaction field sphere centered at origin

rfbulkd bulk dielectric constant of reaction field continuum

rfterms number of terms to use in reaction field summation

**SCALES parameter scale factors for optimization**

scale multiplicative factor for each optimization parameter

set\_scale logical flag to show if scale factors have been set

**SEQUEN sequence information for a biopolymer**

nseq total number of residues in biopolymer sequences

nchain number of separate biopolymer sequence chains

ichain first and last residue in each biopolymer chain

seqtyp residue type for each residue in the sequence

seq three-letter code for each residue in the sequence

chnnam one-letter identifier for each sequence chain

**SHAKE definition of Shake/Rattle constraints**

krat ideal distance value for rattle constraint

nrat number of rattle distance constraints to apply

nratx number of atom group spatial constraints to apply

irat atom numbers of atoms in a rattle constraint

iratx group number of group in a spatial constraint

kratx spatial constraint type (1=plane, 2=line, 3=point)

ratimage flag to use minimum image for rattle constraint

use\_rattle logical flag to set use of rattle contraints

**SHUNT polynomial switching function coefficients**

off distance at which the potential energy goes to zero

off2 square of distance at which the potential goes to zero

cut distance at which switching of the potential begins

cut2 square of distance at which the switching begins

c0 zeroth order coefficient of multiplicative switch

c1 first order coefficient of multiplicative switch

c2 second order coefficient of multiplicative switch

c3 third order coefficient of multiplicative switch

c4 fourth order coefficient of multiplicative switch

c5 fifth order coefficient of multiplicative switch

f0 zeroth order coefficient of additive switch function

f1 first order coefficient of additive switch function

f2 second order coefficient of additive switch function

f3 third order coefficient of additive switch function

f4 fourth order coefficient of additive switch function

f5 fifth order coefficient of additive switch function

f6 sixth order coefficient of additive switch function

f7 seventh order coefficient of additive switch function

**SIZES parameter values to set array dimensions**

"sizes.i" sets values for critical array dimensions used throughout the software; these parameters will fix the size of the largest systems that can be handled; values too large for the computer's memory and/or swap space to accomodate will result in poor performance or outright failure

parameter: maximum allowed number of:

maxatm atoms in the molecular system

maxval atoms directly bonded to an atom

maxgrp user-defined groups of atoms

maxtyp force field atom type definitions

maxclass force field atom class definitions

maxprm lines in the parameter file

maxkey lines in the keyword file

maxrot bonds for torsional rotation

maxvar optimization variables (vector storage)

maxopt optimization variables (matrix storage)

maxhess off-diagonal Hessian elements

maxlight sites for method of lights neighbors

maxvib vibrational frequencies

maxgeo distance geometry points

maxcell unit cells in replicated crystal

maxring 3-, 4-, or 5-membered rings

maxfix geometric constraints and restraints

maxbio biopolymer atom definitions

maxres residues in the macromolecule

maxamino amino acid residue types

maxnuc nucleic acid residue types

maxbnd covalent bonds in molecular system

maxang bond angles in molecular system

maxtors torsional angles in molecular system

maxbitor bitorsions in molecular system

maxpi atoms in conjugated pisystem

maxpib covalent bonds involving pisystem

maxpit torsional angles involving pisystem

**SOCKET control parameters for socket communication**

runtyp calculation type for passing socket information

cstep current optimization or dynamics step number

cdt current dynamics cumulative simulation time

cenergy current potential energy from simulation

cdx current gradient components along the x-axis

cdy current gradient components along the y-axis

cdz current gradient components along the z-axis

skt\_init logical flag set to true after socket initialization

use\_socket logical flag governing use of external sockets

use\_gui logical flag to show TINKER was invoked from GUI

closing logical flag to indicate JVM and server shutdown

**SOLUTE parameters for continuum solvation models**

rsolv atomic radius of each atom for continuum solvation

vsolv atomic volume of each atom for continuum solvation

asolv atomic solvation parameters (kcal/mole/Ang\*\*2)

