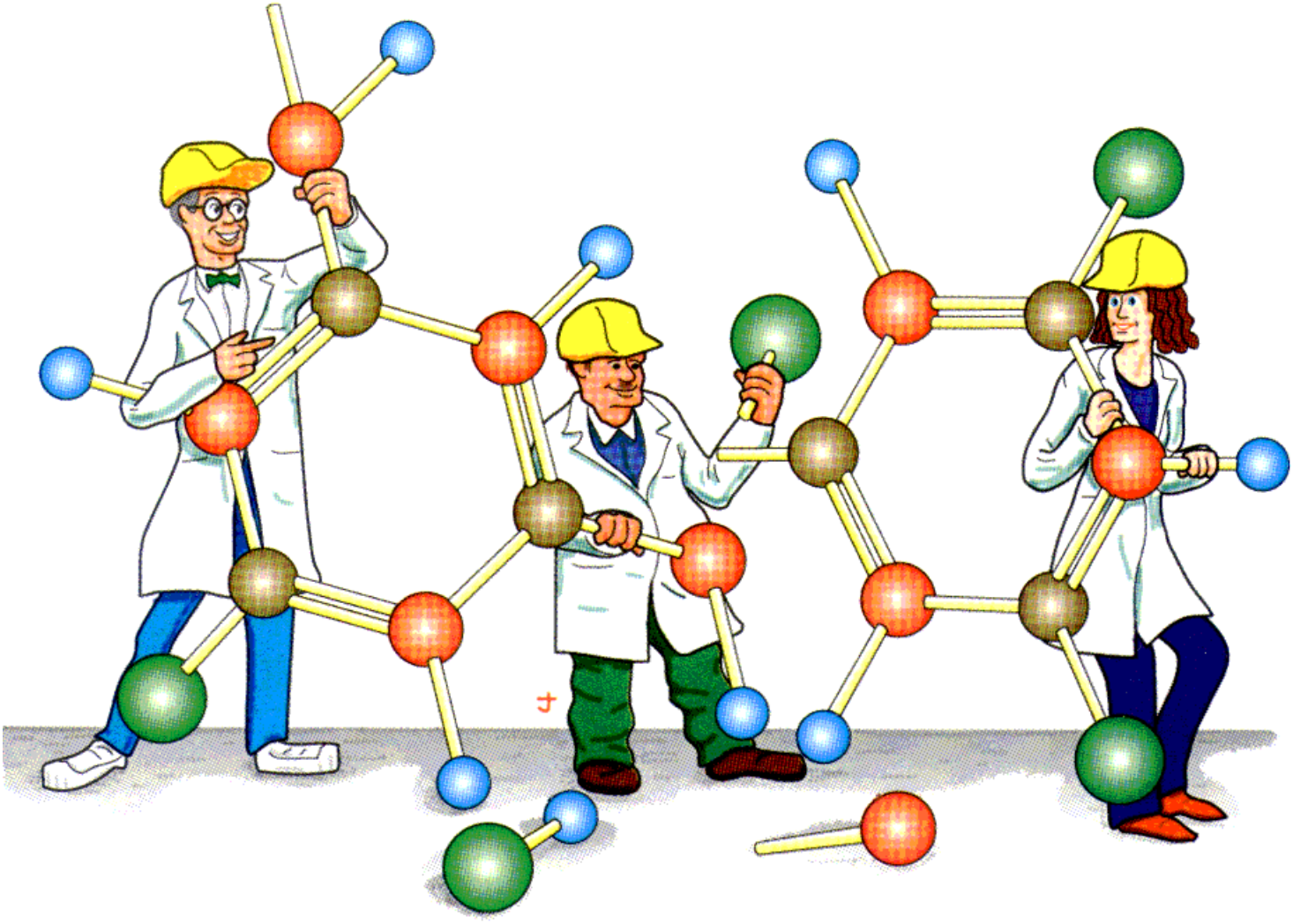
TINKER

Software Tools for Molecular Design



Version 6.0 October 2011

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Courtesy of Prof. R. T. Paine, Univ. of New Mexico

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1. Introduction to the Software

What is the TINKER Software?

Welcome to the TINKER molecular modeling package! TINKER is designed to be an easily used and flexible system of programs and routines for molecular mechanics and dynamics as well as other energy-based and structural manipulation calculations. It is intended to be modular enough to enable development of new computational methods and efficient enough to meet most production calculation needs. Rather than incorporating all the functionality in one monolithic program, TINKER provides a set of relatively small programs that interoperate to perform complex computations. New programs can be easily added by modelers with only limited programming experience.

Features and Capabilities

The series of major programs included in the distribution system perform the following core tasks:

(1) building protein and nucleic acid models from sequence
(2) energy minimization and structural optimization
(3) analysis of energy distribution within a structure
(4) molecular dynamics and stochastic dynamics
(5) simulated annealing with a choice of cooling schedules
(6) normal modes and vibrational frequencies
(7) conformational search and global optimization
(8) transition state location and conformational pathways
(9) fitting of energy parameters to crystal data
(10) distance geometry with pairwise metrization
(11) molecular volumes and surface areas
(12) free energy changes for structural mutations
(13) advanced algorithms based on potential smoothing

Many of the various energy minimization and molecular dynamics computations can be performed on full or partial structures, over Cartesian, internal or rigid body coordinates, and including a variety of boundary conditions and crystal cell types. Other programs are available to generate timing data and allow checking of potential function derivatives for coding errors. Special features are available to facilitate input and output of protein and nucleic acid structures. However, the basic core routines have no knowledge of biopolymer structure and can be used for general molecular systems.

Due to its emphasis on ease of modification, TINKER differs from many other currently available molecular modeling packages in that the user is expected to be willing to write simple ``front-end'' programs and make some alterations at the source code level. The main programs provided should be considered as templates for the users to change according to their wishes. All subroutines are internally documented and structured programming practices are adhered to throughout. The result, it is hoped, will be a calculational system which can be tailored to local needs and desires.

The core TINKER system consists of nearly 135,000 lines of source written entirely in a portable Fortran77 superset. Use is made of only some very common extensions that aid in writing highly structured code. The current version of the package has been ported to a wide range of computers with no or extremely minimal changes. Tested systems include: Red Hat Linux, Microsoft Windows 9X/NT/2000/XP, Apple OS9 and OSX, HP/Compaq/DEC Alphas under Tru64 Unix and OpenVMS, Hewlett-Packard, IBM, Silicon Graphics and Sun workstations under each vendor's Unix. At present, our new code is written on various Linux platforms, and occasionally tested for compatibility on

various of the other machine and OS combinations listed above. At present, we are in the process of converting our primary development efforts from Fortran77 to a more modern Fortran dialect. A machine-translated C version of TINKER is currently available, and a hand-translated optimized C version of a previous TINKER release is available for inspection. Conversion to C or C++ is under consideration, but not being actively pursued at this time.

The basic design of the energy function engine used by the TINKER system allows usage of several different parameter sets. At present we are distributing parameters that implement AMBER ff94 and ff96, CHARMM19 and 27, MM2, MM3, OPLS-UA, OPLS-AA, Liam Dang's polarizable potentials, and our own AMOEBA (Atomic Multipole Optimized Energetics for Biomolecular Applications) parameters. In most cases, the source code separates the geometric manipulations needed for energy derivatives from the actual form of the energy function itself. Several other literature parameter sets are being considered for possible future development (ENCAD, MMFF-94, MM4, UFF, *etc.)*, and many of the alternative potential function forms reported in the literature can be implemented directly or after minor code changes.

Much of the software in the TINKER package has been heavily used and well tested, but some modules are still in a fairly early stage of development. Further work on the TINKER system is planned in three main areas: (1) extension and improvement of the potential energy parameters including additional parameterization and testing of our polarizable multipole AMOEBA force field, (2) coding of new computational algorithms including additional methods for free energy determination, torsional Monte Carlo and molecular dynamics sampling, advanced methods for long range interactions, better transition state location, and further application of the potential smoothing paradigm, and (3) further development of Force Field Explorer, a Java-based GUI front-end to the TINKER programs that provides for calculation setup, launch and control as well as basic molecular visualization.

Contact Information

Questions and comments regarding the TINKER package, including suggestions for improvements and changes should be made to the author:

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In addition, an Internet web site containing an online version of this User's Guide, the most recent distribution version of the full TINKER package and other useful information can be found at **`http://dasher.wustl.edu/tinker`**, the Home Page for the TINKER Molecular Modeling Package.

2. Installation on your Computer

How to Obtain a Copy of TINKER

The TINKER package is distributed on the Internet via either the web site or the anonymous ftp account on **dasher.wustl.edu** with an IP number of 128.252.208.48. This node is a web and file server located in the Ponder lab at Washington University School of Medicine. The package is available via the web and standard browsers from the TINKER home page at **http://dasher.wustl.edu/tinker/**. Alternatively TINKER can be downloaded by logging into **dasher.wustl.edu** via anonymous ftp (Username: **anonymous**, Password: "**your email address**") and downloading the software from the /pub/tinker subdirectory. The complete TINKER distributions as well as individual files can be downloaded from this site.

The easiest way to get TINKER running on your machine is to use the self-extracting installation kit for either Linux, Windows, or Macintosh OS X 10.3. The installer will guide you through complete setup of TINKER and the Force Field Explorer (FFE) GUI, and perform all required configuration chores. The installer kits for the three supported systems are **tinker4.2-linux.sh**, **tinker4.2-windows.exe** and **tinker4.2-macosx.sit**. The Linux and Windows kits each contain a private copy of a Java and Java3D run-time environment for use with the package. The Macintosh version requires an OS X 10.3 (Panther) system for installation. The native Java implementation is used on Macs, and the Java3D package must be downloaded from Apple and installed prior to using TINKER with Force Field Explorer.

Prebuilt TINKER Executables

The TINKER package is also available as compressed Unix tar archives, Windows zip files, and as a complete set of uncompressed source and data files. Binaries are provided for machines running Windows 9X/ME/NT/2000/XP, Linux, and Apple Mac OS X. All of these executables are present in standard compressed formats as individual programs or as complete sets of executables. It is expected that other Unix users and PC users who need specially customized versions, will build binaries for their specific system. Sites with access to the Unix tar, compress and uncompress commands should simply obtain the archive file **tinker.tar.Z**. Alternatively, **tinker.tar.gz** and **tinker.zip** containing identical distributions compressed to GNU gzip and Windows ZIP format are also provided. If you choose to download individual files, you will need at a minimum the contents of the /doc, /source and /params subdirectories. Also required are the compile/build scripts from the subdirectory named for your machine type. Other areas contain test cases and examples, benchmark results, machine-translated C code, and the Force Field Explorer Java GUI for TINKER. The entire TINKER package, after building the executables, will require from about 40 to over 150 megabytes of disk space depending on the components installed and the use of shared libraries in the executables.

Building your Own Executables

The compilation and building of the TINKER executables should be easy for most of the common workstation and PC class computers. We provide in the /make area a Unix-style Makefile that with some modification can be used to build TINKER on most Unix machines. As a simpler alternative to Makefiles for the Unix versions, we also provide machine-specific directories with three separate shell scripts to compile the source, build an object library, and link binary executables. Three similar command files are provided for Windows, Macintosh and Open VMS systems. Compilation on Unix workstations should use the vendor supplied Fortran compiler, if available. The public domain GNU

g77 Fortran compiler available from **http://gcc.gnu.org/** is also capable of building TINKER on Linux and other Unix-based machines. The Linux executables we provide are built with the Intel Fortran for Linux 8.0 compiler. The Portland Group (PGI) and Absoft ProFortran compilers have also been tested under Linux, both of which generate executables roughly comparable in speed to the Intel compiler. On Linux, the g77 executables tend to exhibit degraded performance compared with executables from commercial compilers. Some benchmark results are provided in a later section of this User's Guide For the Macintosh we distribute executables built under Apple OS X 10.3 with the GNU g77 compiler. TINKER also builds on the Macintosh using the Absoft ProFortran compiler. For PCs running Windows 9X/NT/2000/XP, the distributed TINKER executables are built under the Intel Fortran for Windows 8.0 compiler. Alternative Windows compilers such as Compaq Visual Fortran, Lahey/Fujitsu and The Portland Group compilers, and GNU g77 under Cygwin have been tested and shown to build TINKER correctly. Please see the README files in each of the machine-specific areas for further information.

The first step in building TINKER using the script files is to run the appropriate **compile.make** script for your operating system and compiler version. Next you must use a **library.make** script to create an archive of object code modules. Finally, run a **link.make** script to produce the complete set of TINKER executables. The executables can be renamed and moved to wherever you like by editing and running the ``rename'' script. These steps will produce executables that can run from the command line, but without the capability to interact with the FFE GUI. Building FFE-enabled TINKER executables involves replacing the **sockets.f** source file with sockets.c, and included the object from the C code in the TINKER object library. Then executables must be linked against Java libraries in addition to the usual resources. Sample **compgui.make** and **linkgui.make** scripts are provided for systems capable of building GUI-enabled executables.

Regardless of your target machine, only a few small pieces of code can possibly require attention prior to building. The first two are the system dependent time and date routines found in **clock.f** and **calendar.f** respectively. Next is the **openend.f** routine that facilitates appending data to the end of an existing disk file. Please uncomment the sections of these routines needed for your computer type. Version of these system dependent routines suitable for each system are also provided in the directory for each machine/OS type. The final set of possible source alterations are to the master array dimensions found in the include file **sizes.i**. The most basic limit is on the number of atoms allowed, ``maxatm''. This parameter can be set to 10000 or more on most workstations. Personal computers with minimal memory may need a lower limit, perhaps 1000 atoms, depending on available memory, swap space and other resources. A description of the other parameter values is contained in the header of the file. Note that in order to keep the code completely transparent, TINKER does not implement any sort of dynamic memory allocation or heap data structure. This requires that **sizes.i** dimensioning values be set at least as large as the biggest problem you intend to run. Obviously, you should not set the array sizes to unnecessarily large values, since this can tax your compute resources and may result in performance degradation or overt failure of the executables.

Documentation and Other Information

The documentation for the TINKER programs, including the guide you are currently reading, is located in the /pub/tinker/doc subdirectory. The documentation was prepared using the Applixware Words and Graphics programs. Portable versions of the documentation are provided as ascii text in **.txt** files and in Adobe Acrobat **.pdf** file formats. Please read and return by mail the TINKER license. In particular, we note that TINKER is not ``Open Source'' as users are prohibited from redistribution of original or modified TINKER source code or binaries to other parties. While our intent is to distribute the TINKER code to anyone who wants it, the Ponder Lab would like to remain the sole distribution site and keep track of researchers using the package. The returned license forms

also help us justify further development of TINKER. When new modules and capabilities become available, and when the almost inevitable bugs are uncovered, we will attempt to notify those who have returned a license form. Finally, we remind you that this software is copyrighted, and ask that it not be redistributed in any form.

Where to Direct Questions

Specific questions about the building or use of the TINKER package should be directed to **tinker@dasher.wustl.edu**. TINKER related questions or comments of more general interest can be sent to the Computational Chemistry List (**http://www.ccl.net/**) run by Jan Labanowski at the University of Notre Dame. The TINKER developers monitor this list and will respond to the list or the individual poster as appropriate.

3. Types of Input & Output Files

This section describes the basic file types used by the TINKER package. Let's say you wish to perform a calculation on a particular small organic molecule. Assume that the file name chosen for our input and output files is **sample**. Then all of the TINKER files will reside on the computer under the name **sample.xxx** where **.xxx** is any of the several extension types to be described below.

SAMPLE.XYZ

The **.xyz** file is the basic TINKER Cartesian coordinates file type. It contains a title line followed by one line for each atom in the structure. Each line contains: the sequential number within the structure, an atomic symbol or name, X-, Y-, and Z-coordinates, the force field atom type number of the atom, and a list of the atoms connected to the current atom. Except for programs whose basic operation is in torsional space, all TINKER calculations are done from some version of the **.xyz** format.

SAMPLE.INT

The **.int** file contains an internal coordinates representation of the molecular structure. It consists of a title line followed by one line for each atom in the structure. Each line contains: the sequential number within the structure, an atomic symbol or name, the force field atom type number of the atom, and internal coordinates in the usual Z-matrix format. For each atom the internal coordinates consist of a distance to some previously defined atom, and either two bond angles or a bond angle and a dihedral angle to previous atoms. The length, angle and dihedral definitions do not have to represent real bonded interactions. Following the last atom definition are two optional blank line separated sets of atom number pairs. The first list contains pairs of atoms that are covalently bonded, but whose bond length was not used as part of the atom definitions. These pairs are typically used to close ring structures. The second list contains ``bonds'' that are to be broken, *i.e.*, pairs of atoms that are not covalently bonded, but which were used to define a distance in the atom definitions.

SAMPLE.KEY

The keyword parameter file always has the extension **.key** and is optionally present during TINKER calculations. It contains values for any of a wide variety of switches and parameters that are used to change the course of the computation from the default. The detailed contents of this file is explained in a latter section of this User's Guide. If a molecular system specific keyfile, in this case **sample.key**, is not present, the the TINKER program will look in the same directory for a generic file named **tinker.key**.

SAMPLE.DYN

The **.dyn** file contains values needed to restart a molecular or stochastic dynamics computation. It stores the current position, current velocity and current and previous accelerations for each atom, as well as the size and shape of any periodic box or crystal unit cell. This information can be used to start a new dynamics run from the final state of a previous run. Upon startup, the dynamics programs always check for the presence of a **.dyn** file and make use of it whenever possible. The **.dyn** file is updated concurrent with the saving of a new dynamics trajectory snapshot.

SAMPLE.END

The **.end** file type provides a mechanism to gracefully stop a running TINKER calculation. At appropriate checkpoints during a calculation, TINKER will test for the presence of a **sample.end** file, and if found will terminate the calculation after updating the output. The **.end** file can be created at any time during a computation, and will be detected when the next checkpoint is reached. The file may be of zero size, and its contents are unimportant. In the current version of TINKER, the **.end** mechanism is only available within dynamics-based programs.

SAMPLE.001, SAMPLE.002, ...

Several types of computations produce files containing a three or more digit extension (**.001** as shown; or **.002**, **.137**, **.5678**, *etc*.). These are referred to as cycle files, and are used to store various types of output structures. The cycle files from a given computation are identical in internal structure to either the **.xyz** or **.int** files described above. For example, the vibrational analysis program can save the tenth normal mode in **sample.010**. A molecular dynamics-based program might save its tenth 0.1 picosecond frame (or an energy minimizer its tenth partially minimized intermediate) in a file of the same name.

SAMPLE.LOG

The Force Field Explorer interface to TINKER saves results of all calculations launched from the GUI to a log file with the **.log** suffix. Any output that would normally be directed to the screen after starting a program from the command line is appended to this log file by Force Field Explorer.

SAMPLE.ARC

A TINKER archive file is simply a series of **.xyz** Cartesian coordinate files appended together one after another. This file can be used to condense the results from intermediate stages of an optimization, frames from a molecular dynamics trajectory, or set of normal mode vibrations into a single file for storage. TINKER archive files can be displayed as ``movies'' by the Force Field Explorer modeling program.

SAMPLE.PDB

This file type contains coordinate information in the PDB format developed by the Brookhaven Protein Data Bank for deposition of model structures based on macromolecular X-ray diffraction and NMR data. Although TINKER itself does not use **.pdb** files directly for input/output, auxiliary programs are provided with the system for interconverting **.pdb** files with the **.xyz** format described above.

SAMPLE.SEQ

This file type contains the primary sequence of a biopolymer in the standard one-letter code with 50 residues per line. The **.seq** file for a biopolymer is generated automatically when a PDB file is converted to TINKER **.xyz** format or when using the PROTEIN or NUCLEIC programs to build a structure from sequence It is required for the reverse conversion of a TINKER file back to PDB format..

SAMPLE.FRAC

The fractional coordinates corresponding to the asymmetric unit of a crystal unit cell are stored in the **.frac** file. The internal format of this file is identical to the **.xyz** file; except that the coordinates are fractional instead of in Angstrom units.

SAMPLE.XMOL

The ARCHIVE program has the option of converting a series of **.xyz** cycle files into an XMakemol XYZ file. These files can be displayed as a movie using the XMakemol display program. Note that the **.xmol** file format does not contain TINKER atom type information, so it is not possible to convert an **.xmol** file back into a TINKER **.xyz** file.

SAMPLE.CAR

The ARCHIVE program has the option of converting a series of **.xyz** cycle files into an Accelerys InsightII coordinate archive file. These files can be displayed as a movie using the InsightII display program. Note that the **.car** file format does not contain TINKER atom type information, so it is not possible to convert a **.car** file back into a TINKER **.XYZ** file.

PARAMETER FILES

The potential energy parameter files distributed with the TINKER package all end in the extension **.prm**, although this is not required by the programs themselves. Each of these files contains a definition of the potential energy functional forms for that force field as well as values for individual energy parameters. For example, the **mm3pro.prm** file contains the energy parameters and definitions needed for a protein-specific version of the MM3 force field.

4. Potential Energy Programs

This section of the manual contains a brief description of each of the TINKER potential energy programs. A detailed example showing how to run each program is included in a later section. The programs listed below are all part of the main, supported distribution. Additional source code for various unsupported programs can be found in the /other directory of the TINKER distribution.

ALCHEMY

A simple program to perform very basic free energy perturbation calculations. This program is provided mostly for demonstration purposes. For example, we use ALCHEMY in a molecular modeling course laboratory exercise to perform such classic mutations as chloride to bromide and ethane to methanol in water. The present version uses the perturbation formula and windowing with an explicit mapping of atoms involved in the mutation (``AMBER''-style), instead of thermodynamic integration and independent freely propagating groups of mutated atoms (``CHARMM''-style). Some of the code specific to this program is limited to the AMBER and OPLS potential functional forms, but could be easily generalized to handle other potentials. A more general and sophisticated version is currently under development.

ANALYZE

Provides information about a specific molecular structure. The program will ask for the name of a structure file, which must be in the TINKER **.xyz** file format, and the type of analysis desired. Options allow output of: (1) total potential energy of the system, (2) breakdown of the energy by potential function type or over individual atoms, (3) computation of the total dipole moment and its components, moments of inertia and radius of gyration, (4) listing of the parameters used to compute selected interaction energies, (5) energies associated with specified individual interactions.

ANNEAL

Performs a molecular dynamics simulated annealing computation. The program starts from a specified input molecular structure in TINKER **.xyz** format. The trajectory is updated using either a modified Beeman or a velocity Verlet integration method. The annealing protocol is implemented by allowing smooth changes between starting and final values of the system temperature via the Groningen method of coupling to an external bath. The scaling can be linear or sigmoidal in nature. In addition, parameters such as cutoff distance can be transformed along with the temperature. The user must input the desired number of dynamics steps for both the equilibration and cooling phases, a time interval for the dynamics steps, and an interval between coordinate/trajectory saves. All saved coordinate sets along the trajectory are placed in sequentially numbered cycle files.

DYNAMIC

Performs a molecular dynamics (MD) or stochastic dynamics (SD) computation. Starts either from a specified input molecular structure (an **.xyz** file) or from a structure-velocity-acceleration set saved from a previous dynamics trajectory (a restart from a **.dyn** file). MD trajectories are propagated using either a modified Beeman or a velocity Verlet integration method. SD is implemented via our own derivation of a velocity Verlet-based algorithm. In addition the program can perform full crystal calculations, and can operate in constant energy mode or with maintenance of a desired temperature and/or pressure using the Groningen method of coupling to external baths. The user must input the desired number of dynamics steps, a time interval for the dynamics steps, and an interval between coordinate/trajectory saves. Coordinate sets along the trajectory can be saved as sequentially

numbered cycle files or directly to a TINKER archive **.arc** file. At the same time that a point along the trajectory is saved, the complete information needed to restart the trajectory from that point is updated and stored in the **.dyn** file.

GDA

A program to implement Straub's Gaussian Density Annealing algorithm over an effective series of analytically smoothed potential energy surfaces. This method can be viewed as an extended stochastic version of the diffusion equation method of Scheraga, *et al*., and also has many similar features to the TINKER Potential Smoothing and Search (PSS) series of programs. The current version of GDA is similar to but does not exactly reproduce Straub's published method and is limited to argon clusters and other simple systems involving only van der Waals interactions; further modification and development of this code is currently underway in the Ponder research group. As with other programs involving potential smoothing, GDA currently requires use of the **smooth.prm** force field parameters.