rborn Born radius of each atom for GB/SA solvation

drb solvation derivatives with respect to Born radii

doffset dielectric offset to continuum solvation atomic radii

p1 single-atom scale factor for analytical Still GB/SA

p2 1-2 interaction scale factor for analytical Still GB/SA

p3 1-3 interaction scale factor for analytical Still GB/SA

p4 nonbonded scale factor for analytical Still GB/SA

p5 soft cutoff parameter for analytical Still GB/SA

gpol polarization self-energy values for each atom

shct overlap scaling factors for Hawkins-Cramer-Truhlar GB/SA

wace "omega" values for atom class pairs for use with ACE

s2ace "sigma^2" values for atom class pairs for use with ACE

uace "mu" values for atom class pairs for use with ACE

solvtyp solvation model (ASP, SASA, ONION, STILL, HCT, ACE)

**STODYN frictional coefficients for SD trajectory**

friction global frictional coefficient for exposed particle

gamma atomic frictional coefficients for each atom

use\_sdarea logical flag to use surface area friction scaling

**STRBND stretch-bends in the current structure**

ksb force constant for stretch-bend terms

nstrbnd total number of stretch-bend interactions

isb angle and bond numbers used in stretch-bend

**STRTOR stretch-torsions in the current structure**

kst 1-, 2- and 3-fold stretch-torsion force constants

nstrtor total number of stretch-torsion interactions

ist torsion and bond numbers used in stretch-torsion

**SYNTRN definition of synchronous transit path**

t value of the path coordinate (0=reactant, 1=product)

pm path coordinate for extra point in quadratic transit

xmin1 reactant coordinates as array of optimization variables

xmin2 product coordinates as array of optimization variables

xm extra coordinate set for quadratic synchronous transit

**TITLES title for the current molecular system**

ltitle length in characters of the nonblank title string

title title used to describe the current structure

**TORPOT specifics of torsional functional forms**

idihunit convert improper dihedral energy to kcal/mole

itorunit convert improper torsion amplitudes to kcal/mole

torsunit convert torsional parameter amplitudes to kcal/mole

ptorunit convert pi-orbital torsion energy to kcal/mole

storunit convert stretch-torsion energy to kcal/mole

ttorunit convert stretch-torsion energy to kcal/mole

**TORS torsional angles within the current structure**

tors1 1-fold amplitude and phase for each torsional angle

tors2 2-fold amplitude and phase for each torsional angle

tors3 3-fold amplitude and phase for each torsional angle

tors4 4-fold amplitude and phase for each torsional angle

tors5 5-fold amplitude and phase for each torsional angle

tors6 6-fold amplitude and phase for each torsional angle

ntors total number of torsional angles in the system

itors numbers of the atoms in each torsional angle

**TORTOR torsion-torsions in the current structure**

ntortor total number of torsion-torsion interactions

itt atoms and parameter indices for torsion-torsion

**TREE potential smoothing & search tree levels**

maxpss maximum number of potential smoothing levels

etree energy reference value at the top of the tree

ilevel smoothing deformation value at each tree level

nlevel number of levels of potential smoothing used

**UNITS physical constants and unit conversions**

avogadro Avogadro's number (N) in particles/mole

boltzmann Boltzmann constant (kB) in g\*Ang\*\*2/ps\*\*2/K/mole

gasconst ideal gas constant (R) in kcal/mole/K

lightspd speed of light in vacuum (c) in cm/ps

bohr conversion from Bohrs to Angstroms

joule conversion from calories to joules

evolt conversion from Hartree to electron-volts

hartree conversion from Hartree to kcal/mole

electric conversion from electron\*\*2/Ang to kcal/mole

debye conversion from electron-Ang to Debyes

prescon conversion from kcal/mole/Ang\*\*3 to Atm

convert conversion from kcal to g\*Ang\*\*2/ps\*\*2

**UREY Urey-Bradley interactions in the structure**

uk Urey-Bradley force constants (kcal/mole/Ang\*\*2)