MINIMIZE

The MINIMIZE program performs a limited memory L-BFGS minimization of an input structure over Cartesian coordinates using a modified version of the algorithm of Jorge Nocedal. The method requires only the potential energy and gradient at each step along the minimization pathway. It requires storage space proportional to the number of atoms in the structure. The MINIMIZE procedure is recommended for preliminary minimization of trial structures to an *rms* gradient of 1.0 to 0.1 kcal/mole/≈. It has a relatively fast cycle time and is tolerant of poor initial structures, but converges in a slow, linear fashion near the minimum. The user supplies the name of the TINKER **.xyz** coordinates file and a target *rms* gradient value at which the minimization will terminate. Output consists of minimization statistics written to the screen or redirected to an output file, and the new coordinates written to updated **.xyz** files or to cycle files.

MINIROT

The MINIROT program uses the same limited memory L-BFGS method as MINIMIZE, but performs the computation in terms of dihedral angles instead of Cartesian coordinates. Output is saved in an updated **.int** file or in cycle files.

MINRIGID

The MINRIGID program is similar to MINIMIZE except that it operates on rigid bodies starting from a TINKER **.xyz** coordinate file and the rigid body group definitions found in the corresponding **.key** file. Output is saved in an updated **.xyz** file or in cycle files.

MONTE

The MONTE program implements the Monte Carlo Minimization algorithm developed by Harold Scheraga's group and others. The procedure takes Monte Carlo steps for either a single atom or a single torsional angle, then performs a minimization before application of the Metropolis sampling method. This results in effective sampling of a modified potential surface where the only possible energy levels are those of local minima on the original surface. The program can be easily modified to elaborate on the available move set.

NEWTON

A truncated Newton minimization method which requires potential energy, gradient and Hessian information. This procedure has significant advantages over standard Newton methods, and is able to minimize very large structures completely. Several options are provided with respect to minimization method and preconditioning of the Newton equations. The default options are recommended unless the user is familiar with the math involved. This program operates in Cartesian coordinate space and is fairly tolerant of poor input structures. Typical algorithm iteration times are longer than with nonlinear conjugate gradient or variable metric methods, but many fewer iterations are required for complete minimization. NEWTON is usually the best choice for minimizations to the 0.01 to 0.000001 kcal/mole/≈ level of *rms* gradient convergence. Tests for directions of negative curvature can be removed, allowing NEWTON to be used for optimization to conformational transition state structures (this only works if the starting point is very close to the transition state). Input consists of a TINKER **.xyz** coordinates file; output is an updated set of minimized coordinates and minimization statistics.

NEWTROT

The NEWTROT program is similar to NEWTON except that it requires a **.int** file as input and then operates in terms of dihedral angles as the minimization variables. Since the dihedral space Hessian matrix of an arbitrary structure is often indefinite, this method will often not perform as well as the other, simpler dihedral angle based minimizers.

OPTIMIZE

The OPTIMIZE program performs a optimally conditioned variable metric minimization of an input structure over Cartesian coordinates using an algorithm due to William Davidon. The method does not perform line searches, but requires computation of energies and gradients as well as storage for an estimate of the inverse Hessian matrix. The program operates on Cartesian coordinates from a TINKER **.xyz** file. OPTIMIZE will typically converge somewhat faster and more completely than MINIMIZE. However, the need to store and manipulate a full inverse Hessian estimate limits its use to structures containing less than a few hundred atoms on workstation class machines. As with the other minimizers, OPTIMIZE needs input coordinates and an *rms* gradient cutoff criterion. The output coordinates are saved in updated **.xyz** files or as cycle files.

OPTIROT

The OPTIROT program is similar to OPTIMIZE except that it operates on dihedral angles starting from a TINKER **.int** internal coordinate file. This program is usually the preferred method for most dihedral angle optimization problems since Truncated Newton methods appear, in our hands, to lose some of their efficacy in moving from Cartesian to torsional coordinates.

OPTRIGID

The OPTRIGID program is similar to OPTIMIZE except that it operates on rigid bodies starting from a TINKER **.xyz** coordinate file and the rigid body atom group definitions found in the corresponding **.key** file. Output is saved in an updated **.xyz** file or in cycle files.

PATH

A program that implements a variant of Elber's Lagrangian multiplier-based reaction path following algorithm. The program takes as input a pair of structural minima as TINKER **.xyz** files, and then generates a user specified number of points along a path through conformational space connecting the input structures. The intermediate structures are output as TINKER cycle files, and the higher

energy intermediates can be used as input to a Newton-based optimization to locate conformational transition states.

PSS

Implements our version of a potential smoothing and search algorithm for the global optimization of molecular conformation. An initial structure in **.xyz** format is first minimized in Cartesian coordinates on a series of increasingly smoothed potential energy surfaces. Then the smoothing procedure is reversed with minimization on each successive surface starting from the coordinates of the minimum on the previous surface. A local search procedure is used during the backtracking to explore for alternative minima better than the one found during the current minimization. The final result is usually a very low energy conformation or, in favorable cases, the global energy minimum conformation. The minimum energy coordinate sets found on each surface during both the forward smoothing and backtracking procedures are placed in sequentially numbered cycle files.

PSSRIGID

This program implements the potential smoothing and search method as described above for the PSS program, but performs the computation in terms of keyfile-defined rigid body atom groups instead of Cartesian coordinates. Output is saved in numbered cycle files with the **.xyz** file format.

PSSROT

This program implements the potential smoothing and search method as described above for the PSS program, but performs the computation in terms of a set of user-specified dihedral angles instead of Cartesian coordinates. Output is saved in numbered cycle files with the **.int** file format.

SADDLE

A program for the location of a conformational transition state between two potential energy minima. SADDLE uses a conglomeration of ideas from the Bell-Crighton quadratic path and the Halgren-Lipscomb synchronous transit methods. The basic idea is to perform a nonlinear conjugate gradient optimization in a subspace orthogonal to a suitably defined reaction coordinate. The program requires as input the coordinates (TINKER **.xyz** files) of the two minima and an *rms* gradient convergence criterion for the optimization. The current estimate of the transition state structure is written to the file TSTATE.XYZ. Crude transition state structures generated by SADDLE can sometimes be refined using the NEWTON program. Optionally, a scan of the interconversion pathway can be made at each major iteration.

SCAN

A program for general conformational search of an entire potential energy surface via a basin hopping method. The program takes as input a TINKER **.xyz** coordinates file which is then minimized to find the first local minimum for a search list. A series of activations along various normal modes from this initial minimum are used as seed points for additional minimizations. Whenever a previously unknown local minimum is located it is added to the search list. When all minima on the search list have been subjected to the normal mode activation without locating additional new minima, the program terminates. The individual local minima are written to cycle files as they are discovered. While the SCAN program can be used on standard undeformed potential energy surfaces, we have found it to be most useful for quickly ``scanning'' a smoothed energy surface to enumerate the major basins of attraction spaning the entire surface.

SNIFFER

A program that implements the Sniffer global optimization algorithm of Butler and Slaminka, a discrete version of Griewank's global search trajectory method. The program takes an input TINKER **.xyz** coordinates file and shakes it vigorously via a modified dynamics trajectory before, hopefully, settling into a low lying minimum. Some trial and error is often required as the current implementation is sensitive to various parameters and tolerances that govern the computation. At present, these parameters are not user accessible, and must be altered in the source code. However, this method can do a good job of quickly optimizing conformation within a limited range of convergence.

TESTGRAD

The TESTGRAD program computes and compares the analytical and numerical first derivatives (*i.e.*, the gradient vector) of the potential energy for a Cartesian coordinate input structure. The output can be used to test or debug the current potential or any added user defined energy terms.

TESTHESS

The TESTHESS program computes and compares the analytical and numerical second derivatives (*i.e.*, the Hessian matrix) of the potential energy for a Cartesian coordinate input structure. The output can be used to test or debug the current potential or any added user defined energy terms.

TESTLIGHT

A program to compare the efficiency of different nonbonded neighbor methods for the current molecular system. The program times the computation of energy and gradient for the van der Waals and charge-charge electrostatic potential terms using a simple double loop over all interactions and using the Method of Lights algorithm to select neighbors. The results can be used to decide whether the Method of Lights has any CPU time advantage for the current structure. Both methods should give exactly the same answer in all cases, since the identical individual interactions are computed by both methods. The default double loop method is faster when cutoffs are not used, or when the cutoff sphere contains about half or more of the total system of unit cell. In cases where the cutoff sphere is much smaller than the system size, the Method of Lights can be much faster since it avoids unnecessary calculation of distances beyond the cutoff range.

TESTROT

The TESTROT program computes and compares the analytical and numerical first derivatives (*i.e.*, the gradient vector) of the potential energy with respect to dihedral angles. Input is a TINKER **.int** internal coordinate file. The output can be used to test or debug the current potential functions or any added user defined energy terms.

TIMER

A simple program to provide timing statistics for energy function calls within the TINKER package. TIMER requires an input **.xyz** file and outputs the CPU time (wall clock time on some machine types) needed to perform a specified number of energy, gradient and Hessian evaluations.

TIMEROT

This program is similar to TIMER, only it operates over dihedral angles via input of a TINKER **.int** internal coordinate file. In the current version, the torsional Hessian is computed numerically from the analytical torsional gradient.

VIBRATE

A program to perform vibrational analysis by computing and diagonalizing the full Hessian matrix (*i.e.*, the second partial derivatives) for an input structure (a TINKER **.xyz** file). Eigenvalues and eigenvectors of the mass weighted Hessian (*i.e.*, the vibrational frequencies and normal modes) are also calculated. Structures corresponding to individual normal mode motions can be saved in cycle files.

VIBROT

The program VIBROT forms the torsional Hessian matrix via numerical differentiation of the analytical torsional gradient. The Hessian is then diagonalized and the eigenvalues are output. The present version does not compute the kinetic energy matrix elements needed to convert the Hessian into the torsional normal modes; this will be added in a later version. The required input is a TINKER **.int** internal coordinate file.

XTALFIT

The XTALFIT program is of use in the automated fitting of potential parameters to crystal structure and thermodynamic data. XTALFIT takes as input several crystal structures (TINKER **.xyz** files with unit cell parameters in corresponding keyfiles) as well as information on lattice energies and dipole moments of monomers. The current version uses a nonlinear least squares optimization to fit van der Waals and electrostatic parameters to the input data. Bounds can be placed on the values of the optimization parameters.

XTALMIN

A program to perform full crystal minimizations. The program takes as input the structure coordinates and unit cell lattice parameters. It then alternates cycles of Newton-style optimization of the structure and conjugate gradient optimization of the crystal lattice parameters. This alternating minimization is slower than more direct optimization of all parameters at once, but is somewhat more robust in our hands. The symmetry of the original crystal is not enforced, so interconversion of crystal forms may be observed in some cases.

5. Additional Utility Programs & Scripts

This section of the manual contains a brief description of each of the TINKER structure manipulation, geometric calculation and auxiliary programs. A detailed example showing how to run each program is included in a later section. The programs listed below are all part of the main, supported distribution. Additional source code for various unsupported programs can be found in the /other directory of the TINKER distribution.

ARCHIVE

A program for concatenating TINKER cycle files into a single archive file; useful for storing the intermediate results of minimizations, dynamics trajectories, and so on. The archive file can be written in TINKER format, or in formats usable with MSI's InsightII (their CAR file with **.msi** extension) or with XMakemol (their file format with **`.xmol`** extension). Only active atoms are written into the InsightII and XMakemol output files, allowing display of partial structures. The program can also extract individual cycle files from a TINKER archive.

CORRELATE

A program to compute time correlation functions from collections of TINKER cycle files. Its use requires a user supplied function **property** that computes the value of the property for which a time correlation is desired for two input structures. A sample routine is supplied that computes either a velocity autocorrelation function or an *rms* structural superposition as a function of time. The main body of the program organizes the overall computation in an efficient manner and outputs the final time correlation function.

CRYSTAL

A program for the manipulation of crystal structures including interconversion of fractional and Cartesian coordinates, generation of the unit cell from an asymmetric unit, and building of a crystalline block of specified size via replication of a single unit cell. The present version can handle about 25 of the most common space groups, others can easily be added as needed by modification of the routine **symmetry**.

DIFFUSE

A program to compute the self-diffusion constant for a homogeneous liquid via the Einstein equation. A previously saved dynamics trajectory is read in and ``unfolded'' to reverse translation of molecules due to use of periodic boundary conditions. The average motion over all molecules is then used to compute the self-diffusion constant. While the current program assumes a homogeneous system, it should be easy to modify the code to handle diffusion of individual molecules or other desired effects.

DISTGEOM

A program to perform distance geometry calculations using variations on the classic metric matrix method. A user specified number of structures consistent with keyfile input distance and dihedral restraints is generated. Bond length and angle restraints are derived from the input structure. Trial distances between the triangle smoothed lower and upper bounds can be chosen via any of several metrization methods, including a very effective partial random pairwise scheme. The correct radius of gyration of the structure is automatically maintained by choosing trial distances from Gaussian distributions of appropriate mean and width. The initial embedded structures can be further refined

against a geometric restraint-only potential using either a sequential minimization protocol or simulated annealing.

DOCUMENT

The DOCUMENT program is provided as a minimal listing and documentation tool. It operates on the TINKER source code, either individual files or the complete source listing produced by the command script **`listing.make`**, to generate lists of routines, common blocks or valid keywords. In addition, the program has the ability to output a formatted parameter listing from the standard TINKER parameter files.

INTEDIT

A program to allow interactive inspection and alteration of the internal coordinate definitions and values of a TINKER structure. If the structure is altered, the user has the option to write out a new internal coordinates file upon exit.

INTXYZ

A program to convert a TINKER **`.int`** internal coordinates formatted file into a TINKER **`.xyz`** Cartesian coordinates formatted file.

NUCLEIC

A program for automated building of nucleic acid structures. Upon interactive input of a nucleotide sequence with optional phosphate backbone angles, the program builds internal and Cartesian coordinates. Standard bond lengths and angles are used. Both DNA and RNA sequences are supported as are A-, B- and Z-form structures. Double helixes of complementary sequence can be automatically constructed via a rigid docking of individual strands.

PDBXYZ

A program for converting a Brookhaven Protein Data Bank file (a PDB file) into a TINKER **`.xyz`** Cartesian coordinate file. If the PDB file contains only protein/peptide amino acid residues, then standard protein connectivity is assumed, and transferred to the **.xyz** file. For non-protein portions of the PDB file, atom connectivity is determined by the program based on interatomic distances. The program also has the ability to add or remove hydrogen atoms from a protein as required by the force field specified during the computation.

POLARIZE

A program for computing molecular polarizability from an atom-based distributed model of polarizability. A damped interaction model due to Thole is optionally via keyfile settings. A TINKER **`.xyz`** file is required as input. The output consists of the overall polarizability tensor in the global coordinates and its eigenvalues.

PRMEDIT

A program for formatting and renumbering TINKER force field parameter files. When atom types or classes are added to a parameter file, this utility program has the ability to renumber all the atom records sequentially, and alter type and class numbers in all other parameter entries to maintain consistency.

PROTEIN

A program for automated building of peptide and protein structures. Upon interactive input of an amino acid sequence with optional phi/psi/omega/chi angles, D/L chirality, etc., the program builds internal and Cartesian coordinates. Standard bond lengths and angles are assumed for the peptide. The program will optionally convert the structure to a cyclic peptide, or add either or both N- and C-terminal capping groups. Atom type numbers are automatically assigned for the specified force field. The final coordinates and a sequence file are produced as the output.

RADIAL

A program to compute the pair radial distribution function between two atom types. The user supplies the two atom names for which the distribution function is to be computed, and the width of the distance bins for data analysis. A previously saved dynamics trajectory is read as input. The raw radial distribution and a spline smoothed version are then output from zero to a distance equal to half the minimum periodic box dimension. The atom names are matched to the atom name column of the TINKER **.xyz** file, independent of atom type.

SPACEFILL

A program to compute the volume and surface areas of molecules. Using a modified version of Connolly's original analytical description of the molecular surface, the program determines either the van der Waals, accessible or molecular (contact/reentrant) volume and surface area. Both surface area and volume are broken down into their geometric components, and surface area is decomposed into the convex contribution for each individual atom. The probe radius is input as a user option, and atomic radii can be set via the keyword file. If TINKER archive files are used as input, the program will compute the volume and surface area of each structure in the input file.

SPECTRUM

A program to compute a power spectrum from velocity autocorrelation data. As input, this program requires a velocity autocorrelation function as produced by the CORRELATE program. This data, along with a user input time step, are Fourier transformed to generate the spectral intensities over a wavelength range. The result is a power spectrum, and the positions of the bands are those predicted for an infrared or Raman spectrum. However, the data is not weighted by molecular dipole moment derivatives as would be required to produce correct IR intensities.

SUPERPOSE

A program to superimpose two molecular structures in 3-dimensions. A variety of options for input of the atom sets to be used during the superposition are presented interactively to the user. The superposition can be mass-weighted if desired, and the coordinates of the second structure superimposed on the first structure are optionally output. If TINKER archive files are used as input, the program will compute all pairwise superpositions between structures in the input files.

SYBYLXYZ

A program for converting a TRIPOS Sybyl MOL2 file into a TINKER **`.xyz`** Cartesian coordinate file. The current version of the program does not attempt to convert the Sybyl atoms types into the active TINKER force field types, *i.e.*, all atoms types are simply set to zero.

XYZEDIT

A program that performs and of a variety of manipulations on an input TINKER .xyz Cartesian coordinates formatted file. The present version of the program has the following interactively selectable options: (1) Offset the Numbers of the Current Atoms, (2) Deletion of Individual Specified Atoms, (3) Deletion of Specified Types of Atoms, (4) Deletion of Atoms outside Cutoff Range, (5) Insertion of Individual Specified Atoms, (6) Replace Old Atom Type with a New Type, (7) Assign Connectivities based on Distance, (8) Convert Units from Bohrs to Angstroms, (9) Invert thru Origin to give Mirror Image, (10) Translate Center of Mass to the Origin, (11) Translate a Specified Atom to the Origin, (12) Translate and Rotate to Inertial Frame, (13) Move to Specified Rigid Body Coordinates, (14) Create and Fill a Periodic Boundary Box, (15) Soak Current Molecule in Box of Solvent, (16) Append another XYZ file to Current One. In most cases, multiply options can be applied sequentially to an input file. At the end of the editing process, a new version of the original **.xyz** file is written as output.

XYZINT

A program for converting a TINKER **.xyz** Cartesian coordinate formatted file into a TINKER **.int** internal coordinates formatted file. This program can optionally use an existing internal coordinates file as a template for the connectivity information.

XYZPDB

A program for converting a TINKER **.xyz** Cartesian coordinate file into a Brookhaven Protein Data Bank file (a PDB file).

XYZSYBYL

A program to convert a TINKER **.xyz** Cartesian coordinates file into a TRIPOS Sybyl MOL2 file. The conversion generates only the MOLECULE, ATOM, BOND and SUBSTRUCTURE record type in the MOL2 file. Generic Sybyl atom types are used in most cases; while these atom types may need to be altered in some cases, Sybyl is usually able to correctly display the resulting MOL2 file.

6. Special Features & Methods

This section contains several short notes with further information about TINKER methodology, algorithms and special features. The discussion is not intended to be exhaustive, but rather to explain features and capabilities so that users can make more complete use of the package.

File Version Numbers

All of the input and output file types routinely used by the TINKER package are capable of existing as multiple versions of a base file name. For example, if the program XYZINT is run on the input file **molecule.xyz**, the output internal coordinates file will be written to **molecule.int**. If a file named **molecule.int** is already present prior to running XYZINT, then the output will be written instead to the next available version, in this case to **molecule.int_2**. In fact the output is generally written to the lowest available, previously unused version number (**molecule.int_3**, **molecule.int_4**, *etc.*, as high as needed). Input file names are handled similarly. If simply **molecule** or **molecule.xyz** is entered as the input file name upon running XYZINT, then the highest version of **molecule.xyz** will be used as the actual input file. If an explicit version number is entered as part of the input file name, then the specified version will be used as the input file.

The version number scheme will be recognized by many older users as a holdover from the VMS origins of the first version of the TINKER software. It has been maintained to make it easier to chain together multiple calculations that may create several new versions of a given file, and to make it more difficult to accidently overwrite a needed result. The version scheme applies to most uses of many common TINKER file types such as **.xyz**, **.int**, **.key**, **.arc**. It is not used when an overwritten file ``update'' is obviously the correct action, for example, the **.dyn** molecular dynamics restart files. For those users who prefer a more Unix-like operation, and do not desire use of file versions, this feature can be turned off by adding the NOVERSION keyword to the applicable TINKER keyfile.

The version scheme as implemented in TINKER does have two known quirks. First, it becomes impossible to directly use the original unversioned copy of a file if higher version numbers are present. For example, if the files **molecule.xyz** and **molecule.xyz_2** both exist, then **molecule.xyz** cannot be accessed as input by XYZINT. If **molecule.xyz** is entered in response to the input file name question, **molecule.xyz_2** (or the highest present version number) will be used as input. The only workaround is to copy or rename **molecule.xyz** to something else, say **molecule.new**, and use that name for the input file. Secondly, missing version numbers always end the search for the highest available version number; *i.e.*, version numbers are assumed to be consecutive and without gaps. For example, if **molecule.xyz**, **molecule.xyz_2** and **molecule.xyz_4** are present, but not **molecule.xyz_3**, then **molecule.xyz_2** will be used as input to XYZINT if **molecule** is given as the input file name. Similarly, output files will fill in gaps in an already existing set of file versions.

Command Line Options

Many operating systems or compiler supplied-libraries make available something like the standard Unix iargc and getarg routines for capturing command line arguments. On these machines most of the TINKER programs support a selection of command line arguments and options. The name of the keyfile to be used for a calculation is read from the argument following a **-k** (equivalent to either **-key** or **-keyfile**, case insensitive) command line argument. Note that the **-k** options can appear anywhere on the command line following the executable name. All other command line arguments, excepting the name of the executable program itself, are treated as input arguments. These input

arguments are read from left to right and interpreted in order as the answers to questions that would be asked by an interactive invocation of the same TINKER program. For example, the following command line:

```
newton molecule -k test a a 0.01
```

will invoke the NEWTON program on the structure file **molecule.xyz** using the keyfile **test.key**, automatic mode **[a]** for both the method and preconditioning, and **0.01** for the RMS gradient per atom termination criterion in kcal/mole/≈. Provided that the force field parameter set, *etc*. is provided in **test.key**, the above compuation will procede directly from the command line invocation without further interactive input.

Use on Microsoft Windows Systems

TINKER executables for Microsoft PC systems should be run from the DOS or Command Prompt window available under the various versions of Windows. The TINKER executable directory should be added to your path via the autoexec.bat file or similar. If using Win2000 or XP, set the number of scrollable lines in the Command Prompt window to a very large number, so that you will be able to inspect screen output after it flies by. With Win95/98, these Command Prompt windows are only able to scroll a small number of lines (*amazing!*), so TINKER programs which generate large amounts of screen output should be run such that output will be redirected to a file. This can be accomplished by running the TINKER program in batch mode or by using the Unix-like output redirection build into DOS. For example, the command:

```
dynamic < molecule.inp > molecule.log
```

will run the TINKER dynamic program taking input from the file **molecule.inp** and sending output to **molecule.log**. Also note that command line options as described above are available with the distributed TINKER executables.

Another alternative, particularly attractive to those already familiar with Linux or Unix systems, is to download the Cygwin package currently available under GPL license from the site **http://source.redhat.com/cygwin/**. The cygwin tools provide many of the GNU tools, including a bash shell window from which TINKER programs can be run.

If the distributed TINKER executables are run directly from Windows by double clicking on the program icon, then the program will run in its own window. However, upon completion of the program the window will close and screen output will be lost. Any output files written by the program will, of course, still be available. The Windows behavior can be changed by adding the EXIT-PAUSE keyword to the keyfile. This keyword causes the executation window to remain open after completion until the ``Enter'' key is pressed.

Use on Apple Macintosh Systems

The TINKER executables are best run under Mac OS X in a ``terminal'' application window where behavior is identical to that in a Linux terminal. At present the Force Field Explorer GUI for TINKER will not run on OS X since the required Java3D extensions are unavailable.

We have discontinued active support for Mac OS 9. However, the OS 9 versions of TINKER are run by double clicking on a program icon. The program will run in its own window to which all ``screen'' output will be directed. Upon program termination the window will remain active pending a final return entered by the user which will close the window. Prior to the final return, the contents of the screen window can be saved to a file via the clipboard for permanent storage. Note that Macintosh

OS9 uses a colon instead of a forward- or back-slash as the directory separator, so keyfiles transfered from other machines will need to be altered accordingly.

Atom Types *vs*. Atom Classes

Manipulation of atom types and the proliferation of parameters as atoms are further subdivided into new types is the bane of force field calculation. For example, if each topologically distinct atom arising from the 20 natural amino acids is given a different atom type, then about 300 separate type are required (this ignores the different N- and C-terminal forms of the residues, diastereotopic hydrogens, *etc*.). However, all these types lead to literally thousands of different force field parameters. In fact, there are many thousands of distinct torsional parameters alone. It is impossible at present to fully optimize each of these parameters; and even if we could, a great many of the parameters would be nearly identical. Two somewhat complimentary solutions are available to handle the proliferation of parameters. The first is to specify the molecular fragments to which a given parameter can be applied in terms of a chemical structure language, SMILES strings for example. Some commercial systems, such as the TRIPOS Sybyl software, make use of such a scheme to parse structures and assign force field parameters.

A second general approach is to use hierarchical cascades of parameter groups. TINKER uses a simple version of this scheme. Each TINKER force field atom has both an atom *type* number and an atom *class* number. The types are subsets of the atom classes, *i.e.*, several different atom types can belong to the same atom class. Force field parameters that are somewhat less sensitive to local environment, such as local geometry terms, are then provided and assigned based on atom class. Other energy parameters, such as electrostatic parameters, that are very environment dependent are assigned over the atom types. This greatly reduces the number of independent multiple-atom parameters like the four-atom torsional parameters.

Calculations on Partial Structures

Two methods are available for performing energetic calculations on portions or substructures within a full molecular system. TINKER allows division of the entire system into *active* and *inactive* parts which can be defined via keywords. In subsequent calculations, such as minimization or dynamics, only the active portions of the system are allowed to move. The force field engine responds to the active/inactive division by computing all energetic interactions involving at least one active atom; *i.e.*, any interaction whose energy can change with the motion of one or more active atoms is computed.

The second method for partial structure computation involves dividing the original system into a set of atom *groups*. As before, the groups can be specified via appropriate keywords. The current TINKER implementation allows specification of up to a maximum number of groups as given in the **`sizes.i`** dimensioning file. The groups must be disjoint in that no atom can belong to more than one group. Further keywords allow the user to specify which intra- and intergroup sets of energetic interactions will contribute to the total force field energy. Weights for each set of interactions in the total energy can also be input. A specific energetic interaction is assigned to a particular intra- or intergroup set if all the atoms involved in the interaction belong to the group (intra-) or pair of groups (inter-). Interactions involving atoms from more than two groups are not computed.

Note that the groups method and active/inactive method use different assignment procedures for individual interactions. The active/inactive scheme is intended for situations where only a portion of a system is allowed to move, but the total energy needs to reflect the presence of the remaining inactive portion of the structure. The groups method is intended for use in rigid body calculations, and is needed for certain kinds of free energy perturbation calculations.

Metal Complexes and Hypervalent Species

The distribution version of TINKER comes dimensioned for a maximum atomic coordination number of four as needed for standard organic compounds. In order to use TINKER for calculations on species containing higher coordination numbers, simply change the value of the parameter **maxval** in the master dimensioning file **sizes.i** and rebuilt the package. Note that this parameter value should not be set larger than necessary since large values can slow the execution of portions of some TINKER programs.

Many molecular mechanics approaches to inorganic and metal structures use an angle bending term which is softer than the usual harmonic bending potential. TINKER implements a Fourier bending term similar to that used by the Landis group's SHAPES force field. The parameters for specific Fourier angle terms are supplied via the ANGLEF parameter and keyword format. Note that a Fourier term will only be used for a particular angle if a corresponding harmonic angle term is not present in the parameter file.

We are now collaborating with Anders Carlsson's group in St. Louis to add his transition metal ligand field term to TINKER. Support for this additional potential functional form is already in the TINKER source code, and we plan to release the energy routines after further testing and parameterization.

Neighbor Methods for Nonbonded Terms

In addition to standard double loop methods, the Method of Lights is available to speed neighbor searching. This method based on taking intersections of sorted atom lists can be much faster for problems where the cutoff distance is significantly smaller than half the maximal cell dimension. The current version of TINKER does not implement the ``neighbor list'' schemes common to many other simulation packages.

Periodic Boundary Conditions

Both spherical cutoff images or replicates of a cell are supported by all TINKER programs that implement periodic boundary conditions. Whenever the cutoff distance is too large for the minimum image to be the only relevant neighbor (*i.e.*, half the minimum box dimension for orthogonal cells), TINKER will automatically switch from the image formalism to use of replicated cells.

Distance Cutoffs for Energy Functions

Polynomial energy switching over a window is used for terms whose energy is small near the cutoff distance. For monopole electrostatic interactions, which are quite large in typical cutoff ranges, a two polynomial multiplicative-additive shifted energy switch unique to TINKER is applied. The TINKER method is similar in spirit to the force switching methods of Steinbach and Brooks, *J. Comput. Chem.*, ***15***, 667-683 (1994). While the particle mesh Ewald method is preferred when periodic boundary conditions are present, TINKER's shifted energy switch with reasonable switching windows is quite satisfactory for most routine modeling problems. The shifted energy switch minimizes the perturbation of the energy and the gradient at the cutoff to acceptable levels. Problems should arise only if the property you wish to monitor is known to require explicit inclusion of long range components (*i.e.*, calculation of the dielectric constant, *etc.*).

Ewald Summations Methods

TINKER contains a versions of the Ewald summation technique for inclusion of long range electrostatic interactions via periodic boundaries. The particle mesh Ewald (PME) method is available for simple charge-charge potentials, while regular Ewald is provided for polarizable atomic multipole interactions. The accuracy and speed of the regular and PME calculations is dependent on

several interrelated parameters. For both methods, the Ewald coefficient and real-space cutoff distance must be set to reasonable and complementary values. Additional control variables for regular Ewald are the fractional coverage and number of vectors used in reciprocal space. For PME the additional control values are the B-spline order and charge grid dimensions. Complete control over all of these parameters is available via the TINKER keyfile mechanism. By default TINKER will select a set of parameters which provide a reasonable compromise between accuracy and speed, but these should be checked and modified as necessary for each individual system.

Continuum Solvation Models

Several alternative continuum solvation algorithms are contained within TINKER. All of these are accessed via the SOLVATE keyword and its modifiers. Two simple surface area methods are implemented: the ASP method of Eisenberg and McLachlan, and the SASA method from Scheraga's group. These methods are applicable to any of the standard TINKER force fields. Various schemes based on the generalized Born formalism are also available: the original 1990 numerical ``Onion-shell'' GB/SA method from Still's group, the 1997 analytical GB/SA method also due to Still, a pairwise descreening algorithm originally proposed by Hawkins, Cramer and Truhlar, and the analytical continuum solvation (ACE) method of Schaefer and Karplus. At present, the generalized Born methods should only be used with force fields having simple partial charge electrostatic interactions.

Some further comments are in order regarding the GB/SA-style solvation models. The ``Onion-shell'' model is provided mostly for comparison purposes. It uses an exact, analytical surface area calculation for the cavity term and the numerical scheme described in the original paper for the polarization term. This method is very slow, especially for large systems, and does not contain the contribution of the Born radii chain rule term to the first derivatives. We recommend its use only for single-point energy calculations. The other GB/SA methods (``analytical'' Still, H-C-T pairwise descreening, and ACE) use an approximate cavity term based on Born radii, and do contain fully correct derivatives including the Born radii chain rule contribution. These methods all scale in CPU time with the square of the size of the system, and can be used with minimization, molecular dynamics and large molecules.

Finally, we note that the ACE solvation model should not be used with the current version of TINKER. The algorithm is fully implemented in the source code, but parameterization is not complete. As of late 2000, parameter values are only available in the literature for use of ACE with the older CHARMM19 force field. We plan to develop values for use with more modern all-atom force fields, and these will be incorporated into TINKER sometime in the future.

Polarizable Multipole Electrostatics

Atomic multipole electrostatics through the quadrupole moment is supported by the current version of TINKER, as is either mutual or direct dipole polarization. Ewald summation is available for inclusion of long range interactions. Calculations are implemented via a mixture of the CCP5 algorithms of W. Smith and the Applequist-Dykstra Cartesian polytensor method. At present analytical energy and Cartesian gradient code is provided.

The TINKER package allows intramolecular polarization to be treated via a version of the interaction damping scheme of Thole. To implement the Thole scheme, it is necessary to set all the **mutual-1x-scale** keywords to a value of one. The other polarization scaling keyword series, **direct-1x-scale** and **polar-1x-scale**, can be set independently to enable a wide variety of polarization models. In order to use an Applequist-style model without polarization damping, simply set the **polar-damp** keyword to zero.

Potential Energy Smoothing

Versions of our Potential Smoothing and Search (PSS) methodology have been implemented within TINKER. This methods belong to the same general family as Scheraga's Diffusion Equation Method, Straub's Gaussian Density Annealing, Shalloway's Packet Annealing and Verschelde's Effective Diffused Potential, but our algorithms reflect our own ongoing research in this area. In many ways the TINKER potential smoothing methods are the deterministic analog of stochastic simulated annealing. The PSS algorithms are very powerful, but are relatively new and are still undergoing modification, testing and calibration within our research group. This version of TINKER also includes a basin-hopping conformational scanning algorithm in the program SCAN which is particularly effective on smoothed potential surfaces.

Distance Geometry Metrization

A much improved and very fast random pairwise metrization scheme is available which allows good sampling during trial distance matrix generation without the usual structural anomalies and CPU constraints of other metrization procedures. An outline of the methodology and its application to NMR NOE-based structure refinement is described in the paper by Hodsdon, *et al*. in *J. Mol. Biol.*, ***264***, 585-602 (1996). We have obtained good results with something like the keyword phrase **`trial-distribution pairwise 5`**, which performs 5% partial random pairwise metrization. For structures over several hundred atoms, a value less than 5 for the percentage of metrization should be fine.

7. Use of the Keyword Control File

Using Keywords to Control TINKER Calculations

This section contains a description of the over 300 keyword parameters which may be used to define or alter the course of a TINKER calculation. The keyword control file is optional in the sense that all of the TINKER programs will run in the absence of a keyfile and will simply use default values or query the user for needed information. However, the keywords allow use of a wide variety of algorithmic and procedural options, many of which are unavailable interactively.

Keywords are read from the keyword control file. All programs look first for a keyfile with the same base name as the input molecular system and ending in the extension **`.key`**. If this file does not exist, then TINKER tries to use a generic keyfile with the name **`tinker.key`** and located in the same directory as the input system. If neither a system-specific nor a generic keyfile is present, TINKER will continue by using default values for keyword options and asking interactive questions as necessary.

TINKER searches the keyfile during the course of a calculation for relevant keywords that may be present. All keywords must appear as the first word on the line. Any blank space to the left of the keyword is ignored, and all contents of the keyfiles are case insensitive. Some keywords take modifiers; *i.e.*, TINKER looks further on the same line for additional information, such as the value of some parameter related to the keyword. Modifier information is read in free format, but must be completely contained on the same line as the original keyword. Any lines contained in the keyfile which do not qualify as valid keyword lines are treated as comments and are simply ignored.

Several keywords take a list of integer values (atom numbers, for example) as modifiers. For these keywords the integers can simply be listed explicitly and separated by spaces, commas or tabs. If a range of numbers is desired, it can be specified by listing the negative of the first number of the range, followed by a separator and the last number of the range. For example, the keyword line **`ACTIVE 4 -9 17 23`** could be used to add atoms 4, 9 through 17, and 23 to the set of active atoms during a TINKER calculation.

Keywords Grouped by Functionality

Listed below are the available TINKER keywords sorted into groups by general function. The section ends with an alphabetical list containing each individual keyword, along with a brief description of its action, possible keyword modifiers, and usage examples.

OUTPUT CONTROL KEYWORDS

ARCHIVE	DEBUG	DIGITS
ECHO	EXIT-PAUSE	NOVERSION
OVERWRITE	PRINTOUT	SAVE-CYCLE
SAVE-FORCE	SAVE-INDUCED	SAVE-VELOCITY
VERBOSE	WRITEOUT	

FORCE FIELD SELECTION KEYWORDS

FORCEFIELD	PARAMETERS

POTENTIAL FUNCTION SELECTION KEYWORDS

ANGANGTERM
ANGLETERM
BONDTERM
CHARGETERM
CHGDPLTERM
DIPOLETERM
EXTRATERM
IMPROPTERM
IMPTORSTERM
METALTERM
MPOLETERM
OPBENDTERM
OPDISTTERM
PITORSTERM
POLARIZETERM
RESTRAINTERM
RXNFIELDTERM
SOLVATETERM
STRBNDTERM
STRTORTERM
TORSIONTERM
TORTORTERM
UREYTERM
VDWTERM

POTENTIAL FUNCTION PARAMETER KEYWORDS

ANGANG
ANGLE
ANGLE3
ANGLE4
ANGLE5
ANGLEF
ATOM
BIOTYPE
BOND
BOND3
BOND4
BOND5
CHARGE
DIPOLE
DIPOLE3
DIPOLE4
DIPOLE5
ELECTNEG
HBOND
IMPROPER
IMPTORS
METAL
MULTIPOLE
OPBEND
OPDIST
PIATOM
PIBOND
PITORS
POLARIZE
SOLVATE
STRBND
STRTORS
TORSION
TORSION4
TORSION5
TORTOR
UREYBRAD
VDW
VDW14
VDWPR

ENERGY UNIT CONVERSION KEYWORDS

ANGLEUNIT
ANGANGUNIT
BONDUNIT
ELECTRIC
IMPROPUNIT
IMPTORUNIT
OPBENDUNIT
OPDISTUNIT
PITORSUNIT
STRBNDUNIT
STRTORUNIT
TORSIONUNIT
TORTORUNIT
UREYUNIT

LOCAL GEOMETRY FUNCTIONAL FORM KEYWORDS

ANGLE-CUBIC
ANGLE-QUARTIC
ANGLE-PENTIC
ANGLE-SEXTIC
BOND-CUBIC
BOND-QUARTIC
BONDTYPE
MM2-STRBND
PISYSTEM
UREY-CUBIC
UREY-QUARTIC

VAN DER WAALS FUNCTIONAL FORM KEYWORDS

A-EXPTERM
B-EXPTERM
C-EXPTERM
DELTA-HALGREN
EPSILONRULE
GAMMA-HALGREN
GAUSSTYPE
RADIUSRULE
RADIUSSIZE
RADIUSTYPE
VDW-12-SCALE
VDW-13-SCALE
VDW-14-SCALE
VDW-15-SCALE
VDW-CORRECTION
VDWINDEX
VDWTYPE

ELECTROSTATICS FUNCTIONAL FORM KEYWORDS

CHG-12-SCALE
CHG-13-SCALE
CHG-14-SCALE

CHG-15-SCALE
CHG-BUFFER
DIELECTRIC
DIRECT-11-SCALE
DIRECT-12-SCALE
DIRECT-13-SCALE
DIRECT-14-SCALE
MPOLE-12-SCALE
MPOLE-13-SCALE
MPOLE-14-SCALE
MPOLE-15-SCALE
MUTUAL-11-SCALE
MUTUAL-12-SCALE
MUTUAL-13-SCALE
MUTUAL-14-SCALE
POLAR-12-SCALE
POLAR-13-SCALE
POLAR-14-SCALE
POLAR-15-SCALE
POLAR-ASPC
POLAR-EPS
POLAR-SOR
POLARIZATION
REACTIONFIELD

NONBONDED CUTOFF KEYWORDS

CHG-CUTOFF
CHG-TAPER
CUTOFF
DPL-CUTOFF
DPL-TAPER
HESS-CUTOFF
LIGHTS
MPOLE-CUTOFF
MPOLE-TAPER
NEIGHBOR-GROUPS
NEUTRAL-GROUPS
POLYMER-CUTOFF
TAPER
TRUNCATE
VDW-CUTOFF
VDW-TAPER

EWALD SUMMATION KEYWORDS

EWALD
EWALD-ALPHA
EWALD-BOUNDARY
EWALD-CUTOFF
PME-GRID
PME-ORDER

CRYSTAL LATTICE & PERIODIC BOUNDARY KEYWORDS

A-AXIS
B-AXIS
C-AXIS
ALPHA
BETA
GAMMA
NO-SYMMETRY
OCTAHEDRON
SPACEGROUP
X-AXIS
Y-AXIS
Z-AXIS

NEIGHBOR LIST KEYWORDS

CHG-LIST
LIST-BUFFER
MPOLE-LIST
NEIGHBOR-LIST
VDW-LIST

OPTIMIZATION KEYWORDS

ANGMAX
CAPPA
FCTMIN
HGUESS
INTMAX
LBFGS-VECTORS
MAXITER
NEWHESS
NEXTITER
SLOPEMAX
STEEPEST-DESCENT
STEPMAX
STEPMIN

MOLECULAR DYNAMICS KEYWORDS

BEEMAN-MIXING
DEGREES-FREEDOM
INTEGRATOR
REMOVE-INERTIA

THERMOSTAT & BAROSTAT KEYWORDS

ANISO-PRESSURE
BAROSTAT
COLLISION
COMPRESS
FRICTION
FRICTION-SCALING
TAU-PRESSURE
TAU-TEMPERATURE
THERMOSTAT

VOLUME-MOVE	VOLUME-SCALE	VOLUME-TRIAL

TRANSITION STATE KEYWORDS

DIVERGE	GAMMAMIN	REDUCE
SADDLEPOINT		

DISTANCE GEOMETRY KEYWORDS

TRIAL-DISTANCE	TRIAL-DISTRIBUTION

VIBRATIONAL ANALYSIS KEYWORDS

IDUMP	VIB-ROOTS	VIB-TOLERANCE

IMPLICIT SOLVATION KEYWORDS

BORN-RADIUS	GK-RADIUS	GKC
GKR	SOLVENT-PRESSURE	SURFACE-TENSION

POISSON-BOLTZMANN KEYWORDS

AGRID	APBS-GRID	BCFL
CGCENT	CGRID	FGCENT
FGRID	ION	MG-AUTO
MG-MANUAL	PB-RADIUS	PDIE
SDENS	SDIE	SMIN
SRAD	SRFM	SWIN

MATHEMATICAL ALGORITHM KEYWORDS

FFT-PACKAGE	RANDOMSEED

PARALLELIZATION KEYWORDS

OPENMP-THREADS

FREE ENERGY PERTURBATION KEYWORDS

CHG-LAMBDA	DPL-LAMBDA	LAMBDA
LIGAND	MPOLE-LAMBDA	MUTATE
POLAR-LAMBDA	VDW-LAMBDA	

PARTIAL STRUCTURE KEYWORDS

ACTIVE	GROUP	GROUP-INTER
GROUP-INTRA	GROUP-MOLECULE	GROUP-SELECT
INACTIVE		

CONSTRAINT & RESTRAINT KEYWORDS

BASIN	ENFORCE-CHIRALITY	RATTLE
RATTLE-DISTANCE	RATTLE-EPS	RATTLE-LINE
RATTLE-ORIGIN	RATTLE-PLANE	RESTRAIN-ANGLE

RESTRAIN-DISTANCE	RESTRAIN-GROUPS	RESTRAIN-POSITION
RESTRAIN-TORSION	SPHERE	WALL

PARAMETER FITTING KEYWORDS

FIT-ANGLE	FIT-BOND	FIT-OPBEND
FIT-STRBND	FIT-TORSION	FIT-UREY
FIX-ANGLE	FIX-BOND	FIX-DIPOLE
FIX-MONOPOLE	FIX-OPBEND	FIX-QUADRUPOLE
FIX-STRBND	FIX-TORSION	FIX-UREY
POTENTIAL-ATOMS	POTENTIAL-FIT	POTENTIAL-OFFSET
POTENTIAL-SHELLS	POTENTIAL-SPACING	TARGET-DIPOLE
TARGET-QUADRUPOLE		

POTENTIAL SMOOTHING KEYWORDS

DEFORM	DIFFUSE-CHARGE	DIFFUSE-TORSION
DIFFUSE-VDW	SMOOTHING	

Description of Individual Keywords

The following is an alphabetical list of the TINKER keywords along with a brief description of the action of each keyword and required or optional parameters that can be used to extend or modify each keyword. The format of possible modifiers, if any, is shown in brackets following each keyword.

A-AXIS [real] Sets the value of the a-axis length for a crystal unit cell, or, equivalently, the X-axis length for a periodic box. The length value in Angstroms is listed after the keyword.

A-EXPTERM [real] Sets the value of the ``A'' premultiplier term in the Buckingham van der Waals function, *i.e.*, the value of A in the formula $E_{vdw} = \varepsilon \{ A \exp[-B(R_o/R)] - C (R_o/R)^6 \}$.

ACTIVE [integer list] Sets the list of active atoms during a TINKER computation. Individual potential energy terms are computed when at least one atom involved in the term is active. For Cartesian space calculations, active atoms are those allowed to move. For torsional space calculations, rotations are allowed when all atoms on one side of the rotated bond are active. Multiple ACTIVE lines can be present in the keyfile and are treated cumulatively. On each line the keyword can be followed by one or more atom numbers or atom ranges. The presence of any ACTIVE keyword overrides any INACTIVE keywords in the keyfile.

ALPHA [real] Sets the value of the α angle of a crystal unit cell, *i.e.*, the angle between the b-axis and c-axis of a unit cell, or, equivalently, the angle between the Y-axis and Z-axis of a periodic box. The default value in the absence of the ALPHA keyword is 90 degrees.

ANGANG [1 integer & 3 reals] This keyword provides the values for a single angle-angle cross term potential parameter.

ANGANGTERM [NONE/ONLY] This keyword controls use of the angle-angle cross term potential energy. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

ANGANGUNIT [real] Sets the scale factor needed to convert the energy value computed by the angle-angle cross term potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default of $(\pi/180)^2$ = 0.0003046 is used, if the ANGANGUNIT keyword is not given in the force field parameter file or the keyfile.

ANGLE [3 integers & 4 reals] This keyword provides the values for a single bond angle bending parameter. The integer modifiers give the atom class numbers for the three kinds of atoms involved in the angle which is to be defined. The real number modifiers give the force constant value for the angle and up to three ideal bond angles in degrees. In most cases only one ideal bond angle is given, and that value is used for all occurrences of the specified bond angle. If all three ideal angles are given, the values apply when the central atom of the angle is attached to 0, 1 or 2 additional hydrogen atoms, respectively. This ``hydrogen environment'' option is provided to implement the corresponding feature of Allinger's MM force fields. The default units for the force constant are kcal/mole/radian^2, but this can be controlled via the ANGLEUNIT keyword.

ANGLE-CUBIC [real] Sets the value of the cubic term in the Taylor series expansion form of the bond angle bending potential energy. The real number modifier gives the value of the coefficient as a multiple of the quadratic coefficient. This term multiplied by the angle bending energy unit conversion factor, the force constant, and the cube of the deviation of the bond angle from its ideal value gives the cubic contribution to the angle bending energy. The default value in the absence of the ANGLE-CUBIC keyword is zero; *i.e.*, the cubic angle bending term is omitted.

ANGLE-PENTIC [real] Sets the value of the fifth power term in the Taylor series expansion form of the bond angle bending potential energy. The real number modifier gives the value of the coefficient as a multiple of the quadratic coefficient. This term multiplied by the angle bending energy unit conversion factor, the force constant, and the fifth power of the deviation of the bond angle from its ideal value gives the pentic contribution to the angle bending energy. The default value in the absence of the ANGLE-PENTIC keyword is zero; *i.e.*, the pentic angle bending term is omitted.