ul ideal 1-3 distance values in Angstroms

nurey total number of Urey-Bradley terms in the system

iury numbers of the atoms in each Urey-Bradley interaction

**URYPOT specifics of Urey-Bradley functional form**

cury cubic coefficient in Urey-Bradley potential

qury quartic coefficient in Urey-Bradley potential

ureyunit convert Urey-Bradley energy to kcal/mole

**USAGE atoms active during energy computation**

nuse number of active atoms used in energy calculation

use true if an atom is active, false if inactive

**VDW van der Waals parameters for current structure**

radmin minimum energy distance for each atom class pair

epsilon well depth parameter for each atom class pair

radmin4 minimum energy distance for 1-4 interaction pairs

epsilon4 well depth parameter for 1-4 interaction pairs

radhbnd minimum energy distance for hydrogen bonding pairs

epshbnd well depth parameter for hydrogen bonding pairs

kred value of reduction factor parameter for each atom

ired attached atom from which reduction factor is applied

nvdw total number van der Waals active sites in the system

ivdw number of the atom for each van der Waals active site

**VDWPOT specifics of van der Waals functional form**

abuck value of "A" constant in Buckingham vdw potential

bbuck value of "B" constant in Buckingham vdw potential

cbuck value of "C" constant in Buckingham vdw potential

ghal value of "gamma" in buffered 14-7 vdw potential

dhal value of "delta" in buffered 14-7 vdw potential

v2scale factor by which 1-2 vdw interactions are scaled

v3scale factor by which 1-3 vdw interactions are scaled

v4scale factor by which 1-4 vdw interactions are scaled

v5scale factor by which 1-5 vdw interactions are scaled

igauss coefficients of Gaussian fit to vdw potential

ngauss number of Gaussians used in fit to vdw potential

vdwtyp type of van der Waals potential energy function

radtyp type of parameter (sigma or R-min) for atomic size

radsiz atomic size provided as radius or diameter

radrule combining rule for atomic size parameters

epsrule combining rule for vdw well depth parameters

gausstyp type of Gaussian fit to van der Waals potential

**VIRIAL components of internal virial tensor**

vir total internal virial Cartesian tensor components

**WARP parameters for potential surface smoothing**

m2 second moment of the GDA gaussian for each atom

deform value of the smoothing deformation parameter

difft diffusion coefficient for torsional potential

diffv diffusion coefficient for van der Waals potential

diffc diffusion coefficient for charge-charge potential

use\_smooth flag to use a potential energy smoothing method

use\_dem flag to use diffusion equation method potential

use\_gda flag to use gaussian density annealing potential

use\_tophat flag to use analytical tophat smoothed potential

use\_stophat flag to use shifted tophat smoothed potential

**XTALS crystal structures for parameter fitting**

e0\_lattice ideal lattice energy for the current crystal

moment\_0 ideal dipole moment for monomer from crystal

nxtal number of crystal structures to be stored

nvary number of potential parameters to optimize

ivary index for the types of potential parameters

vary atom numbers involved in potential parameters

iresid crystal structure to which each residual refers

rsdtyp experimental variable for each of the residuals

vartyp type of potential parameter to be optimized

**ZCLOSE ring openings and closures for Z-matrix**

nadd number of added bonds between Z-matrix atoms

iadd numbers of the atom pairs defining added bonds

ndel number of bonds between Z-matrix bonds to delete

idel numbers of the atom pairs defining deleted bonds

**ZCOORD Z-matrix internal coordinate definitions**

zbond bond length used to define each Z-matrix atom

zang bond angle used to define each Z-matrix atom

ztors angle or torsion used to define Z-matrix atom

iz defining atom numbers for each Z-matrix atom