ANGLE-QUARTIC [real] Sets the value of the quartic term in the Taylor series expansion form of the bond angle bending potential energy. The real number modifier gives the value of the coefficient as a multiple of the quadratic coefficient. This term multiplied by the angle bending energy unit conversion factor, the force constant, and the forth power of the deviation of the bond angle from its ideal value gives the quartic contribution to the angle bending energy. The default value in the absence of the ANGLE-QUARTIC keyword is zero; *i.e.*, the quartic angle bending term is omitted.

ANGLE-SEXTIC [real] Sets the value of the sixth power term in the Taylor series expansion form of the bond angle bending potential energy. The real number modifier gives the value of the coefficient as a multiple of the quadratic coefficient. This term multiplied by the angle bending energy unit conversion factor, the force constant, and the sixth power of the deviation of the bond angle from its ideal value gives the sextic contribution to the angle bending energy. The default value in the absence of the ANGLE-SEXTIC keyword is zero; *i.e.*, the sextic angle bending term is omitted.

ANGLE3 [3 integers & 4 reals] This keyword provides the values for a single bond angle bending parameter specific to atoms in 3-membered rings. The integer modifiers give the atom class numbers for the three kinds of atoms involved in the angle which is to be defined. The real number modifiers give the force constant value for the angle and up to three ideal bond angles in degrees. If all three ideal angles are given, the values apply when the central atom of the angle is attached to 0, 1 or 2 additional hydrogen atoms, respectively. The default units for the force constant are kcal/mole/radian^2, but this can be controlled via the ANGLEUNIT keyword. If any ANGLE3 keywords are present, either in the master force field parameter file or the keyfile, then TINKER requires that

special ANGLE3 parameters be given for all angles in 3-membered rings. In the absence of any ANGLE3 keywords, standard ANGLE parameters will be used for bonds in 3-membered rings.

ANGLE4 [3 integers & 4 reals] This keyword provides the values for a single bond angle bending parameter specific to atoms in 4-membered rings. The integer modifiers give the atom class numbers for the three kinds of atoms involved in the angle which is to be defined. The real number modifiers give the force constant value for the angle and up to three ideal bond angles in degrees. If all three ideal angles are given, the values apply when the central atom of the angle is attached to 0, 1 or 2 additional hydrogen atoms, respectively. The default units for the force constant are kcal/mole/radian^2, but this can be controlled via the ANGLEUNIT keyword. If any ANGLE4 keywords are present, either in the master force field parameter file or the keyfile, then TINKER requires that special ANGLE4 parameters be given for all angles in 4-membered rings. In the absence of any ANGLE4 keywords, standard ANGLE parameters will be used for bonds in 4-membered rings.

ANGLE5 [3 integers & 4 reals] This keyword provides the values for a single bond angle bending parameter specific to atoms in 5-membered rings. The integer modifiers give the atom class numbers for the three kinds of atoms involved in the angle which is to be defined. The real number modifiers give the force constant value for the angle and up to three ideal bond angles in degrees. If all three ideal angles are given, the values apply when the central atom of the angle is attached to 0, 1 or 2 additional hydrogen atoms, respectively. The default units for the force constant are kcal/mole/radian^2, but this can be controlled via the ANGLEUNIT keyword. If any ANGLE5 keywords are present, either in the master force field parameter file or the keyfile, then TINKER requires that special ANGLE5 parameters be given for all angles in 5-membered rings. In the absence of any ANGLE5 keywords, standard ANGLE parameters will be used for bonds in 5-membered rings.

ANGLEF [3 integers & 3 reals] This keyword provides the values for a single bond angle bending parameter for a SHAPES-style Fourier potential function. The integer modifiers give the atom class numbers for the three kinds of atoms involved in the angle which is to be defined. The real number modifiers give the force constant value for the angle, the angle shift in degrees, and the periodicity value. Note that the force constant should be given as the ``harmonic'' value and not the native Fourier value. The default units for the force constant are kcal/mole/radian^2, but this can be controlled via the ANGLEUNIT keyword.

ANGLETERM [NONE/ONLY] This keyword controls use of the bond angle bending potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

ANGLEUNIT [real] Sets the scale factor needed to convert the energy value computed by the bond angle bending potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default value of $(\pi/180)^2$ = 0.0003046 is used, if the ANGLEUNIT keyword is not given in the force field parameter file or the keyfile.

ANGMAX [real] Set the maximum permissible angle between the current optimization search direction and the negative of the gradient direction. If this maximum angle value is exceeded, the optimization routine will note an error condition and may restart from the steepest descent direction. The default value in the absence of the ANGMAX keyword is usually 88 degrees for conjugate gradient methods and 180 degrees (*i.e.*, disabled) for variable metric optimizations.

ANISO-PRESSURE This keyword invokes use of full anisotropic pressure during dynamics simulations. When using this option, the three axis lengths and axis angles vary separately in

response to the pressure tensor. The default, in the absence of the keyword, is isotropic pressure based on the average of the diagonal of the pressure tensor.

ARCHIVE This keyword causes TINKER molecular dynamics-based programs to write trajectories directly to a single plain-text archive file with the **`.arc`** format. If an archive file already exists at the start of the calculation, then the newly generated trajectory is appended to the end of the existing file. The default in the absence of this keyword is to write the trajectory snapshots to consecutively numbered cycle files.

ATOM [2 integers, name, quoted string, integer, real & integer] This keyword provides the values needed to define a single force field atom type.

B-AXIS [real] Sets the value of the b-axis length for a crystal unit cell, or, equivalently, the Y-axis length for a periodic box. The length value in Angstroms is listed after the keyword. If the keyword is absent, the b-axis length is set equal to the a-axis length.

B-EXPTERM [real] Sets the value of the ``B'' exponential factor in the Buckingham van der Waals function, *i.e.*, the value of B in the formula $E_{vdw} = \varepsilon \{ A \exp[-B(R_o/R)] - C (R_o/R)^6 \}$.

BAROSTAT [BERENDSEN] This keyword selects a barostat algorithm for use during molecular dynamics. At present only one modifier is available, a Berendsen bath coupling method. The default in the absence of the BAROSTAT keyword is to use the BERENDSEN algorithm.

BASIN [2 reals] Presence of this keyword turns on a ``basin'' restraint potential function that serves to drive the system toward a compact structure. The actual function is a Gaussian of the form $E_{basin} = \Sigma A \exp[-B R^2]$, summed over all pairs of atoms where R is the distance between atoms. The A and B values are the depth and width parameters given as modifiers to the BASIN keyword. This potential is currently used to control the degree of expansion during potential energy smooth procedures through the use of shallow, broad basins.

BETA [real] Sets the value of the β angle of a crystal unit cell, *i.e.*, the angle between the a-axis and c-axis of a unit cell, or, equivalently, the angle between the X-axis and Z-axis of a periodic box. The default value in the absence of the BETA keyword is to set the β angle equal to the α angle as given by the keyword ALPHA.

BIOTYPE [integer, name, quoted string & integer] This keyword provides the values to define the correspondence between a single biopolymer atom type and its force field atom type.

BOND [2 integers & 2 reals] This keyword provides the values for a single bond stretching parameter. The integer modifiers give the atom class numbers for the two kinds of atoms involved in the bond which is to be defined. The real number modifiers give the force constant value for the bond and the ideal bond length in ≈. The default units for the force constant are kcal/mole/$\approx^2$, but this can be controlled via the BONDUNIT keyword.

BOND-CUBIC [real] Sets the value of the cubic term in the Taylor series expansion form of the bond stretching potential energy. The real number modifier gives the value of the coefficient as a multiple of the quadratic coefficient. This term multiplied by the bond stretching energy unit conversion factor, the force constant, and the cube of the deviation of the bond length from its ideal value gives the cubic contribution to the bond stretching energy. The default value in the absence of the BOND-CUBIC keyword is zero; *i.e.*, the cubic bond stretching term is omitted.

BOND-QUARTIC [real] Sets the value of the quartic term in the Taylor series expansion form of the bond stretching potential energy. The real number modifier gives the value of the coefficient as a multiple of the quadratic coefficient. This term multiplied by the bond stretching energy unit conversion factor, the force constant, and the forth power of the deviation of the bond length from its ideal value gives the quartic contribution to the bond stretching energy. The default value in the absence of the BOND-QUARTIC keyword is zero; *i.e.*, the quartic bond stretching term is omitted.

BOND3 [2 integers & 2 reals] This keyword provides the values for a single bond stretching parameter specific to atoms in 3-membered rings. The integer modifiers give the atom class numbers for the two kinds of atoms involved in the bond which is to be defined. The real number modifiers give the force constant value for the bond and the ideal bond length in ≈. The default units for the force constant are kcal/mole/$\approx^2$, but this can be controlled via the BONDUNIT keyword. If any BOND3 keywords are present, either in the master force field parameter file or the keyfile, then TINKER requires that special BOND3 parameters be given for all bonds in 3-membered rings. In the absence of any BOND3 keywords, standard BOND parameters will be used for bonds in 3-membered rings.

BOND4 [2 integers & 2 reals] This keyword provides the values for a single bond stretching parameter specific to atoms in 4-membered rings. The integer modifiers give the atom class numbers for the two kinds of atoms involved in the bond which is to be defined. The real number modifiers give the force constant value for the bond and the ideal bond length in ≈. The default units for the force constant are kcal/mole/$\approx^2$, but this can be controlled via the BONDUNIT keyword. If any BOND4 keywords are present, either in the master force field parameter file or the keyfile, then TINKER requires that special BOND4 parameters be given for all bonds in 4-membered rings. In the absence of any BOND4 keywords, standard BOND parameters will be used for bonds in 4-membered rings

BOND5 [2 integers & 2 reals] This keyword provides the values for a single bond stretching parameter specific to atoms in 5-membered rings. The integer modifiers give the atom class numbers for the two kinds of atoms involved in the bond which is to be defined. The real number modifiers give the force constant value for the bond and the ideal bond length in ≈. The default units for the force constant are kcal/mole/$\approx^2$, but this can be controlled via the BONDUNIT keyword. If any BOND5 keywords are present, either in the master force field parameter file or the keyfile, then TINKER requires that special BOND5 parameters be given for all bonds in 5-membered rings. In the absence of any BOND5 keywords, standard BOND parameters will be used for bonds in 5-membered rings

BONDTERM [NONE/ONLY] This keyword controls use of the bond stretching potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

BONDTYPE [TAYLOR/MORSE/GAUSSIAN] Chooses the functional form of the bond stretching potential. The TAYLOR option selects a Taylor series expansion containing terms from harmonic through quartic. The MORSE option selects a Morse potential fit to the ideal bond length and stretching force constant parameter values. The GAUSSIAN option uses an inverted Gaussian with amplitude equal to the Morse bond dissociation energy and width set to reproduce the vibrational frequency of a harmonic potential. The default is to use the TAYLOR potential.

BONDUNIT [real] Sets the scale factor needed to convert the energy value computed by the bond stretching potential into units of kcal/mole. The correct value is force field dependent and typically

provided in the header of the master force field parameter file. The default value of 1.0 is used, if the BONDUNIT keyword is not given in the force field parameter file or the keyfile.

C-AXIS [real] Sets the value of the C-axis length for a crystal unit cell, or, equivalently, the Z-axis length for a periodic box. The length value in Angstroms is listed after the keyword. If the keyword is absent, the C-axis length is set equal to the A-axis length.

C-EXPTERM [real] Sets the value of the ``C'' dispersion multiplier in the Buckingham van der Waals function, *i.e.*, the value of C in the formula $E_{vdw} = \varepsilon \{ A \exp[-B(R_o/R)] - C (R_o/R)^6 \}$.

CAPPA [real] This keyword is used to set the normal termination criterion for the line search phase of TINKER optimization routines. The line search exits successfully if the ratio of the current gradient projection on the line to the projection at the start of the line search falls below the value of CAPPA. A default value of 0.1 is used in the absence of the CAPPA keyword.

CHARGE [1 integer & 1 real] This keyword provides a value for a single atomic partial charge electrostatic parameter. The integer modifier, if positive, gives the atom type number for which the charge parameter is to be defined. Note that charge parameters are given for atom types, not atom classes. If the integer modifier is negative, then the parameter value to follow applies only to the individual atom whose atom number is the negative of the modifier. The real number modifier gives the values of the atomic partial charge in electrons.

CHARGETERM [NONE/ONLY] This keyword controls use of the charge-charge potential energy term between pairs of atomic partial charges. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

CHG-12-SCALE [real] This keyword provides a multiplicative scale factor that is applied to charge-charge electrostatic interactions between 1-2 connected atoms, *i.e.*, atoms that are directly bonded. The default value of 0.0 is used, if the CHG-12-SCALE keyword is not given in either the parameter file or the keyfile.

CHG-13-SCALE [real] This keyword provides a multiplicative scale factor that is applied to charge-charge electrostatic interactions between 1-3 connected atoms, *i.e.*, atoms separated by two covalent bonds. The default value of 0.0 is used, if the CHG-13-SCALE keyword is not given in either the parameter file or the keyfile.

CHG-14-SCALE [real] This keyword provides a multiplicative scale factor that is applied to charge-charge electrostatic interactions between 1-4 connected atoms, *i.e.*, atoms separated by three covalent bonds. The default value of 1.0 is used, if the CHG-14-SCALE keyword is not given in either the parameter file or the keyfile.

CHG-15-SCALE [real] This keyword provides a multiplicative scale factor that is applied to charge-charge electrostatic interactions between 1-5 connected atoms, *i.e.*, atoms separated by four covalent bonds. The default value of 1.0 is used, if the CHG-15-SCALE keyword is not given in either the parameter file or the keyfile.

CHG-CUTOFF [real] Sets the cutoff distance value in Angstroms for charge-charge electrostatic potential energy interactions. The energy for any pair of sites beyond the cutoff distance will be set to zero. Other keywords can be used to select a smoothing scheme near the cutoff distance. The default

cutoff distance in the absence of the CHG-CUTOFF keyword is infinite for nonperiodic systems and 9.0 for periodic systems.

CHG-TAPER [real] This keyword allows modification of the cutoff window for charge-charge electrostatic potential energy interactions. It is similar in form and action to the TAPER keyword, except that its value applies only to the charge-charge potential. The default value in the absence of the CHG-TAPER keyword is to begin the cutoff window at 0.65 of the corresponding cutoff distance.

CHGDPLTERM [NONE/ONLY] This keyword controls use of the charge-dipole potential energy term between atomic partial charges and bond dipoles. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

COLLISION [real] Sets the value of the random collision frequency used in the Andersen stochastic collision dynamics thermostat. The supplied value has units of fs^{-1} $atom^{-1}$ and is multiplied internal to TINKER by the time step in fs and $N^{-2/3}$ where N is the number of atoms. The default value used in the absence of the COLLISION keyword is 0.1 which is appropriate for many systems but may need adjustment to achieve adequate temperature control without perturbing the dynamics.

COMPRESS [real] Sets the value of the bulk solvent isothermal compressibility in Atm^{-1} for use during pressure computation and scaling in molecular dynamics computations. The default value used in the absence of the COMPRESS keyword is 0.000046, appropriate for water. This parameter serves as a scale factor for the Groningen-style pressure bath coupling time, and its exact value should not be of critical importance.

CUTOFF [real] Sets the cutoff distance value for all nonbonded potential energy interactions. The energy for any of the nonbonded potentials of a pair of sites beyond the cutoff distance will be set to zero. Other keywords can be used to select a smoothing scheme near the cutoff distance, or to apply different cutoff distances to various nonbonded energy terms.

DEBUG Turns on printing of detailed information and intermediate values throughout the progress of a TINKER computation; not recommended for use with large structures or full potential energy functions since a summary of every individual interaction will usually be output.

DEFORM [real] Sets the amount of diffusion equation-style smoothing that will be applied to the potential energy surface when using the SMOOTH force field. The real number option is equivalent to the ``time'' value in the original Piela, *et al.* formalism; the larger the value, the greater the smoothing. The default value is zero, meaning that no smoothing will be applied.

DEGREES-FREEDOM [integer] This keyword allows manual setting of the number of degrees of freedom during a dynamics calculation. The integer modifier is used by thermostating methods and in other places as the number of degrees of freedom, overriding the value determined by the TINKER code at dynamics startup. In the absence of the keyword, the programs will automatically compute the correct value based on the number of atoms active during dynamics, bond or other constrains, and use of periodic boundary conditions.

DELTA-HALGREN [real] Sets the value of the δ parameter in Halgren's buffered 14-7 vdw potential energy functional form. In the absence of the DELTA-HALGREN keyword, a default value of 0.07 is used.

DIELECTRIC [real] Sets the value of the bulk dielectric constant used to damp all electrostatic interaction energies for any of the TINKER electrostatic potential functions. The default value is force field dependent, but is usually equal to 1.0 (for Allinger's MM force fields the default is 1.5).

DIFFUSE-CHARGE [real] This keyword is used during potential function smoothing procedures to specify the effective diffusion coefficient to be applied to the smoothed form of the Coulomb's Law charge-charge potential function. In the absence of the DIFFUSE-CHARGE keyword, a default value of 3.5 is used.

DIFFUSE-TORSION [real] This keyword is used during potential function smoothing procedures to specify the effective diffusion coefficient to be applied to the smoothed form of the torsion angle potential function. In the absence of the DIFFUSE-TORSION keyword, a default value of 0.0225 is used.

DIFFUSE-VDW [real] This keyword is used during potential function smoothing procedures to specify the effective diffusion coefficient to be applied to the smoothed Gaussian approximation to the Lennard-Jones van der Waals potential function. In the absence of the DIFFUSE-VDW keyword, a default value of 1.0 is used.

DIGITS [integer] This keyword controls the number of digits of precision output by TINKER in reporting potential energies and atomic coordinates. The allowed values for the integer modifier are 4, 6 and 8. Input values less than 4 will be set to 4, and those greater than 8 will be set to 8. Final energy values reported by most TINKER programs will contain the specified number of digits to the right of the decimal point. The number of decimal places to be output for atomic coordinates is generally two larger than the value of DIGITS. In the absence of the DIGITS keyword a default value of 4 is used, and energies will be reported to 4 decimal places with coordinates to 6 decimal places.

DIPOLE [2 integers & 2 reals] This keyword provides the values for a single bond dipole electrostatic parameter. The integer modifiers give the atom type numbers for the two kinds of atoms involved in the bond dipole which is to be defined. The real number modifiers give the value of the bond dipole in Debyes and the position of the dipole site along the bond. If the bond dipole value is positive, then the first of the two atom types is the positive end of the dipole. For a negative bond dipole value, the first atom type listed is negative. The position along the bond is an optional modifier that gives the postion of the dipole site as a fraction between the first atom type (position=0) and the second atom type (position=1). The default for the dipole position in the absence of a specified value is 0.5, placing the dipole at the midpoint of the bond.

DIPOLE3 [2 integers & 2 reals] This keyword provides the values for a single bond dipole electrostatic parameter specific to atoms in 3-membered rings. The integer modifiers give the atom type numbers for the two kinds of atoms involved in the bond dipole which is to be defined. The real number modifiers give the value of the bond dipole in Debyes and the position of the dipole site along the bond. The default for the dipole position in the absence of a specified value is 0.5, placing the dipole at the midpoint of the bond. If any DIPOLE3 keywords are present, either in the master force field parameter file or the keyfile, then TINKER requires that special DIPOLE3 parameters be given for all bond dipoles in 3-membered rings. In the absence of any DIPOLE3 keywords, standard DIPOLE parameters will be used for bonds in 3-membered rings.

DIPOLE4 [2 integers & 2 reals] This keyword provides the values for a single bond dipole electrostatic parameter specific to atoms in 4-membered rings. The integer modifiers give the atom type numbers for the two kinds of atoms involved in the bond dipole which is to be defined. The real number modifiers give the value of the bond dipole in Debyes and the position of the dipole site along the bond. The default for the dipole position in the absence of a specified value is 0.5, placing the

dipole at the midpoint of the bond. If any DIPOLE4 keywords are present, either in the master force field parameter file or the keyfile, then TINKER requires that special DIPOLE4 parameters be given for all bond dipoles in 4-membered rings. In the absence of any DIPOLE4 keywords, standard DIPOLE parameters will be used for bonds in 4-membered rings.

DIPOLE5 [2 integers & 2 reals] This keyword provides the values for a single bond dipole electrostatic parameter specific to atoms in 5-membered rings. The integer modifiers give the atom type numbers for the two kinds of atoms involved in the bond dipole which is to be defined. The real number modifiers give the value of the bond dipole in Debyes and the position of the dipole site along the bond. The default for the dipole position in the absence of a specified value is 0.5, placing the dipole at the midpoint of the bond. If any DIPOLE5 keywords are present, either in the master force field parameter file or the keyfile, then TINKER requires that special DIPOLE5 parameters be given for all bond dipoles in 5-membered rings. In the absence of any DIPOLE5 keywords, standard DIPOLE parameters will be used for bonds in 5-membered rings.

DIPOLETERM [NONE/ONLY] This keyword controls use of the dipole-dipole potential energy term between pairs of bond dipoles. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

DIRECT-11-SCALE [real] This keyword provides a multiplicative scale factor that is applied to the permanent (direct) field due to atoms within a polarization group during an induced dipole calculation, *i.e.*, atoms that are in the same polarization group as the atom being polarized. The default value of 0.0 is used, if the DIRECT-11-SCALE keyword is not given in either the parameter file or the keyfile.

DIRECT-12-SCALE [real] This keyword provides a multiplicative scale factor that is applied to the permanent (direct) field due to atoms in 1-2 polarization groups during an induced dipole calculation, *i.e.*, atoms that are in polarization groups directly connected to the group containing the atom being polarized. The default value of 0.0 is used, if the DIRECT-12-SCALE keyword is not given in either the parameter file or the keyfile.

DIRECT-13-SCALE [real] This keyword provides a multiplicative scale factor that is applied to the permanent (direct) field due to atoms in 1-3 polarization groups during an induced dipole calculation, *i.e.*, atoms that are in polarization groups separated by one group from the group containing the atom being polarized. The default value of 0.0 is used, if the DIRECT-13-SCALE keyword is not given in either the parameter file or the keyfile.

DIRECT-14-SCALE [real] This keyword provides a multiplicative scale factor that is applied to the permanent (direct) field due to atoms in 1-4 polarization groups during an induced dipole calculation, *i.e.*, atoms that are in polarization groups separated by two groups from the group containing the atom being polarized. The default value of 1.0 is used, if the DIRECT-14-SCALE keyword is not given in either the parameter file or the keyfile.

DIVERGE [real] This keyword is used by the SADDLE program to set the maximum allowed value of the ratio of the gradient length along the path to the total gradient norm at the end of a cycle of minimization perpendicular to the path. If the value provided by the DIVERGE keyword is exceeded, then another cycle of maximization along the path is required. A default value of 0.005 is used in the absence of the DIVERGE keyword.

DPL-CUTOFF [real] Sets the cutoff distance value in Angstroms for bond dipole-bond dipole electrostatic potential energy interactions. The energy for any pair of bond dipole sites beyond the

cutoff distance will be set to zero. Other keywords can be used to select a smoothing scheme near the cutoff distance. The default cutoff distance in the absence of the DPL-CUTOFF keyword is essentially infinite for nonperiodic systems and 10.0 for periodic systems.

DPL-TAPER [real] This keyword allows modification of the cutoff windows for bond dipole-bond dipole electrostatic potential energy interactions. It is similar in form and action to the TAPER keyword, except that its value applies only to the vdw potential. The default value in the absence of the DPL-TAPER keyword is to begin the cutoff window at 0.75 of the dipole cutoff distance.

ECHO [text string] The presence of this keyword causes whatever text follows it on the line to be copied directly to the output file. This keyword is also active in parameter files. It has no default value; if no text follows the ECHO keyword, a blank line is placed in the output file.

ELECTNEG [3 integers & 1 real] This keyword provides the values for a single electronegativity bond length correction parameter. The first two integer modifiers give the atom class numbers of the atoms involved in the bond to be corrected. The third integer modifier is the atom class of an electronegative atom. In the case of a primary correction, an atom of this third class must be directly bonded to an atom of the second atom class. For a secondary correction, the third class is one atom removed from an atom of the second class. The real number modifier is the value in ≈ by which the original ideal bond length is to be corrected.

ENFORCE-CHIRALITY This keyword causes the chirality found at chiral tetravalent centers in the input structure to be maintained during TINKER calculations. The test for chirality is not exhaustive; two identical monovalent atoms connected to a center cause it to be marked as non-chiral, but large equivalent substituents are not detected. Trivalent ``chiral'' centers, for example the alpha carbon in united-atom protein structures, are not enforced as chiral.

EPSILONRULE [GEOMETRIC/ARITHMETIC/HARMONIC/HHG] This keyword selects the combining rule used to derive the ε value for van der Waals interactions. The default in the absence of the EPSILONRULE keyword is to use the GEOMETRIC mean of the individual ε values of the two atoms involved in the van der Waals interaction.

EWALD This keyword turns on the use of Ewald summation during computation of electrostatic interactions in periodic systems. In the current version of TINKER, regular Ewald is used for polarizable atomic multipoles, and smooth particle mesh Ewald (PME) is used for charge-charge interactions. Ewald summation is not available for interactions involving bond-centered dipoles. By default, in the absence of the EWALD keyword, distance-based cutoffs are used for electrostatic interactions.

EWALD-ALPHA [real] Sets the value of the Ewald coefficient which controls the width of the Gaussian screening charges during particle mesh Ewald summation. In the absence of the EWALD-ALPHA keyword, a value is chosen which causes interactions outside the real-space cutoff to be below a fixed tolerance. For most standard applications of Ewald summation, the program default should be used.

EWALD-BOUNDARY This keyword invokes the use of insulating (*ie,* vacuum) boundary conditions during Ewald summation, corresponding to the media surrounding the system having a dielectric value of 1. The default in the absence of the EWALD-BOUNDARY keyword is to use conducting (*ie,* tinfoil) boundary conditions where the surrounding media is assumed to have an infinite dielectric value.

EWALD-CUTOFF [real] Sets the value in Angstroms of the real-space distance cutoff for use during Ewald summation. By default, in the absence of the EWALD-CUTOFF keyword, a value of 9.0 is used.

EXIT-PAUSE This keyword causes TINKER programs to pause and wait for a carriage return at the end of executation prior to returning control to the operating system. This is useful to keep the execution window open following termination on machines running Microsoft Windows or Apple MacOS. The default in the absence of the EXIT-PAUSE keyword, is to return control to the operating system immediately at program termination.

EXTRATERM [NONE/ONLY] This keyword controls use of the user defined extra potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

FCTMIN [real] This keyword sets a convergence criterion for successful completion of a TINKER optimization. If the value of the optimization objective function, typically the potential energy, falls below the value set by FCTMIN, then the optimization is deemed to have converged. The default value in the absence of the FCTMIN keyword is -1000000, effectively removing this criterion as a possible agent for termination.

FORCEFIELD [name] This keyword provides a name for the force field to be used in the current calculation. Its value is usually set in the master force field parameter file for the calculation (see the PARAMETERS keyword) instead of in the keyfile.

FRICTION [real] Sets the value of the frictional coefficient in ps^{-1} for use with stochastic dynamics. The default value used in the absence of the FRICTION keyword is 91.0, which is generally appropriate for water.

FRICTION-SCALING This keyword turns on the use of atomic surface area-based scaling of the frictional coefficient during stochastic dynamics. When in use, the coefficient for each atom is multiplied by that atom's fraction of exposed surface area. The default in the absence of the keyword is to omit the scaling and use the full coefficient value for each atom.

GAMMA [real] Sets the value of the γ angle of a crystal unit cell, *i.e.*, the angle between the a-axis and b-axis of a unit cell, or, equivalently, the angle between the X-axis and Y-axis of a periodic box. The default value in the absence of the GAMMA keyword is to set the γ angle equal to the α angle as given by the keyword ALPHA.

GAMMA-HALGREN [real] Sets the value of the γ parameter in Halgren's buffered 14-7 vdw potential energy functional form. In the absence of the DELTA-HALGREN keyword, a default value of 0.12 is used.

GAMMAMIN [real] Sets the convergence target value for γ during searches for maxima along the quadratic synchronous transit used by the SADDLE program. The value of γ is the square of the ratio of the gradient projection along the path to the total gradient. A default value of 0.00001 is used in the absence of the GAMMAMIN keyword.

GAUSSTYPE [LJ-2/LJ-4/MM2-2/MM3-2/IN-PLACE] This keyword specifies the underlying vdw form that a Gaussian vdw approximation will attempt to fit.number of terms to be used in a Gaussian approximation of the Lennard-Jones van der Waals potential. The text modifier gives the name of the functional form to be used. Thus LJ-2 as a modifier will result in a 2-Gaussian fit to a Lennard-Jones

vdw potential. The GAUSSTYPE keyword only takes effect when VDWTYPE is set to GAUSSIAN. This keyword has no default value.

GROUP [integer, integer list] This keyword defines an atom group as a substructure within the full input molecular structure. The value of the first integer is the group number which must be in the range from 1 to the maximum number of allowed groups. The remaining intergers give the atom or atoms contained in this group as one or more atom numbers or ranges. Multiple keyword lines can be used to specify additional atoms in the same group. Note that an atom can only be in one group, the last group to which it is assigned is the one used.

GROUP-INTER This keyword assigns a value of 1.0 to all inter-group interactions and a value of 0.0 to all intra-group interactions. For example, combination with the GROUP-MOLECULE keyword provides for rigid-body calculations.

GROUP-INTRA This keyword assigns a value of 1.0 to all intra-group interactions and a value of 0.0 to all inter-group interactions.

GROUP-MOLECULE This keyword sets each individual molecule in the system to be a separate atom group, but does not assign weights to group-group interactions.

GROUP-SELECT [2 integers, real] This keyword gives the weight in the final potential energy of a specified set of intra- or intergroup interactions. The integer modifiers give the group numbers of the groups involved. If the two numbers are the same, then an intragroup set of interactions is specified. The real modifier gives the weight by which all energetic interactions in this set will be multiplied before incorporation into the final potential energy. If omitted as a keyword modifier, the weight will be set to 1.0 by default. If any SELECT-GROUP keywords are present, then any set of interactions not specified in a SELECT-GROUP keyword is given a zero weight. The default when no SELECT-GROUP keywords are specified is to use all intergroup interactions with a weight of 1.0 and to set all intragroup interactions to zero.

HBOND [2 integers & 2 reals] This keyword provides the values for the MM3-style directional hydrogen bonding parameters for a single pair of atoms. The integer modifiers give the pair of atom class numbers for which hydrogen bonding parameters are to be defined. The two real number modifiers give the values of the minimum energy contact distance in ≈ and the well depth at the minimum distance in kcal/mole.

HESS-CUTOFF [real] This keyword defines a lower limit for significant Hessian matrix elements. During computation of the Hessian matrix of partial second derivatives, any matrix elements with absolute value below HESS-CUTOFF will be set to zero and omitted from the sparse matrix Hessian storage scheme used by TINKER. For most calculations, the default in the absence of this keyword is zero, i.e., all elements will be stored. For most Truncated Newton optimizations the Hessian cutoff will be chosen dynamically by the optimizer.

HGUESS [real] Sets an initial guess for the average value of the diagonal elements of the scaled inverse Hessian matrix used by the optimally conditioned variable metric optimization routine. A default value of 0.4 is used in the absence of the HGUESS keyword.

IMPROPER [4 integers & 2 reals] This keyword provides the values for a single CHARMM-style improper dihedral angle parameter.

IMPROPTERM [NONE/ONLY] This keyword controls use of the CHARMM-style improper dihedral angle potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

IMPROPUNIT [real] Sets the scale factor needed to convert the energy value computed by the CHARMM-style improper dihedral angle potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default value of 1.0 is used, if the IMPROPUNIT keyword is not given in the force field parameter file or the keyfile.

IMPTORS [4 integers & up to 3 real/real/integer triples] This keyword provides the values for a single AMBER-style improper torsional angle parameter. The first four integer modifiers give the atom class numbers for the atoms involved in the improper torsional angle to be defined. By convention, the third atom class of the four is the trigonal atom on which the improper torsion is centered. The torsional angle computed is literally that defined by the four atom classes in the order specified by the keyword. Each of the remaining triples of real/real/integer modifiers give the half-amplitude, phase offset in degrees and periodicity of a particular improper torsional term, respectively. Periodicities through 3-fold are allowed for improper torsional parameters.

IMPTORSTERM [NONE/ONLY] This keyword controls use of the AMBER-style improper torsional angle potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

IMPTORSUNIT [real] Sets the scale factor needed to convert the energy value computed by the AMBER-style improper torsional angle potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default value of 1.0 is used, if the IMPTORSUNIT keyword is not given in the force field parameter file or the keyfile.

INACTIVE [integer list] Sets the list of inactive atoms during a TINKER computation. Individual potential energy terms are not computed when all atoms involved in the term are inactive. For Cartesian space calculations, inactive atoms are not allowed to move. For torsional space calculations, rotations are not allowed when there are inactive atoms on both sides of the rotated bond. Multiple INACTIVE lines can be present in the keyfile, and on each line the keyword can be followed by one or more atom numbers or ranges. If any INACTIVE keys are found, all atoms are set to active except those listed on the INACTIVE lines. The ACTIVE keyword overrides all INACTIVE keywords found in the keyfile.

INTEGRATE [VERLET/BEEMAN/STOCHASTIC/RIGIDBODY] Chooses the integration method for propagation of dynamics trajectories. The keyword is followed on the same line by the name of the option. Standard Newtonian MD can be run using either VERLET for the Velocity Verlet method, or BEEMAN for the velocity form of Bernie Brook's ``Better Beeman'' method. A Velocity Verlet-based stochastic dynamics trajectory is selected by the STOCHASTIC modifier. A rigid-body dynamics method is selected by the RIGIDBODY modifier. The default integration scheme is MD using the BEEMAN method.

INTMAX [integer] Sets the maximum number of interpolation cycles that will be allowed during the line search phase of an optimization. All gradient-based TINKER optimization routines use a common line search routine involving quadratic extrapolation and cubic interpolation. If the value of INTMAX is reached, an error status is set for the line search and the search is repeated with a much

smaller initial step size. The default value in the absence of this keyword is optimization routine dependent, but is usually in the range 5 to 10.

LAMBDA [real] This keyword sets the value of the λ path parameter for free energy perturbation calculations. The real number modifier specifies the position along the mutation path and must be a number in the range from 0 (initial state) to 1 (final state). The actual atoms involved in the mutation are given separately in individual MUTATE keyword lines.

LBFGS-VECTORS [integer] Sets the number of correction vectors used by the limited-memory L-BFGS optimization routine. The current maximum allowable value, and the default in the absence of the LBFGS-VECTORS keyword is 15.

LIGHTS This keyword turns on Method of Lights neighbor generation for the partial charge electrostatics and any of the van der Waals potentials. This method will yield identical energetic results to the standard double loop method. Method of Lights will be faster when the volume of a sphere with radius equal to the nonbond cutoff distance is significantly less than half the volume of the total system (*i.e.*, the full molecular system, the crystal unit cell or the periodic box). It requires less storage than pairwise neighbor lists.

LIST-BUFFER [real] Sets the size of the neighbor list buffer in Angstroms. This value is added to the actual cutoff distance to determine which pairs will be kept on the neighbor list. The same buffer value is used for all neighbor lists. The default value in the absence of 2.0 is used in the absence of the LIST-BUFFER keyword.

MAXITER [integer] Sets the maximum number of minimization iterations that will be allowed for any TINKER program that uses any of the nonlinear optimization routines. The default value in the absence of this keyword is program dependent, but is always set to a very large number.

METAL This keyword provides the values for a single transition metal ligand field parameter. ***Note this keyword is present in the code, but not active in the current version of TINKER.***

METALTERM [NONE/ONLY] This keyword controls use of the transition metal ligand field potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

MM2-STRBND This keyword switches the behavior of the stretch-bend potential function to match the formulation used by the MM2 force field. In MM2, stretching of bonds to attached hydrogen atoms is not including in computing the stretch-bend cross term energy. The default behavior in the absence of this keyword is to include stretching of attached hydrogen atoms as in the MM3 force field.

MPOLE-12-SCALE [real] This keyword provides a multiplicative scale factor that is applied to permanent atomic multipole electrostatic interactions between 1-2 connected atoms, *i.e.*, atoms that are directly bonded. The default value of 0.0 is used, if the MPOLE-12-SCALE keyword is not given in either the parameter file or the keyfile.

MPOLE-13-SCALE [real] This keyword provides a multiplicative scale factor that is applied to permanent atomic multipole electrostatic interactions between 1-3 connected atoms, *i.e.*, atoms separated by two covalent bonds. The default value of 0.0 is used, if the MPOLE-13-SCALE keyword is not given in either the parameter file or the keyfile.

MPOLE-14-SCALE [real] This keyword provides a multiplicative scale factor that is applied to permanent atomic multipole electrostatic interactions between 1-4 connected atoms, *i.e.*, atoms separated by three covalent bonds. The default value of 1.0 is used, if the MPOLE-14-SCALE keyword is not given in either the parameter file or the keyfile.

MPOLE-15-SCALE [real] This keyword provides a multiplicative scale factor that is applied to permanent atomic multipole electrostatic interactions between 1-5 connected atoms, *i.e.*, atoms separated by four covalent bonds. The default value of 1.0 is used, if the MPOLE-15-SCALE keyword is not given in either the parameter file or the keyfile.

MPOLE-CUTOFF [real] Sets the cutoff distance value in Angstroms for atomic multipole potential energy interactions. The energy for any pair of sites beyond the cutoff distance will be set to zero. Other keywords can be used to select a smoothing scheme near the cutoff distance. The default cutoff distance in the absence of the MPOLE-CUTOFF keyword is infinite for nonperiodic systems and 9.0 for periodic systems.

MPOLE-TAPER [real] This keyword allows modification of the cutoff window for atomic multipole potential energy interactions. It is similar in form and action to the TAPER keyword, except that its value applies only to the atomic multipole potential. The default value in the absence of the MPOLE-TAPER keyword is to begin the cutoff window at 0.65 of the corresponding cutoff distance.

MPOLETERM [NONE/ONLY] This keyword controls use of the atomic multipole electrostatics potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

MULTIPOLE [5 lines with: 3 or 4 integers & 1 real; 3 reals; 1 real; 2 reals; 3 reals] This keyword provides the values for a set of atomic multipole parameters at a single site. A complete keyword entry consists of three consequtive lines, the first line containing the MULTIPOLE keyword and the two following lines. The first line contains three integers which define the atom type on which the multipoles are centered, and the Z-axis and X-axis defining atom types for this center. The optional fourth integer contains the Y-axis defining atom type, and is only required for locally chiral multipole sites. The real number on the first line gives the monopole (atomic charge) in electrons. The second line contains three real numbers which give the X-, Y- and Z-components of the atomic dipole in electron-≈. The final three lines, consisting of one, two and three real numbers give the upper triangle of the traceless atomic quadrupole tensor in electron-$≈^2$.

MUTATE [3 integers] This keyword is used to specify atoms to be mutated during free energy perturbation calculations. The first integer modifier gives the atom number of an atom in the current system. The final two modifier values give the atom types corresponding the the $\lambda=0$ and $\lambda=1$ states of the specified atom.

MUTUAL-11-SCALE [real] This keyword provides a multiplicative scale factor that is applied to the induced (mutual) field due to atoms within a polarization group during an induced dipole calculation, *i.e.*, atoms that are in the same polarization group as the atom being polarized. The default value of 1.0 is used, if the MUTUAL-11-SCALE keyword is not given in either the parameter file or the keyfile.

MUTUAL-12-SCALE [real] This keyword provides a multiplicative scale factor that is applied to the induced (mutual) field due to atoms in 1-2 polarization groups during an induced dipole

calculation, *i.e.*, atoms that are in polarization groups directly connected to the group containing the atom being polarized. The default value of 1.0 is used, if the MUTUAL-12-SCALE keyword is not given in either the parameter file or the keyfile.

MUTUAL-13-SCALE [real] This keyword provides a multiplicative scale factor that is applied to the induced (mutual) field due to atoms in 1-3 polarization groups during an induced dipole calculation, *i.e.*, atoms that are in polarization groups separated by one group from the group containing the atom being polarized. The default value of 1.0 is used, if the MUTUAL-13-SCALE keyword is not given in either the parameter file or the keyfile.

MUTUAL-14-SCALE [real] This keyword provides a multiplicative scale factor that is applied to the induced (mutual) field due to atoms in 1-4 polarization groups during an induced dipole calculation, *i.e.*, atoms that are in polarization groups separated by two groups from the group containing the atom being polarized. The default value of 1.0 is used, if the MUTUAL-14-SCALE keyword is not given in either the parameter file or the keyfile.

NEIGHBOR-GROUPS This keyword causes the attached atom to be used in determining the charge-charge neighbor distance for all monovalent atoms in the molecular system. Its use causes all monovalent atoms to be treated the same as their attached atoms for purposes of including or scaling 1-2, 1-3 and 1-4 interactions. This option works only for the simple charge-charge electrostatic potential; it does not affect bond dipole or atomic multipole potentials. The NEIGHBOR-GROUPS scheme is similar to that used by some common force fields such as ENCAD.

NEIGHBOR-LIST This keyword turns on pairwise neighbor lists for partial charge electrostatics, polarize multipole electrostatics and any of the van der Waals potentials. This method will yield identical energetic results to the standard double loop method.

NEUTRAL-GROUPS This keyword causes the attached atom to be used in determining the charge-charge interaction cutoff distance for all monovalent atoms in the molecular system. Its use reduces cutoff discontinuities by avoiding splitting many of the largest charge separations found in typical molecules. Note that this keyword does not rigorously implement the usual concept of a ``neutral group'' as used in the literature with AMBER/OPLS and other force fields. This option works only for the simple charge-charge electrostatic potential; it does not affect bond dipole or atomic multipole potentials.

NEWHESS [integer] Sets the number of algorithmic iterations between recomputation of the Hessian matrix. At present this keyword applies exclusively to optimizations using the Truncated Newton method. The default value in the absence of this keyword is 1, *i.e.,* the Hessian is computed on every iteration.

NEXTITER [integer] Sets the iteration number to be used for the first iteration of the current computation. At present this keyword applies to optimization procedures where its use can effect convergence criteria, timing of restarts, and so forth. The default in the absence of this keyword is to take the initial iteration as iteration 1.

NOSE-MASS [real] This keyword sets the mass of particles making up the Nose-Hoover chain in that thermostating method. The default in the absence of the NOSE-MASS keyword is to use a mass of 0.1.

NOVERSION Turns off the use of version numbers appended to the end of filenames as the method for generating filenames for updated copies of an existing file. The presence of this keyword results in direct use of input file names without a search for the highest available version, and requires the

entry of specific output file names in many additional cases. By default, in the absence of this keyword, TINKER generates and attaches version numbers in a manner similar to the Digital OpenVMS operating system. For example, subsequent new versions of the file **molecule.xyz** would be written first to the file **molecule.xyz_2**, then to **molecule.xyz_3**, *etc*.

OCTAHEDRON Specifies that the periodic ``box'' is a truncated octahedron with maximal distance across the truncated octahedron as given by the A-AXIS keyword. All other unit cell and periodic box size-defining keywords are ignored if the OCTAHEDRON keyword is present.

OPBEND [2 integers & 1 real] This keyword provides the values for a single Allinger MM-style out-of-plane angle bending potential parameter. The first integer modifier is the atom class of the central trigonal atom and the second integer is the atom class of the out-of-plane atom. The real number modifier gives the force constant value for the out-of-plane angle. The default units for the force constant are kcal/mole/radian^2, but this can be controlled via the OPBENDUNIT keyword.

OPBENDTERM [NONE/ONLY] This keyword controls use of the Allinger MM-style out-of-plane bending potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

OPBENDUNIT [real] Sets the scale factor needed to convert the energy value computed by the Allinger MM-style out-of-plane bending potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default of $(\pi/180)^2$ = 0.0003046 is used, if the OPBENDUNIT keyword is not given in the force field parameter file or the keyfile.

OPDIST [4 integers & 1 real] This keyword provides the values for a single out-of-plane distance potential parameter. The first integer modifier is the atom class of the central trigonal atom and the three following integer modifiers are the atom classes of the three attached atoms. The real number modifier is the force constant for the harmonic function of the out-of-plane distance of the central atom. The default units for the force constant are kcal/mole/$\approx^2$, but this can be controlled via the OPDISTUNIT keyword.

OPDISTTERM [NONE/ONLY] This keyword controls use of the out-of-plane distance potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

OPDISTUNIT [real] Sets the scale factor needed to convert the energy value computed by the out-of-plane distance potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default value of 1.0 is used, if the OPDISTUNIT keyword is not given in the force field parameter file or the keyfile.

OVERWRITE Causes TINKER programs, such as minimizations, that output intermediate coordinate sets to create a single disk file for the intermediate results which is successively overwritten with the new intermediate coordinates as they become available. This keyword is essentially the opposite of the SAVECYCLE keyword.

PARAMETERS [file name] Provides the name of the force field parameter file to be used for the current TINKER calculation. The standard file name extension for parameter files, **.prm**, is an optional part of the file name modifier. The default in the absence of the PARAMETERS keyword is to

look for a parameter file with the same base name as the molecular system and ending in the **.prm** extension. If a valid parameter file is not found, the user will asked to provide a file name interactively.

PIATOM [1 integer & 3 reals] This keyword provides the values for the pisystem MO potential parameters for a single atom class belonging to a pisystem.

PIBOND [2 integers & 2 reals] This keyword provides the values for the pisystem MO potential parameters for a single type of pisystem bond.

PIBOND4 [2 integers & 2 reals] This keyword provides the values for the pisystem MO potential parameters for a single type of pisystem bond contained in a 4-membered ring.

PIBOND5 [2 integers & 2 reals] This keyword provides the values for the pisystem MO potential parameters for a single type of pisystem bond contained in a 5-membered ring.

PISYSTEM [integer list] This keyword sets the atoms within a molecule that are part of a conjugated π-system. The keyword is followed on the same line by a list of atom numbers and/or atom ranges that constitute the π-system. The Allinger MM force fields use this information to set up an MO calculation used to scale bond and torsion parameters involving π-system atoms.

PITORS [2 integers & 1 real] This keyword provides the values for a single pi-orbital torsional angle potential parameter. The two integer modifiers give the atom class numbers for the atoms involved in the central bond of the torsional angle to be parameterized. The real modifier gives the value of the 2-fold Fourier amplitude for the torsional angle between p-orbitals centered on the defined bond atom classes. The default units for the stretch-torsion force constant can be controlled via the PITORSUNIT keyword.

PITORSTERM [NONE/ONLY] This keyword controls use of the pi-orbital torsional angle potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

PITORSUNIT [real] Sets the scale factor needed to convert the energy value computed by the pi-orbital torsional angle potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default value of 1.0 is used, if the PITORSUNIT keyword is not given in the force field parameter file or the keyfile.

PME-GRID [3 integers] This keyword sets the dimensions of the charge grid used during particle mesh Ewald summation. The three modifiers give the size along the X-, Y- and Z-axes, respectively. If either the Y- or Z-axis dimensions are omitted, then they are set equal to the X-axis dimension. The default in the absence of the PME-GRID keyword is to set the grid size along each axis to the smallest power of 2, 3 and/or 5 which is at least as large as 1.5 times the axis length in Angstoms. Note that the FFT used by PME is not restricted to, but is most efficient for, grid sizes which are powers of 2, 3 and/or 5.

PME-ORDER [integer] This keyword sets the order of the B-spline interpolation used during particle mesh Ewald summation. A default value of 8 is used in the absence of the PME-ORDER keyword.

POLAR-12-SCALE [real] This keyword provides a multiplicative scale factor that is applied to polarization interactions between 1-2 polarization groups, *i.e.*, pairs of atoms that are in directly connected polarization groups. The default value of 0.0 is used, if the POLAR-12-SCALE keyword is not given in either the parameter file or the keyfile.

POLAR-13-SCALE [real] This keyword provides a multiplicative scale factor that is applied to polarization interactions between 1-3 polarization groups, *i.e.*, pairs of atoms that are in polarization groups separated by one other group. The default value of 0.0 is used, if the POLAR-13-SCALE keyword is not given in either the parameter file or the keyfile.

POLAR-14-SCALE [real] This keyword provides a multiplicative scale factor that is applied to polarization interactions between 1-4 polarization groups, *i.e.*, pairs of atoms that are in polarization groups separated by two other groups. The default value of 1.0 is used, if the POLAR-14-SCALE keyword is not given in either the parameter file or the keyfile.

POLAR-15-SCALE [real] This keyword provides a multiplicative scale factor that is applied to polarization interactions between 1-5 polarization groups, *i.e.*, pairs of atoms that are in polarization groups separated by three other groups. The default value of 1.0 is used, if the POLAR-15-SCALE keyword is not given in either the parameter file or the keyfile.

POLAR-DAMP [2 reals] Controls the strength of the damping function applied to induced dipoles and dipole polarization interaction energies. The first modifier sets the radius in Angstoms of a hypothetical atom with unit polarizability, while the second modifier sets the scale factor for the exponent of the damping function. The default values for the radius and the scale factor are 1.662 and 1.0, respectively. Damping is eliminated entirely by using this keyword to set the radius value to zero.

POLAR-EPS [real] This keyword sets the convergence criterion applied during computation of self-consistent induced dipoles. The calculation is deemed to have converged when the *rms* change (in Debyes) of the induced dipoles at all polarizable sites is less than the value specified with this keyword. The default value in the absence of the keyword is 10^{-6} Debyes.

POLAR-SOR [real] Sets a successive overrelaxation (SOR) factor for use in computation of induced atomic dipoles. Optimal values for this keyword will speed the induced dipole calculation, and poor values can result in convergence failure. The default value in the absence of the POLAR-SOR keyword is 0.7 which often a reasonable value when short-range intramolecular polarization is present. For models lacking intramolecular polarization, keyword values closer to 1.0 may be optimal.

POLARIZATION [DIRECT/MUTUAL] Selects between the use of direct and mutual dipole polarization for force fields that incorporate the polarization term. The DIRECT modifier avoids an iterative calculation by using only the permanent electric field in computation of induced dipoles. The MUTUAL option, which is the default in the absence of the POLARIZATION keyword, iterates the induced dipoles to self-consistency.

POLARIZE [1 integer, 1 real & up to 4 integers] This keyword provides the values for a single atomic dipole polarizability parameter. The integer modifier, if positive, gives the atom type number for which a polarizability parameter is to be defined. If the first integer modifier is negative, then the parameter value to follow applies only to the individual atom whose atom number is the negative of the modifier. The real number modifier gives the value of the dipole polarizability in $\approx^3$. The final integer modifiers list the atom type numbers of atoms directly bonded to the current atom and which will be considered to be part of the current atom's polarization group.

POLARIZETERM [NONE/ONLY] This keyword controls use of the atomic dipole polarization potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

POLYMER-CUTOFF [real] Sets the value of an additional cutoff parameter needed for infinite polymer systems. This value must be set to less than half the minimal periodic box dimension and should be greater than the largest possible interatomic distance that can be subject to scaling or exclusion as a local electrostatic or van der Waals interaction. The default in the absence of the POLYMER-CUTOFF keyword is 5.5 Angstroms.

PRINTOUT [integer] A general parameter for iterative procedures such as minimizations that sets the number of iterations between writes of status information to the standard output. The default value in the absence of the keyword is 1, *i.e.*, the calculation status is given every iteration.

RADIUSRULE [ARITHMETIC/GEOMETRIC/CUBIC-MEAN] Sets the functional form of the radius combining rule for heteroatomic van der Waals potential energy interactions. The default in the absence of the RADIUSRULE keyword is to use the arithmetic mean combining rule to get radii for heteroatomic interactions.

RADIUSSIZE [RADIUS/DIAMETER] Determines whether the atom size values given in van der Waals parameters read from VDW keyword statements are interpreted as atomic radius or diameter values. The default in the absence of the RADIUSSIZE keyword is to assume that vdw size parameters are given as radius values.

RADIUSTYPE [R-MIN/SIGMA] Determines whether atom size values given in van der Waals parameters read from VDW keyword statements are interpreted as potential minimum (R_{min}) or LJ-style sigma (σ) values. The default in the absence of the RADIUSTYPE keyword is to assume that vdw size parameters are given as R_{min} values.

RANDOMSEED [integer] Followed by an integer value, this keyword sets the initial seed value for the random number generator used by TINKER. Setting RANDOMSEED to the same value as an earlier run will allow exact reproduction of the earlier calculation. (Note that this will not hold across different machine types.) RANDOMSEED should be set to a positive integer less than about 2 billion. In the absence of the RANDOMSEED keyword the seed is chosen ``randomly'' based upon the number of seconds that have elapsed in the current decade.

RATTLE [BONDS/ANGLES/DIATOMIC/TRIATOMIC/WATER] Invokes the rattle algorithm, a velocity version of shake, on portions of a molecular system during a molecular dynamic calculation. The RATTLE keyword can be followed by any of the modifiers shown, in which case all occurrences of the modifier species are constrained at ideal values taken from the bond and angle parameters of the force field in use. In the absence of any modifier, RATTLE constrains all bonds to hydrogen atoms at ideal bond lengths.

RATTLE-DISTANCE [2 integers] This keyword allows the use of a ``Rattle'' constraint between the two atoms whose numbers are specified on the keyword line. If the two atoms are involved in a covalent bond, then their distance is constrained to the ideal bond length from the force field. For nonbonded atoms, the rattle constraint is fixed at their distance in the input coordinate file.

RATTLE-LINE [integer] This keyword

RATTLE-ORIGIN [integer] This keyword

RATTLE-PLANE [integer] This keyword

REACTIONFIELD [2 reals & 1 integer] This keyword provides parameters needed for the reaction field potential energy calculation. The two real modifiers give the radius of the dielectric cavity and the ratio of the bulk dielectric outside the cavity to that inside the cavity. The integer modifier gives the number of terms in the reaction field summation to be used. In the absence of the REACTIONFIELD keyword, the default values are a cavity of radius 1000000 ≈, a dielectric ratio of 80 and use of only the first term of the reaction field summation.

REDUCE [real] Specifies the fraction between zero and one by which the path between starting and final conformational state will be shortened at each major cycle of the transition state location algorithm implemented by the SADDLE program. This causes the path endpoints to move up and out of the terminal structures toward the transition state region. In favorable cases, a nonzero value of the REDUCE modifier can speed convergence to the transition state. The default value in the absence of the REDUCE keyword is zero.

RESTRAIN-ANGLE [3 integers & 3 reals] This keyword implements a flat-welled harmonic potential that can be used to restrain the angle between three atoms to lie within a specified angle range. The integer modifiers contain the atom numbers of the three atoms whose angle is to be restrained. The first real modifier is the force constant in kcal/degree^2 for the restraint. The last two real modifiers give the lower and upper bounds in degrees on the allowed angle values. If the angle lies between the lower and upper bounds, the restraint potential is zero. Outside the bounds, the harmonic restraint is applied. If the angle range modifiers are omitted, then the atoms are restrained to the angle found in the input structure. If the force constant is also omitted, a default value of 10.0 is used.

RESTRAIN-DISTANCE [2 integers & 3 reals] This keyword implements a flat-welled harmonic potential that can be used to restrain two atoms to lie within a specified distance range. The integer modifiers contain the atom numbers of the two atoms to be restrained. The first real modifier specifies the force constant in kcal/≈^{2} for the restraint. The next two real modifiers give the lower and upper bounds in ≈ngstroms on the allowed distance range. If the interatomic distance lies between these lower and upper bounds, the restraint potential is zero. Outside the bounds, the harmonic restraint is applied. If the distance range modifiers are omitted, then the atoms are restrained to the interatomic distance found in the input structure. If the force constant is also omitted, a default value of 100.0 is used.

RESTRAIN-GROUPS [2 integers & 3 reals] This keyword implements a flat-welled harmonic distance restraint between the centers-of-mass of two groups of atoms. The integer modifiers are the numbers of the two groups which must be defined separately via the GROUP keyword. The first real modifier is the force constant in kcal/≈^{2} for the restraint. The last two real modifiers give the lower and upper bounds in ≈ngstroms on the allowed intergroup center-of-mass distance values. If the distance range modifiers are omitted, then the groups are restrained to the distance found in the input structure. If the force constant is also omitted, a default value of 100.0 is used.

RESTRAIN-POSITION [1 integer & 5 reals] This keyword provides the ability to restrain an individual atom to a specified coordinate position. The initial integer modifier contains the atom number of the atom to be restrained. The first real modifier sets the force constant in kcal/≈^{2} for the harmonic restraint potential. The next three real number modifiers give the X-, Y- and Z-coordinates

to which the atom is tethered. The final real modifier defines a sphere around the specified coordinates within which the restraint value is zero. If the exclusion sphere radius is omitted, it is taken to be zero. If the coordinates are omitted, then the atom is restrained to the origin. If the force constant is also omitted, a default value of 100.0 is used.

RESTRAIN-TORSION [4 integers & 3 reals] This keyword implements a flat-welled harmonic potential that can be used to restrain the torsional angle between four atoms to lie within a specified angle range. The initial integer modifiers contains the atom numbers of the four atoms whose torsional angle, computed in the atom order listed, is to be restrained. The first real modifier gives a force constant in kcal/degree^2 for the restraint. The last two real modifiers give the lower and upper bounds in degrees on the allowed torsional angle values. The angle values given can wrap around across -180 and +180 degrees. Outside the allowed angle range, the harmonic restraint is applied. If the angle range modifiers are omitted, then the atoms are restrained to the torsional angle found in the input structure. If the force constant is also omitted, a default value of 1.0 is used.

RESTRAINTERM [NONE/ONLY] This keyword controls use of the restraint potential energy terms. In the absence of a modifying option, this keyword turns on use of these potentials. The NONE option turns off use of these potential energy terms. The ONLY option turns off all potential energy terms except for these terms.

RXNFIELDTERM [NONE/ONLY] This keyword controls use of the reaction field continuum solvation potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

SADDLEPOINT The presence of this keyword allows Newton-style second derivative-based optimization routine used by NEWTON, NEWTROT and other programs to converge to saddlepoints as well as minima on the potential surface. By default, in the absence of the SADDLEPOINT keyword, checks are applied that prevent convergence to stationary points having directions of negative curvature.

SAVE-CYCLE This keyword causes TINKER programs, such as minimizations, that output intermediate coordinate sets to save each successive set to the next consecutively numbered cycle file. The SAVE-CYCLE keyword is the opposite of the OVERWRITE keyword.

SAVE-FORCE This keyword causes TINKER molecular dynamics calculations to save the values of the force components on each atom to a separate cycle file. These files are written whenever the atomic coordinate snapshots are written during the dynamics run. Each atomic force file name contains as a suffix the cycle number followed by the letter **f**.

SAVE-INDUCED This keyword causes TINKER molecular dynamics calculations that involve polarizable atomic multipoles to save the values of the induced dipole components on each polarizable atom to a separate cycle file. These files are written whenever the atomic coordinate snapshots are written during the dynamics run. Each induced dipole file name contains as a suffix the cycle number followed by the letter **u**.

SAVE-VELOCITY This keyword causes TINKER molecular dynamics calculations to save the values of the velocity components on each atom to a separate cycle file. These files are written whenever the atomic coordinate snapshots are written during the dynamics run. Each velocity file name contains as a suffix the cycle number followed by the letter **v**.

SLOPEMAX [real] This keyword and its modifying value set the maximum allowed size of the ratio between the current and initial projected gradients during the line search phase of conjugate gradient or truncated Newton optimizations. If this ratio exceeds SLOPEMAX, then the initial step size is reduced by a factor of 10. The default value is usually set to 10000.0 when not specified via the SLOPEMAX keyword.

SMOOTHING [DEM/GDA/TOPHAT/STOPHAT] This keyword activates the potential energy smoothing methods. Several variations are available depending on the value of the modifier used: DEM= Diffusion Equation Method with a standard Gaussian kernel; GDA= Gaussian Density Annealing as proposed by the Straub group; TOPHAT= a local DEM-like method using a finite range ``tophat'' kernel; STOPHAT= shifted tophat smoothing.

SOLVATE [ASP/SASA/ONION/STILL/HCT/ACE/GBSA] Use of this keyword during energy calculations with any of the standard force fields turns on a continuum solvation free energy term. Several algorithms are available based on the modifier used: ASP= Eisenberg-McLachlan ASP method using the Wesson-Eisenberg vacuum-to-water parameters; SASA= the Ooi-Scheraga SASA method; ONION= the original 1990 Still ``Onion-shell'' GB/SA method; STILL= the 1997 analytical GB/SA method from Still's group; HCT= the pairwise descreening method of Hawkins, Cramer and Truhlar; ACE= the Analytical Continuum Electrostatics solvation method from the Karplus group; GBSA= equivalent to the STILL modifier. At present, GB/SA-style methods are only valid for force fields that use simple partial charge electrostatics.

SOLVATETERM [NONE/ONLY] This keyword controls use of the macroscopic solvation potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

SPACEGROUP [name] This keyword selects the space group to be used in manipulation of crystal unit cells and asymmetric units. The name option must be chosen from one of the following currently implemented space groups: P1, P1(-), P21, Cc, P21/a, P21/n, P21/c, C2/c, P212121, Pna21, Pn21a, Cmc21, Pccn, Pbcn, Pbca, P41, I41/a, P4(-)21c, P4(-)m2, R3c, P6(3)/mcm, Fm3(-)m, Im3(-)m.

SPHERE [4 reals, or 1 integer & 1 real] This keyword provides an alternative to the ACTIVE and INACTIVE keywords for specification of subsets of active atoms. If four real number modifiers are provided, the first three are taken as X-, Y- and Z-coordinates and the fourth is the radius of a sphere centered at these coordinates. In this case, all atoms within the sphere at the *start* of the calculation are active *throughout* the calculation, while all other atoms are inactive. Similarly if one integer and real number are given, an ``active'' sphere with radius set by the real is centered on the system atom with atom number given by the integer modifier. Multiple SPHERE keyword lines can be present in a single keyfile, and the list of active atoms specified by the spheres is cumulative.

STEEPEST-DESCENT This keyword forces the L-BFGS optimization routine used by the MINIMIZE program and other programs to perform steepest descent minimization. This option can be useful in conjunction with small step sizes for following minimum energy paths, but is generally inferior to the L-BFGS default for most optimization purposes.

STEPMAX [real] This keyword and its modifying value set the maximum size of an individual step during the line search phase of conjugate gradient or truncated Newton optimizations. The step size is computed as the norm of the vector of changes in parameters being optimized. The default value depends on the particular TINKER program, but is usually in the range from 1.0 to 5.0 when not specified via the STEPMAX keyword.

STEPMIN [real] This keyword and its modifying value set the minimum size of an individual step during the line search phase of conjugate gradient or truncated Newton optimizations. The step size is computed as the norm of the vector of changes in parameters being optimized. The default value is usually set to about 10^{-16} when not specified via the STEPMIN keyword.

STRBND [1 integer & 3 reals] This keyword provides the values for a single stretch-bend cross term potential parameter. The integer modifier gives the atom class number for the central atom of the bond angle involved in stretch-bend interactions. The real number modifiers give the force constant values to be used when the central atom of the angle is attached to 0, 1 or 2 additional hydrogen atoms, respectively. The default units for the stretch-bend force constant are kcal/mole/≈-degree, but this can be controlled via the STRBNDUNIT keyword.

STRBNDTERM [NONE/ONLY] This keyword controls use of the bond stretching-angle bending cross term potential energy. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

STRBNDUNIT [real] Sets the scale factor needed to convert the energy value computed by the bond stretching-angle bending cross term potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default value of 1.0 is used, if the STRBNDUNIT keyword is not given in the force field parameter file or the keyfile.

STRTORS [2 integers & 1 real] This keyword provides the values for a single stretch-torsion cross term potential parameter. The two integer modifiers give the atom class numbers for the atoms involved in the central bond of the torsional angles to be parameterized. The real modifier gives the value of the stretch-torsion force constant for all torsional angles with the defined central bond atom classes. The default units for the stretch-torsion force constant can be controlled via the STRTORUNIT keyword.

STRTORTERM [NONE/ONLY] This keyword controls use of the bond stretching-torsional angle cross term potential energy. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

STRTORUNIT [real] Sets the scale factor needed to convert the energy value computed by the bond stretching-torsional angle cross term potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default value of 1.0 is used, if the STRTORUNIT keyword is not given in the force field parameter file or the keyfile.

TAPER [real] This keyword allows modification of the cutoff windows for nonbonded potential energy interactions. The nonbonded terms are smoothly reduced from their standard value at the beginning of the cutoff window to zero at the far end of the window. The far end of the window is specified via the CUTOFF keyword or its potential function specific variants. The modifier value supplied with the TAPER keyword sets the beginning of the cutoff window. The modifier can be given either as an absolute distance value in Angstroms, or as a fraction between zero and one of the CUTOFF distance. The default value in the absence of the TAPER keyword ranges from 0.65 to 0.9 of the CUTOFF distance depending on the type of potential function. The windows are implemented via polynomial-based switching functions, in some cases combined with energy shifting.

TAU-PRESSURE [real] Sets the coupling time in picoseconds for the Groningen-style pressure bath coupling used to control the system pressure during molecular dynamics calculations. A default value of 2.0 is used for TAU-PRESSURE in the absence of the keyword.

TAU-TEMPERATURE [real] Sets the coupling time in picoseconds for the Groningen-style temperature bath coupling used to control the system temperature during molecular dynamics calculations. A default value of 0.1 is used for TAU-TEMPERATURE in the absence of the keyword.

THERMOSTAT [BERENDSEN/ANDERSEN] This keyword selects a thermostat algorithm for use during molecular dynamics. Two modifiers are available, a Berendsen bath coupling method, and an Andersen stochastic collision method. The default in the absence of the THERMOSTAT keyword is to use the BERENDSEN algorithm.

TORSION [4 integers & up to 6 real/real/integer triples] This keyword provides the values for a single torsional angle parameter. The first four integer modifiers give the atom class numbers for the atoms involved in the torsional angle to be defined. Each of the remaining triples of real/real/integer modifiers give the amplitude, phase offset in degrees and periodicity of a particular torsional function term, respectively. Periodicities through 6-fold are allowed for torsional parameters.

TORSION4 [4 integers & up to 6 real/real/integer triples] This keyword provides the values for a single torsional angle parameter specific to atoms in 4-membered rings. The first four integer modifiers give the atom class numbers for the atoms involved in the torsional angle to be defined. The remaining triples of real number and integer modifiers operate as described above for the TORSION keyword.

TORSION5 [4 integers & up to 6 real/real/integer triples] This keyword provides the values for a single torsional angle parameter specific to atoms in 5-membered rings. The first four integer modifiers give the atom class numbers for the atoms involved in the torsional angle to be defined. The remaining triples of real number and integer modifiers operate as described above for the TORSION keyword.

TORSIONTERM [NONE/ONLY] This keyword controls use of the torsional angle potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

TORSIONUNIT [real] Sets the scale factor needed to convert the energy value computed by the torsional angle potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default value of 1.0 is used, if the TORSIONUNIT keyword is not given in the force field parameter file or the keyfile.

TORTOR [7 integers, then multiple lines of 2 integers and 1 real] This keyword is used to provide the values for a single torsion-torsion parameter. The first five integer modifiers give the atom class numbers for the atoms involved in the two adjacent torsional angles to be defined. The last two integer modifiers contain the number of data grid points that lie along each axis of the torsion-torsion map. For example, this value will be 13 for a 30 degree torsional angle spacing, *i.e.*, 360/30 = 12, but 13 values are required since data values for -180 and +180 degrees must both be supplied. The subsequent lines contain the torsion-torsion map data as the integer values in degrees of each torsional angle and the target energy value in kcal/mole.

TORTORTERM [NONE/ONLY] This keyword controls use of the torsion-torsion potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

TORTORUNIT [real] Sets the scale factor needed to convert the energy value computed by the torsion-torsion potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default value of 1.0 is used, if the TORTORUNIT keyword is not given in the force field parameter file or the keyfile.

TRIAL-DISTANCE [CLASSIC/RANDOM/TRICOR/HAVEL integer/PAIRWISE integer] Sets the method for selection of a trial distance matrix during distance geometry computations. The keyword takes a modifier that selects the method to be used. The HAVEL and PAIRWISE modifiers also require an additional integer value that specifies the number of atoms used in metrization and the percentage of metrization, respectively. The default in the absence of this keyword is to use the PAIRWISE method with 100 percent metrization. Further information on the various methods is given with the description of the TINKER distance geometry program.

TRIAL-DISTRIBUTION [real] Sets the initial value for the mean of the Gaussian distribution used to select trial distances between the lower and upper bounds during distance geometry computations. The value given must be between 0 and 1 which represent the lower and upper bounds respectively. This keyword is rarely needed since TINKER will usually be able to choose a reasonable value by default.

TRUNCATE Causes all distance-based nonbond energy cutoffs to be sharply truncated to an energy of zero at distances greater than the value set by the cutoff keyword(s) without use of any shifting, switching or smoothing schemes. At all distances within the cutoff sphere, the full interaction energy is computed.

UREY-CUBIC [real] Sets the value of the cubic term in the Taylor series expansion form of the Urey-Bradley potential energy. The real number modifier gives the value of the coefficient as a multiple of the quadratic coefficient. The default value in the absence of the UREY-CUBIC keyword is zero; *i.e.*, the cubic Urey-Bradley term is omitted.

UREY-QUARTIC [real] Sets the value of the quartic term in the Taylor series expansion form of the Urey-Bradley potential energy. The real number modifier gives the value of the coefficient as a multiple of the quadratic coefficient. The default value in the absence of the UREY-QUARTIC keyword is zero; *i.e.*, the quartic Urey-Bradley term is omitted.

UREYBRAD [3 integers & 2 reals] This keyword provides the values for a single Urey-Bradley cross term potential parameter. The integer modifiers give the atom class numbers for the three kinds of atoms involved in the angle for which a Urey-Bradley term is to be defined. The real number modifiers give the force constant value for the term and the target value for the 1-3 distance in ≈. The default units for the force constant are kcal/mole/$\approx^2$, but this can be controlled via the UREYUNIT keyword.

UREYTERM [NONE/ONLY] This keyword controls use of the Urey-Bradley potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

UREYUNIT [real] Sets the scale factor needed to convert the energy value computed by the Urey-Bradley potential into units of kcal/mole. The correct value is force field dependent and typically provided in the header of the master force field parameter file. The default value of 1.0 is used, if the UREYUNIT keyword is not given in the force field parameter file or the keyfile.

VDW [1 integer & 3 reals] This keyword provides values for a single van der Waals parameter. The integer modifier, if positive, gives the atom class number for which vdw parameters are to be defined. Note that vdw parameters are given for atom classes, not atom types. The three real number modifiers give the values of the atom size in ≈, homoatomic well depth in kcal/mole, and an optional reduction factor for univalent atoms.

VDW-12-SCALE [real] This keyword provides a multiplicative scale factor that is applied to van der Waals potential interactions between 1-2 connected atoms, *i.e.*, atoms that are directly bonded. The default value of 0.0 is used, if the VDW-12-SCALE keyword is not given in either the parameter file or the keyfile.

VDW-13-SCALE [real] This keyword provides a multiplicative scale factor that is applied to van der Waals potential interactions between 1-3 connected atoms, *i.e.*, atoms separated by two covalent bonds. The default value of 0.0 is used, if the VDW-13-SCALE keyword is not given in either the parameter file or the keyfile.

VDW-14-SCALE [real] This keyword provides a multiplicative scale factor that is applied to van der Waals potential interactions between 1-4 connected atoms, *i.e.*, atoms separated by three covalent bonds. The default value of 1.0 is used, if the VDW-14-SCALE keyword is not given in either the parameter file or the keyfile.

VDW-15-SCALE [real] This keyword provides a multiplicative scale factor that is applied to van der Waals potential interactions between 1-5 connected atoms, *i.e.*, atoms separated by four covalent bonds. The default value of 1.0 is used, if the VDW-15-SCALE keyword is not given in either the parameter file or the keyfile.

VDW-CUTOFF [real] Sets the cutoff distance value in Angstroms for van der Waals potential energy interactions. The energy for any pair of van der Waals sites beyond the cutoff distance will be set to zero. Other keywords can be used to select a smoothing scheme near the cutoff distance. The default cutoff distance in the absence of the VDW-CUTOFF keyword is infinite for nonperiodic systems and 9.0 for periodic systems.

VDW-TAPER [real] This keyword allows modification of the cutoff windows for van der Waals potential energy interactions. It is similar in form and action to the TAPER keyword, except that its value applies only to the vdw potential. The default value in the absence of the VDW-TAPER keyword is to begin the cutoff window at 0.9 of the vdw cutoff distance.

VDW14 [1 integer & 2 reals] This keyword provides values for a single van der Waals parameter for use in 1-4 nonbonded interactions. The integer modifier, if positive, gives the atom class number for which vdw parameters are to be defined. Note that vdw parameters are given for atom classes, not atom types. The two real number modifiers give the values of the atom size in ≈ and the homoatomic well depth in kcal/mole. Reduction factors, if used, are carried over from the VDW keyword for the same atom class.

VDWPR [2 integers & 2 reals] This keyword provides the values for the vdw parameters for a single special heteroatomic pair of atoms. The integer modifiers give the pair of atom class numbers

for which special vdw parameters are to be defined. The two real number modifiers give the values of the minimum energy contact distance in ≈ and the well depth at the minimum distance in kcal/mole.

VDWTERM [NONE/ONLY] This keyword controls use of the van der Waals repulsion-dispersion potential energy term. In the absence of a modifying option, this keyword turns on use of the potential. The NONE option turns off use of this potential energy term. The ONLY option turns off all potential energy terms except for this one.

VDWTYPE [LENNARD-JONES / BUCKINGHAM / BUFFERED-14-7 / MM3-HBOND / GAUSSIAN] Sets the functional form for the van der Waals potential energy term. The text modifier gives the name of the functional form to be used. The GAUSSIAN modifier value implements a two or four Gaussian fit to the corresponding Lennard-Jones function for use with potential energy smoothing schemes. The default in the absence of the VDWTYPE keyword is to use the standard two parameter Lennard-Jones function.

VERBOSE Turns on printing of secondary and informational output during a variety of TINKER computations; a subset of the more extensive output provided by the DEBUG keyword.

WALL [real] Sets the radius of a spherical boundary used to maintain droplet boundary conditions. The real modifier specifies the desired approximate radius of the droplet. In practice, an artificial van der Waals wall is constructed at a fixed buffer distance of 2.5 ≈ outside the specified radius. The effect is that atoms which attempt to move outside the region defined by the droplet radius will be forced toward the center.

WRITEOUT [integer] A general parameter for iterative procedures such as minimizations that sets the number of iterations between writes of intermediate results (such as the current coordinates) to disk file(s). The default value in the absence of the keyword is 1, *i.e.*, the intermediate results are written to file on every iteration. Whether successive intermediate results are saved to new files or replace previously written intermediate results is controlled by the OVERWRITE and SAVE-CYCLE keywords.

8. Force Field Parameter Sets

The TINKER package is distributed with several force field parameter sets, implementing a selection of widely used literature force fields as well as the TINKER force field currently under construction in the Ponder lab. We try to exactly reproduce the intent of the original authors of our distributed, third-party force fields. In all cases the parameter sets have been validated against literature reports, results provided by the original developers, or calculations made with the authentic programs. With the few exceptions noted below, TINKER calculations can be treated as authentic results from the genuine force fields. A brief description of each parameter set, including some still in preparation and not distributed with the current version, is provided below with lead literature references for the force field:

AMOEBA.PRM

Parameters for the AMOEBA polarizable atomic multipole force field. As of the current TINKER release, we have completed parametrization for a number of ions and small organic molecules. For further information, or if you are interested in developing or testing parameters for other small molecules, please contact the Ponder lab.

P. Ren and J. W. Ponder, A Consistent Treatment of Inter- and Intramolecular Polarization in Molecular Mechanics Calculations, ***J. Comput. Chem.***, *23*, 1497-1506 (2002)

P. Ren and J. W. Ponder, Polarizable Atomic Multipole Water Model for Molecular Mechanics Simulation, ***J. Phys. Chem. B***, *107*, 5933-5947 (2003)

P. Ren and J. W. Ponder, Ion Solvation Thermodynamics from Simulation with a Polarizable Force Field, A. Grossfield, ***J. Am. Chem. Soc.***, *125*, 15671-15682 (2003)

AMOEBAPRO.PRM

Preliminary protein parameters for the AMOEBA polarizable atomic multipole force field. While the distributed parameters are still subject to minor alteration as we continue validation, they are now stable enough for other groups to begin using them. For further information, or if you are interested in testing the protein parameter set, please contact the Ponder lab.

J. W. Ponder and D. A. Case, Force Fields for Protein Simulation, ***Adv. Prot. Chem.***, *66*, 27-85 (2003)

P. Ren and J. W. Ponder, Polarizable Atomic Multipole-based Potential for Proteins: Model and Parameterization, *in preparation*

AMBER94.PRM

AMBER *ff94* parameters for proteins and nucleic acids. Note that with their ``Cornell'' force field, the Kollman group has devised separate, fully independent partial charge values for each of the N- and C-terminal amino acid residues. At present, the terminal residue charges for TINKER's version maintain the correct formal charge, but redistributed somewhat at the alpha carbon atoms from the original Kollman group values. The total magnitude of the redistribution is less than 0.01 electrons in most cases.

W. D. Cornell, P. Cieplak, C. I. Bayly, I. R. Gould, K. M. Merz, Jr., D. M. Ferguson, D. C. Spellmeyer, T. Fox, J. W. Caldwell and P. A. Kollman, A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules, ***J. Am. Chem. Soc.***, *117*, 5179-5197 (1995) [*ff*94]

G. Moyna, H. J. Williams, R. J. Nachman and A. I. Scott, Conformation in Solution and Dynamics of a Structurally Constrained Linear Insect Kinin Pentapeptide Analogue, ***Biopolymers***, *49*, 403-413 (1999) [AIB charges]

W. S. Ross and C. C. Hardin, Ion-Induced Stabilization of the G-DNA Quadruplex: Free Energy Perturbation Studies, ***J. Am. Chem. Soc.***, *116*, 4363-4366 (1994) [alkali metal ions]

J. Aqvist, Ion-Water Interaction Potentials Derived from Free Energy Perturbation Simulations, ***J. Phys. Chem.***, *94*, 8021-8024, 1990 [alkaline earth Ions, radii adapted for Amber combining rule]

Current force field parameter values and suggested procedures for development of parameters for additional molecules are available from the Amber web site in the Case lab at Scripps, http://amber.scripps.edu/

AMBER96.PRM

AMBER *ff96* parameters for proteins and nucleic acids. The only change from the *ff94* parameter set is in the torsional parameters for the protein phi/psi angles. These values were altered to give better agreement with changes of *ff96* with LMP2 QM results from the Friesner lab on alanine dipeptide and tetrapeptide.

P. Kollman, R. Dixon, W. Cornell, T. Fox, C. Chipot and A. Pohorille, The Development/ Application of a 'Minimalist' Organic/Biochemical Molecular Mechanic Force Field using a Combination of *ab Initio* Calculations and Experimental Data, in **Computer Simulation of Biomolecular Systems**, W. F. van Gunsteren, P. K. Weiner, A. J. Wilkinson, eds., Volume 3, 83-96 (1997) [*ff*96]

Current force field parameter values and suggested procedures for development of parameters for additional molecules are available from the Amber web site in the Case lab at Scripps, http://amber.scripps.edu/

AMBER98.PRM

AMBER *ff98* parameters for proteins and nucleic acids. The only change from the *ff94* parameter set is in the glycosidic torsional parameters that control sugar pucker.

T. E. Cheatham III, P. Cieplak and P. A. Kollman, A Modified Version of the Cornell et al. Force Field with Improved Sugar Pucker Phases and Helical Repeat, ***J. Biomol. Struct. Dyn.***, *16*, 845-862 (1999)

Current force field parameter values and suggested procedures for development of parameters for additional molecules are available from the Amber web site in the Case lab at Scripps, http://amber.scripps.edu/

AMBER99.PRM

AMBER *ff99* parameters for proteins and nucleic acids. The original partial charges from the *ff94* parameter set are retained, but many of the bond, angle and torsional parameters have been revised to provide better general agreement with experiment.

J. Wang, P. Cieplak and P. A. Kollman, How Well Does a Restrained Electrostatic Potential (RESP) Model Perform in Calcluating Conformational Energies of Organic and Biological Molecules?, ***J. Comput. Chem.***, *21*, 1049-1074 (2000)

Current force field parameter values and suggested procedures for development of parameters for additional molecules are available from the Amber web site in the Case lab at Scripps, http://amber.scripps.edu/

CHARMM19.PRM

CHARMM19 united-atom parameters for proteins. The nucleic acid parameter are not yet implemented. There are some differences between authentic CHARMM19 and the TINKER version due to replacement of CHARMM impropers by torsions for cases that involve atoms not bonded to the trigonal atom and TINKER's use of all possible torsions across a bond instead of a single torsion per bond.

E. Neria, S. Fischer and M. Karplus, Simulation of Activation Free Energies in Molecular Systems, ***J. Chem. Phys.***, *105*, 1902-1921 (1996)

L. Nilsson and M. Karplus, Empirical Energy Functions for Energy Minimizations and Dynamics of Nucleic Acids, ***J. Comput. Chem.***, *7*, 591-616 (1986)

W. E. Reiher III, Theoretical Studies of Hydrogen Bonding, Ph.D. Thesis, Department of Chemistry, Harvard University, Cambridge, MA, 1985

CHARMM22.PRM

CHARMM27 all-atom parameters for proteins and lipids. Most of the nucleic acid and small model compound parameters are not yet implemented. We plan to provide these additional parameters in due course.

N. Foloppe and A. D. MacKerell, Jr., All-Atom Empirical Force Field for Nucleic Acids: 1) Parameter Optimization Based on Small Molecule and Condensed Phase Macromolecular Target Data, ***J. Comput. Chem.***, *21*, 86-104 (2000) [CHARMM27]

N. Banavali and A. D. MacKerell, Jr., All-Atom Empirical Force Field for Nucleic Acids: 2) Application to Molecular Dynamics Simulations of DNA and RNA in Solution, ***J. Comput. Chem.***, *21*, 105-120 (2000)

A. D. MacKerrell, Jr., *et al.*, All-Atom Empirical Potential for Molecular Modeling and Dynamics Studies of Proteins, ***J. Phys. Chem. B***, *102*, 3586-3616 (1998) [CHARMM22]

A. D. MacKerell, Jr., J. Wiorkeiwicz-Kuczera and M. Karplus, An All-Atom Empirical Energy Function for the Simulation of Nucleic Acids, ***J. Am. Chem. Soc.***, *117*, 11946-11975 (1995)

S. E. Feller, D. Yin, R. W. Pastor and A. D. MacKerell, Jr., Molecular Dynamics Simulation of Unsaturated Lipids at Low Hydration: Parametrization and Comparison with Diffraction Studies, ***Biophysical Journal***, *73*, 2269-2279 (1997) [alkenes]

R. H. Stote and M. Karplus, Zinc Binding in Proteins and Solution - A Simple but Accurate Nonbonded Representation, ***Proteins***, *23*, 12-31 (1995) [zinc ion]

Current and legacy parameter values are available from the CHARMM force field web site on Alex MacKerell's Research Interests page at the University of Maryland School of Pharmacy, https://rxsecure.umaryland.edu/research/amackere/research.html/

DUDEK.PRM

Protein-only parameters for the early 1990's TINKER force field with multipole values of Dudek and Ponder. The current file contains only the multipole values from the 1995 paper by Dudek and Ponder. This set is now superceeded by the more recent TINKER force field developed by Pengyu Ren (see WATER.PRM, below).

M. J. Dudek and J. W. Ponder, Accurate Electrostatic Modelling of the Intramolecular Energy of Proteins, ***J. Comput. Chem.***, *16*, 791-816 (1995)

ENCAD.PRM

ENCAD parameters for proteins and nucleic acids. (*in preparation*)

M. Levitt, M. Hirshberg, R. Sharon and V. Daggett, Potential Energy Function and Parameters for Simulations of the Molecular Dynamics of Protein and Nucleic Acids in Solution, ***Comp. Phys. Commun.***, *91*, 215-231 (1995)

M. Levitt, M. Hirshberg, R. Sharon, K. E. Laidig and V. Daggett, Calibration and Testing of a Water Model for Simulation of the Molecular Dynamics of Protein and Nucleic Acids in Solution, ***J. Phys. Chem. B***, *101*, 5051-5061 (1997) [F3C water]

HOCH.PRM

Simple NMR-NOE force field of Hoch and Stern.

J. C. Hoch and A. S. Stern, A Method for Determining Overall Protein Fold from NMR Distance Restraints, ***J. Biomol. NMR***, *2*, 535-543 (1992)

MM2.PRM

Full MM2(1991) parameters including π-systems. The anomeric and electronegativity correction terms included in some later versions of MM2 are not implemented.

N. L. Allinger, Conformational Analysis. 130. MM2. A Hydrocarbon Force Field Utilizing V1 and V2 Torsional Terms, ***J. Am. Chem. Soc.***, *99*, 8127-8134 (1977)

J. T. Sprague, J. C. Tai, Y. Yuh and N. L. Allinger, The MMP2 Calculational Method, ***J. Comput. Chem.***, *8*, 581-603 (1987)

J. C. Tai and N. L. Allinger, Molecular Mechanics Calculations on Conjugated Nitrogen-Containing Heterocycles, ***J. Am. Chem. Soc.***, *110*, 2050-2055 (1988)

J. C. Tai, J.-H. Lii and N. L. Allinger, A Molecular Mechanics (MM2) Study of Furan, Thiophene, and Related Compounds, ***J. Comput. Chem.***, *10*, 635-647 (1989)

N. L. Allinger, R. A. Kok and M. R. Imam, Hydrogen Bonding in MM2, ***J. Comput. Chem.***, *9*, 591-595 (1988)

L. Norskov-Lauritsen and N. L. Allinger, A Molecular Mechanics Treatment of the Anomeric Effect, ***J. Comput. Chem.***, *5*, 326-335 (1984)

All parameters distributed with TINKER are from the ``MM2 (1991) Parameter Set'', as provided by N. L. Allinger, University of Georgia

MM3.PRM

Full MM3(2000) parameters including pi-systems. The directional hydrogen bonding term and electronegativity bond length corrections are implemented, but the anomeric and Bohlmann correction terms are not implemented.

N. L. Allinger, Y. H. Yuh and J.-H. Lii, Molecular Mechanics. The MM3 Force Field for Hydrocarbons. 1, ***J. Am. Chem. Soc.***, *111*, 8551-8566 (1989)

J.-H. Lii and N. L. Allinger, Molecular Mechanics. The MM3 Force Field for Hydrocarbons. 2. Vibrational Frequencies and Thermodynamics, ***J. Am. Chem. Soc.***, *111*, 8566-8575 (1989)

J.-H. Lii and N. L. Allinger, Molecular Mechanics. The MM3 Force Field for Hydrocarbons. 3. The van der Waals' Potentials and Crystal Data for Aliphatic and Aromatic Hydrocarbons, ***J. Am. Chem. Soc.***, 111, 8576-8582 (1989)

N. L. Allinger, H. J. Geise, W. Pyckhout, L. A. Paquette and J. C. Gallucci, Structures of Norbornane and Dodecahedrane by Molecular Mechanics Calculations (MM3), X-ray Crystallography, and Electron Diffraction, ***J. Am. Chem. Soc.***, *111*, 1106-1114 (1989) [stretch-torsion cross term]

N. L. Allinger, F. Li and L. Yan, Molecular Mechanics. The MM3 Force Field for Alkenes, ***J. Comput. Chem.***, *11*, 848-867 (1990)

N. L. Allinger, F. Li, L. Yan and J. C. Tai, Molecular Mechanics (MM3) Calculations on Conjugated Hydrocarbons, ***J. Comput. Chem.***, *11*, 868-895 (1990)

J.-H. Lii and N. L. Allinger, Directional Hydrogen Bonding in the MM3 Force Field. I, ***J. Phys. Org. Chem.***, *7*, 591-609 (1994)

J.-H. Lii and N. L. Allinger, Directional Hydrogen Bonding in the MM3 Force Field. II, ***J. Comput. Chem.***, *19*, 1001-1016 (1998)

All parameters distributed with TINKER are from the ``MM3 (2000) Parameter Set'', as provided by N. L. Allinger, University of Georgia, August 2000

MM3PRO.PRM

Protein-only version of the MM3 parameters.

J.-H. Lii and N. L. Allinger, The MM3 Force Field for Amides, Polypeptides and Proteins, ***J. Comput. Chem.***, *12*, 186-199 (1991)

OPLSUA.PRM

Complete OPLS-UA with united-atom parameters for proteins and many classes of organic molecules. Explicit hydrogens on polar atoms and aromatic carbons.

W. L. Jorgensen and J. Tirado-Rives, The OPLS Potential Functions for Proteins. Energy Minimizations for Crystals of Cyclic Peptides and Crambin, ***J. Am. Chem. Soc.***, *110*, 1657-1666 (1988) [peptide and proteins]

W. L. Jorgensen and D. L. Severance, Aromatic-Aromatic Interactions: Free Energy Profiles for the Benzene Dimer in Water, Chloroform, and Liquid Benzene, ***J. Am. Chem. Soc.***, *112*, 4768-4774 (1990) [aromatic hydrogens]

S. J. Weiner, P. A. Kollman, D. A. Case, U. C. Singh, C. Ghio, G. Alagona, S. Profeta, Jr. and P. Weiner, A New Force Field for Molecular Mechanical Simulation of Nucleic Acids and Proteins, ***J. Am. Chem. Soc.***, *106*, 765-784 (1984) [united-atom ``AMBER/OPLS'' local geometry]

S. J. Weiner, P. A. Kollman, D. T. Nguyen and D. A. Case, An All Atom Force Field for Simulations of Proteins and Nucleic Acids, ***J. Comput. Chem.***, *7*, 230-252 (1986) [all-atom "AMBER/OPLS" local geometry]

L. X. Dang and B. M. Pettitt, Simple Intramolecular Model Potentials for Water, ***J. Phys. Chem.***, *91*, 3349-3354 (1987) [flexible TIP3P and SPC water]

W. L. Jorgensen, J. D. Madura and C. J. Swenson, Optimized Intermolecular Potential Functions for Liquid Hydrocarbons, ***J. Am. Chem. Soc.***, *106*, 6638-6646 (1984) [hydrocarbons]

W. L. Jorgensen, E. R. Laird, T. B. Nguyen and J. Tirado-Rives, Monte Carlo Simulations of Pure Liquid Substituted Benzenes with OPLS Potential Functions, ***J. Comput. Chem.***, *14*, 206-215 (1993) [substituted benzenes]

E. M. Duffy, P. J. Kowalczyk and W. L. Jorgensen, Do Denaturants Interact with Aromatic Hydrocarbons in Water?, ***J. Am. Chem. Soc.***, *115*, 9271-9275 (1993) [benzene, naphthalene, urea, guanidinium, tetramethyl ammonium]

W. L. Jorgensen and C. J. Swenson, Optimized Intermolecular Potential Functions for Amides and Peptides. Structure and Properties of Liquid Amides, ***J. Am. Chem. Soc.***, *106*, 765-784 (1984) [amides]

W. L. Jorgensen, J. M. Briggs and M. L. Contreras, Relative Partition Coefficients for Organic Solutes form Fluid Simulations, ***J. Phys. Chem.***, *94*, 1683-1686 (1990) [chloroform, pyridine, pyrazine, pyrimidine]

J. M. Briggs, T. B. Nguyen and W. L. Jorgensen, Monte Carlo Simulations of Liquid Acetic Acid and Methyl Acetate with the OPLS Potential Functions, ***J. Phys. Chem.***, *95*, 3315-3322 (1991) [acetic acid, methyl acetate]

H. Liu, F. Muller-Plathe and W. F. van Gunsteren, A Force Field for Liquid Dimethyl Sulfoxide and Physical Properties of Liquid Dimethyl Sulfoxide Calculated Using Molecular Dynamics Simulation, ***J. Am. Chem. Soc.***, *117*, 4363-4366 (1995) [dimethyl sulfoxide]

J. Gao, X. Xia and T. F. George, Importance of Bimolecular Interactions in Developing Empirical Potential Functions for Liquid Ammonia, ***J. Phys. Chem.***, *97*, 9241-9246 (1993) [ammonia]

J. Aqvist, Ion-Water Interaction Potentials Derived from Free Energy Perturbation Simulations, ***J. Phys. Chem.***, *94*, 8021-8024 (1990) [metal ions]

W. S. Ross and C. C. Hardin, Ion-Induced Stabilization of the G-DNA Quadruplex: Free Energy Perturbation Studies, ***J. Am. Chem. Soc.***, *116*, 4363-4366 (1994) [alkali metal ions]

J. Chandrasekhar, D. C. Spellmeyer and W. L. Jorgensen, Energy Component Analysis for Dilute Aqueous Solutions of Li+, Na+, F-, and Cl- Ions, ***J. Am. Chem. Soc.***, *106*, 903-910 (1984) [halide ions]

Most parameters distributed with TINKER are from ``OPLS and OPLS-AA Parameters for Organic Molecules, Ions, and Nucleic Acids'' as provided by W. L. Jorgensen, Yale University, October 1997

OPLSAA.PRM

OPLS-AA force field with all-atom parameters for proteins and many general classes of organic molecules.

W. L. Jorgensen, D. S. Maxwell and J. Tirado-Rives, Development and Testing of the OPLS All-Atom Force Field on Conformational Energetics and Properties of Organic Liquids, ***J. Am. Chem. Soc.***, *117*, 11225-11236 (1996)

D. S. Maxwell, J. Tirado-Rives and W. L. Jorgensen, A Comprehensive Study of the Rotational Energy Profiles of Organic Systems by *Ab Initio* MO Theory, Forming a Basis for Peptide Torsional Parameters, ***J. Comput. Chem.***, *16*, 984-1010 (1995)

W. L. Jorgensen and N. A. McDonald, Development of an All-Atom Force Field for Heterocycles. Properties of Liquid Pyridine and Diazenes, ***THEOCHEM-J. Mol. Struct.***, *424*, 145-155 (1998)

N. A. McDonald and W. L. Jorgensen, Development of an All-Atom Force Field for Heterocycles. Properties of Liquid Pyrrole, Furan, Diazoles, and Oxazoles, ***J. Phys. Chem. B***, *102*, 8049-8059 (1998)

R. C. Rizzo and W. L. Jorgensen, OPLS All-Atom Model for Amines: Resolution of the Amine Hydration Problem, ***J. Am. Chem. Soc.***, *121*, 4827-4836 (1999)

M. L. P. Price, D. Ostrovsky and W. L. Jorgensen, Gas-Phase and Liquid-State Properties of Esters, Nitriles, and Nitro Compounds with the OPLS-AA Force Field, ***J. Comput. Chem.***, *22*, 1340-1352 (2001)

All parameters distributed with TINKER are from ``OPLS and OPLS-AA Parameters for Organic Molecules, Ions, and Nucleic Acids'' as provided by W. L. Jorgensen, Yale University, October 1997

OPLSAAL.PRM

An improved OPLS-AA parameter set for proteins in which the only change is a reworking of many of the backbone and sidechain torsional parameters to give better agreement with LMP2 QM calculations. This parameter set is also known as OPLS(2000).

G. A. Kaminsky, R. A. Friesner, J. Tirado-Rives and W. L. Jorgensen, Evaluation and Reparametrization of the OPLS-AA Force Field for Proteins via Comparison with Accurate Quantum Chemical Calculations on Peptides, ***J. Phys. Chem. B***, *105*, 6474-6487 (2001)

SMOOTH.PRM

Version of OPLS-UA for use with potential smoothing. Largely adapted largely from standard OPLS-UA parameters with modifications to the vdw and improper torsion terms.

R. V. Pappu, R. K. Hart and J. W. Ponder, Analysis and Application of Potential Energy Smoothing and Search Methods for Global Optimization, ***J. Phys, Chem. B***, *102*, 9725-9742 (1998) [smoothing modifications]

SMOOTHAA.PRM

Version of OPLS-AA for use with potential smoothing. Largely adapted largely from standard OPLS-AA parameters with modifications to the vdw and improper torsion terms.

R. V. Pappu, R. K. Hart and J. W. Ponder, Analysis and Application of Potential Energy Smoothing and Search Methods for Global Optimization, ***J. Phys, Chem. B***, *102*, 9725-9742 (1998) [smoothing modifications]

WATER.PRM

The AMOEBA water parameters for a polarizable atomic multipole electrostatics model. This model is equal or better to the best available water models for many bulk and cluster properties.

P. Ren and J. W. Ponder, A Polarizable Atomic Multipole Water Model for Molecular Mechanics Simulation, ***J. Phys. Chem. B***, *107*, 5933-5947 (2003)

P. Ren and J. W. Ponder, Ion Solvation Thermodynamics from Simulation with a Polarizable Force Field, A. Grossfield, ***J. Am. Chem. Soc.***, *125*, 15671-15682 (2003)

P. Ren and J. W. Ponder, Temperature and Pressure Dependence of the AMOEBA Water Model, ***J. Phys. Chem. B***, *108*, xxxx-xxxx (2004)

An earlier version the AMOEBA water model is described in: Yong Kong, Multipole Electrostatic Methods for Protein Modeling with Reaction Field Treatment, Biochemistry & Molecular Biophysics, Washington University, St. Louis, August, 1997 [available from http://dasher.wustl.edu/ponder/]

9. Descriptions of TINKER Routines

The distribution version of the TINKER package contains over 700 separate programs, subroutines and functions. This section contains a brief description of the purpose of most of these code units. Further information can be found in the comments located at the top of each source code file.

ACTIVE Subroutine

"active" sets the list of atoms that are used during each potential energy function calculation

ADDBASE Subroutine

"addbase" builds the Cartesian coordinates for a single nucleic acid base; coordinates are read from the Protein Data Bank file or found from internal coordinates, then atom types are assigned and connectivity data generated

ADDBOND Subroutine

"addbond" adds entries to the attached atoms list in order to generate a direct connection between two atoms

ADDSIDE Subroutine

"addside" builds the Cartesian coordinates for a single amino acid side chain; coordinates are read from the Protein Data Bank file or found from internal coordinates, then atom types are assigned and connectivity data generated

ADJACENT Function

"adjacent" finds an atom connected to atom "i1" other than atom "i2"; if no such atom exists, then the closest atom in space is returned

ALCHEMY Program

"alchemy" computes the free energy difference corresponding to a small perturbation by Boltzmann weighting the potential energy difference over a number of sample states; current version (incorrectly) considers the charge energy to be intermolecular in finding the perturbation energies

ANALYSIS Subroutine

"analysis" calls the series of routines needed to calculate the potential energy and perform energy partitioning analysis in terms of type of interaction or atom number

ANALYZ4 Subroutine

"analyz4" prints the energy to 4 decimal places and number of interactions for each component of the potential energy

ANALYZ6 Subroutine

"analyz6" prints the energy to 6 decimal places and number of interactions for each component of the potential energy

ANALYZ8 Subroutine

"analyz8" prints the energy to 8 decimal places and number of interactions for each component of the potential energy

ANALYZE Program

"analyze" computes and displays the total potential; options are provided to partition the energy by atom or by potential function type; parameters used in computing interactions can also be displayed by atom; output of large energy interactions and of electrostatic and inertial properties is available

ANGLES Subroutine

"angles" finds the total number of bond angles and stores the atom numbers of the atoms defining each angle; for each angle to a trivalent central atom, the third bonded atom is stored for use in out-of-plane bending

ANNEAL Program

"anneal" performs a simulated annealing protocol by means of variable temperature molecular dynamics using either linear, exponential or sigmoidal cooling schedules

ANORM Function

"anorm" finds the norm (length) of a vector; used as a service routine by the Connolly surface area and volume computation

ARCHIVE Program

"archive" is a utility program for coordinate files which concatenates multiple coordinate sets into a single archive file, or extracts individual coordinate sets from an archive

ASET Subroutine

"aset" computes by recursion the A functions used in the evaluation of Slater-type (STO) overlap integrals

ATOMYZE Subroutine

"atomyze" prints the potential energy components broken down by atom and to a choice of precision

ATTACH Subroutine

"attach" generates lists of 1-3, 1-4 and 1-5 connectivities starting from the previously determined list of attached atoms (ie, 1-2 connectivity)

BASEFILE Subroutine

"basefile" extracts from an input filename the portion consisting of any directory name and the base filename

BCUCOF Subroutine

"bcucof" determines the coefficient matrix needed for bicubic interpolation of a function, gradients and cross derivatives

BCUINT Subroutine

"bcuint" performs a bicubic interpolation of the function value on a 2D spline grid

BCUINT1 Subroutine

"bcuint1" performs a bicubic interpolation of the function value and gradient along the directions of a 2D spline grid

BCUINT2 Subroutine

"bcuint2" performs a bicubic interpolation of the function value, gradient and Hessain along the directions of a 2D spline grid

BEEMAN Subroutine

"beeman" performs a single molecular dynamics time step by means of a Beeman multistep recursion formula; the actual coefficients are Brooks' "Better Beeman" values

BETACF Function

"betacf" computes a rapidly convergent continued fraction needed by routine "betai" to evaluate the cumulative Beta distribution

BETAI Function

"betai" evaluates the cumulative Beta distribution function as the probability that a random variable from a distribution with Beta parameters "a" and "b" will be less than "x"

BIGBLOCK Subroutine

"bigblock" replicates the coordinates of a single unit cell to give a larger block of repeated units

BITORS Subroutine

"bitors" finds the total number of bitorsions, pairs of overlapping dihedral angles, and the numbers of the five atoms defining each bitorsion

BMAX Function

"bmax" computes the maximum order of the B functions needed for evaluation of Slater-type (STO) overlap integrals

BNDERR Function

"bnderr" is the distance bound error function and derivatives; this version implements the original and Havel's normalized lower bound penalty, the normalized version is preferred when lower bounds are small (as with NMR NOE restraints), the original penalty is needed if large lower bounds are present

BONDS Subroutine

"bonds" finds the total number of covalent bonds and stores the atom numbers of the atoms defining each bond

BORN Subroutine

"born" computes the Born radius of each atom for use with the various GB/SA solvation models

BORN1 Subroutine

"born1" computes derivatives of the Born radii with respect to atomic coordinates and increments total energy derivatives and virial components for potentials involving Born radii

BOUNDS Subroutine

"bounds" finds the center of mass of each molecule and translates any stray molecules back into the periodic box

BSET Subroutine

"bset" computes by downward recursion the B functions used in the evaluation of Slater-type (STO) overlap integrals

BSPLINE Subroutine

"bspline" calculates the coefficients for an n-th order B-spline approximation

BSPLINE1 Subroutine

"bspline1" calculates the coefficients and derivative coefficients for an n-th order B-spline approximation

BSSTEP Subroutine

"bsstep" takes a single Bulirsch-Stoer step with monitoring of local truncation error to ensure accuracy

CALENDAR Subroutine

"calendar" returns the current time as a set of integer values representing the year, month, day, hour, minute and second

CELLATOM Subroutine

"cellatom" completes the addition of a symmetry related atom to a unit cell by updating the atom type and attachment arrays

CENTER Subroutine

"center" moves the weighted centroid of each coordinate set to the origin during least squares superposition

CERROR Subroutine

"cerror" is the error handling routine for the Connolly surface area and volume computation

CFFTB Subroutine

"cfftb" computes the backward complex discrete Fourier transform, the Fourier synthesis

CFFTB1 Subroutine

CFFTF Subroutine

"cfftf" computes the forward complex discrete Fourier transform, the Fourier analysis

CFFTF1 Subroutine

CFFTI Subroutine

"cffti" initializes the array "wsave" which is used in both forward and backward transforms; the prime factorization of "n" together with a tabulation of the trigonometric functions are computed and stored in "wsave"

CFFTI1 Subroutine

CHIRER Function

"chirer" computes the chirality error and its derivatives with respect to atomic Cartesian coordinates as a sum the squares of deviations of chiral volumes from target values

CHKCLASH Subroutine

"chkclash" determines if there are any atom clashes which might cause trouble on subsequent energy evaluation

CHKPOLE Subroutine

"chkpole" inverts atomic multipole moments as necessary at sites with chiral local reference frame definitions

CHKRING Subroutine

"chkring" tests angles to be constrained for their presence in small rings and removes constraints that are redundant

CHKSIZE Subroutine

"chksize" computes a measure of overall global structural expansion or compaction from the number of excess upper or lower bounds matrix violations

CHKTREE Subroutine

"chktree" tests a minimum energy structure to see if it belongs to the correct progenitor in the existing map

CHKXYZ Subroutine

"chkxyz" finds any pairs of atoms with identical Cartesian coordinates, and prints a warning message

CHOLESKY Subroutine

"cholesky" uses a modified Cholesky method to solve the linear system Ax = b, returning "x" in "b"; "A" is assumed to be a real symmetric positive definite matrix with its diagonal and upper triangle stored by rows

CIRPLN Subroutine

CJKM Function

"cjkm" computes the coefficients of spherical harmonics expressed in prolate spheroidal coordinates

CLIMBER Subroutine

CLIMBRGD Subroutine

CLIMBROT Subroutine

CLIMBTOR Subroutine

CLIMBXYZ Subroutine

CLOCK Subroutine

"clock" determines elapsed CPU time in seconds since the start of the job

CLUSTER Subroutine

"cluster" gets the partitioning of the system into groups and stores a list of the group to which each atom belongs

COLUMN Subroutine

"column" takes the off-diagonal Hessian elements stored as sparse rows and sets up indices to allow column access

COMMAND Subroutine

"command" uses the standard Unix-like iargc/getarg routines to get the number and values of arguments specified on the command line at program runtime

COMPRESS Subroutine

"compress" transfers only the non-buried tori from the temporary tori arrays to the final tori arrays

CONNECT Subroutine

"connect" sets up the attached atom arrays starting from a set of internal coordinates

CONNOLLY Subroutine

"connolly" uses the algorithms from the AMS/VAM programs of Michael Connolly to compute the analytical molecular surface area and volume of a collection of spherical atoms; thus it implements Fred Richards' molecular surface definition as a set of analytically defined spherical and toroidal polygons

CONTACT Subroutine

"contact" constructs the contact surface, cycles and convex faces

CONTROL Subroutine

"control" gets initial values for parameters that determine the output style and information level provided by TINKER

COORDS Subroutine

"coords" converts the three principal eigenvalues/vectors from the metric matrix into atomic coordinates, and calls a routine to compute the rms deviation from the bounds

CORRELATE Program

"correlate" computes the time correlation function of some user-supplied property from individual snapshot frames taken from a molecular dynamics or other trajectory

CREATEJVM Subroutine

CREATESERVER Subroutine

CREATESYSTEM Subroutine

CREATEUPDATE Subroutine

CRYSTAL Program

"crystal" is a utility program which converts between fractional and Cartesian coordinates, and can generate full unit cells from asymmetric units

CUTOFFS Subroutine

"cutoffs" initializes and stores spherical energy cutoff distance windows, Hessian element and Ewald sum cutoffs, and the pairwise neighbor generation method

CYTSY Subroutine

"cytsy" solves a system of linear equations for a cyclically tridiagonal, symmetric, positive definite matrix

CYTSYP Subroutine

"cytsyp" finds the Cholesky factors of a cyclically tridiagonal symmetric, positive definite matrix given by two vectors

CYTSYS Subroutine

"cytsys" solves a cyclically tridiagonal linear system given the Cholesky factors

D1D2 Function

"d1d2" is a utility function used in computation of the reaction field recursive summation elements

DELETE Subroutine

"delete" removes a specified atom from the Cartesian coordinates list and shifts the remaining atoms

DEPTH Function

DESTROYJVM Subroutine

DESTROYSERVER Subroutine

DFTMOD Subroutine

"dftmod" computes the modulus of the discrete Fourier transform of "bsarray", storing it into "bsmod"

DIAGQ Subroutine

"diagq" is a matrix diagonalization routine which is derived from the classical given, housec, and eigen algorithms with several modifications to increase the efficiency and accuracy

DIFFEQ Subroutine

"diffeq" performs the numerical integration of an ordinary differential equation using an adaptive stepsize method to solve the corresponding coupled first-order equations of the general form dyi/dx = f(x,y1,...,yn) for yi = y1,...,yn

DIFFUSE Program

"diffuse" finds the self-diffusion constant for a homogeneous liquid via the Einstein relation from a set of stored molecular dynamics frames; molecular centers of mass are unfolded and mean squared displacements are computed versus time separation

DIST2 Function

"dist2" finds the distance squared between two points; used as a service routine by the Connolly surface area and volume computation

DISTGEOM Program

"distgeom" uses a metric matrix distance geometry procedure to generate structures with interpoint distances that lie within specified bounds, with chiral centers that maintain chirality, and with torsional angles restrained to desired values; the user also has the ability to interactively inspect and alter the triangle smoothed bounds matrix prior to embedding

DMDUMP Subroutine

"dmdump" puts the distance matrix of the final structure into the upper half of a matrix, the distance of each atom to the centroid on the diagonal, and the individual terms of the bounds errors into the lower half of the matrix

DOCUMENT Program

"document" generates a formatted description of all the code modules or common blocks, an index of routines called by each source code module, a listing of all valid keywords, a list of include file dependencies as needed by a Unix-style Makefile, or a formatted force field parameter set summary

DOT Function

"dot" finds the dot product of two vectors

DSTMAT Subroutine

"dstmat" selects a distance matrix containing values between the previously smoothed upper and lower bounds; the distance values are chosen from uniform distributions, in a triangle correlated fashion, or using random partial metrization

DYNAMIC Program

"dynamic" computes a molecular dynamics trajectory in any of several statistical mechanical ensembles with optional periodic boundaries and optional coupling to temperature and pressure baths alternatively a stochastic dynamics trajectory can be generated

EANGANG Subroutine

"eangang" calculates the angle-angle potential energy

EANGANG1 Subroutine

"eangang1" calculates the angle-angle potential energy and first derivatives with respect to Cartesian coordinates

EANGANG2 Subroutine

"eangang2" calculates the angle-angle potential energy second derivatives with respect to Cartesian coordinates using finite difference methods

EANGANG2A Subroutine

"eangang2a" calculates the angle-angle first derivatives for a single interaction with respect to Cartesian coordinates; used in computation of finite difference second derivatives

EANGANG3 Subroutine

"eangang3" calculates the angle-angle potential energy; also partitions the energy among the atoms

EANGLE Subroutine

"eangle" calculates the angle bending potential energy; projected in-plane angles at trigonal centers or Fourier angle bending terms are optionally used

EANGLE1 Subroutine

"eangle1" calculates the angle bending potential energy and the first derivatives with respect to Cartesian coordinates; projected in-plane angles at trigonal centers or Fourier angle bending terms are optionally used

EANGLE2 Subroutine

"eangle2" calculates second derivatives of the angle bending energy for a single atom using a mixture of analytical and finite difference methods; projected in-plane angles at trigonal centers or Fourier angle bending terms are optionally used

EANGLE2A Subroutine

"eangle2a" calculates bond angle bending potential energy second derivatives with respect to Cartesian coordinates

EANGLE2B Subroutine

"eangle2b" computes projected in-plane bending first derivatives for a single angle with respect to Cartesian coordinates; used in computation of finite difference second derivatives

EANGLE3 Subroutine

"eangle3" calculates the angle bending potential energy, also partitions the energy among the atoms; projected in-plane angles at trigonal centers or Fourier angle bending terms are optionally used

EBOND Subroutine

"ebond" calculates the bond stretching energy

EBOND1 Subroutine

"ebond1" calculates the bond stretching energy and first derivatives with respect to Cartesian coordinates

EBOND2 Subroutine

"ebond2" calculates second derivatives of the bond stretching energy for a single atom at a time

EBOND3 Subroutine

"ebond3" calculates the bond stretching energy; also partitions the energy among the atoms

EBUCK Subroutine

"ebuck" calculates the Buckingham exp-6 van der Waals energy

EBUCK0A Subroutine

"ebuck0a" calculates the Buckingham exp-6 van der Waals energy using a pairwise double loop

EBUCK0B Subroutine

"ebuck0b" calculates the Buckingham exp-6 van der Waals energy using the method of lights to locate neighboring atoms

EBUCK0C Subroutine

"ebuck0c" calculates the Buckingham exp-6 van der Waals energy via a Gaussian approximation for potential energy smoothing

EBUCK1 Subroutine

"ebuck1" calculates the Buckingham exp-6 van der Waals energy and its first derivatives with respect to Cartesian coordinates

EBUCK1A Subroutine

"ebuck1a" calculates the Buckingham exp-6 van der Waals energy and its first derivatives using a pairwise double loop

EBUCK1B Subroutine

"ebuck1b" calculates the Buckingham exp-6 van der Waals energy and its first derivatives using the method of lights to locate neighboring atoms

EBUCK1C Subroutine

"ebuck1c" calculates the Buckingham exp-6 van der Waals energy and its first derivatives via a Gaussian approximation for potential energy smoothing

EBUCK2 Subroutine

"ebuck2" calculates the Buckingham exp-6 van der Waals second derivatives for a single atom at a time

EBUCK2A Subroutine

"ebuck2a" calculates the Buckingham exp-6 van der Waals second derivatives using a double loop over relevant atom pairs

EBUCK2B Subroutine

"ebuck2b" calculates the Buckingham exp-6 van der Waals second derivatives via a Gaussian approximation for use with potential energy smoothing

EBUCK3 Subroutine

"ebuck3" calculates the Buckingham exp-6 van der Waals energy and partitions the energy among the atoms

EBUCK3A Subroutine

"ebuck3a" calculates the Buckingham exp-6 van der Waals energy and partitions the energy among the atoms using a pairwise double loop

EBUCK3B Subroutine

"ebuck3b" calculates the Buckingham exp-6 van der Waals energy and also partitions the energy among the atoms using the method of lights to locate neighboring atoms

EBUCK3C Subroutine

"ebuck3c" calculates the Buckingham exp-6 van der Waals energy via a Gaussian approximation for potential energy smoothing

ECHARGE Subroutine

"echarge" calculates the charge-charge interaction energy

ECHARGE0A Subroutine

"echarge0a" calculates the charge-charge interaction energy using a pairwise double loop

ECHARGE0B Subroutine

"echarge0b" calculates the charge-charge interaction energy using the method of lights to locate neighboring atoms

ECHARGE0C Subroutine

"echarge0c" calculates the charge-charge interaction energy for use with potential smoothing methods

ECHARGE0D Subroutine

"echarge0d" calculates the charge-charge interaction energy using a particle mesh Ewald summation

ECHARGE0E Subroutine

"echarge0e" calculates the charge-charge interaction energy using a particle mesh Ewald summation and the method of lights to locate neighboring atoms

ECHARGE1 Subroutine

"echarge1" calculates the charge-charge interaction energy and first derivatives with respect to Cartesian coordinates

ECHARGE1A Subroutine

"echarge1a" calculates the charge-charge interaction energy and first derivatives with respect to Cartesian coordinates using a pairwise double loop

ECHARGE1B Subroutine

"echarge1b" calculates the charge-charge interaction energy and first derivatives with respect to Cartesian coordinates using the method of lights to locate neighboring atoms

ECHARGE1C Subroutine

"echarge1c" calculates the charge-charge interaction energy and first derivatives with respect to Cartesian coordinates for use with potential smoothing methods

ECHARGE1D Subroutine

"echarge1d" calculates the charge-charge interaction energy and first derivatives with respect to Cartesian coordinates using a particle mesh Ewald summation

ECHARGE2 Subroutine

"echarge2" calculates second derivatives of the charge-charge interaction energy for a single atom

ECHARGE2A Subroutine

"echarge2a" calculates second derivatives of the charge-charge interaction energy for a single atom using a pairwise double loop

ECHARGE2B Subroutine

"echarge2b" calculates second derivatives of the charge-charge interaction energy for a single atom for use with potential smoothing methods

ECHARGE2C Subroutine

"echarge2c" calculates second derivatives of the charge-charge interaction energy for a single atom using a particle mesh Ewald summation

ECHARGE3 Subroutine

"echarge3" calculates the charge-charge interaction energy and partitions the energy among the atoms

ECHARGE3A Subroutine

"echarge3a" calculates the charge-charge interaction energy and partitions the energy among the atoms using a pairwise double loop

ECHARGE3B Subroutine

"echarge3b" calculates the charge-charge interaction energy and partitions the energy among the atoms using the method of lights to locate neighboring atoms

ECHARGE3C Subroutine

"echarge3c" calculates the charge-charge interaction energy and partitions the energy among the atoms for use with potential smoothing methods

ECHARGE3D Subroutine

"echarge3d" calculates the charge-charge interaction energy and partitions the energy among the atoms using a particle mesh Ewald summation

ECHARGE3E Subroutine

"echarge3e" calculates the charge-charge interaction energy and partitions the energy among the atoms using a particle mesh Ewald summation and the method of lights to locate neighboring atoms

ECHGDPL Subroutine

"echgdpl" calculates the charge-dipole interaction energy

ECHGDPL1 Subroutine

"echgdpl1" calculates the charge-dipole interaction energy and first derivatives with respect to Cartesian coordinates

ECHGDPL2 Subroutine

"echgdpl2" calculates second derivatives of the charge-dipole interaction energy for a single atom

ECHGDPL3 Subroutine

"echgdpl3" calculates the charge-dipole interaction energy; also partitions the energy among the atoms

EDIPOLE Subroutine

"edipole" calculates the dipole-dipole interaction energy

EDIPOLE1 Subroutine

"edipole1" calculates the dipole-dipole interaction energy and first derivatives with respect to Cartesian coordinates

EDIPOLE2 Subroutine

"edipole2" calculates second derivatives of the dipole-dipole interaction energy for a single atom

EDIPOLE3 Subroutine

"edipole3" calculates the dipole-dipole interaction energy; also partitions the energy among the atoms

EGAUSS Subroutine

"egauss" calculates the Gaussian expansion van der Waals interaction energy

EGAUSS0A Subroutine

"egauss0a" calculates the Gaussian expansion van der Waals interaction energy using a pairwise double loop

EGAUSS0B Subroutine

"egauss0b" calculates the Gaussian expansion van der Waals interaction energy for use with potential energy smoothing

EGAUSS1 Subroutine

"egauss1" calculates the Gaussian expansion van der Waals interaction energy and its first derivatives with respect to Cartesian coordinates

EGAUSS1A Subroutine

"egauss1a" calculates the Gaussian expansion van der Waals interaction energy and its first derivatives using a pairwise double loop

EGAUSS1B Subroutine

"egauss1b" calculates the Gaussian expansion van der Waals interaction energy and its first derivatives for use with stophat potential energy smoothing

EGAUSS2 Subroutine

"egauss2" calculates the Gaussian expansion van der Waals second derivatives for a single atom at a time

EGAUSS2A Subroutine

"egauss2a" calculates the Gaussian expansion van der Waals second derivatives using a pairwise double loop

EGAUSS2B Subroutine

"egauss2b" calculates the Gaussian expansion van der Waals second derivatives for stophat potential energy smoothing

EGAUSS3 Subroutine

"egauss3" calculates the Gaussian expansion van der Waals interaction energy and partitions the energy among the atoms

EGAUSS3A Subroutine

"egauss3a" calculates the Gaussian expansion van der Waals interaction energy and partitions the energy among the atoms using a pairwise double loop

EGAUSS3B Subroutine

"egauss3b" calculates the Gaussian expansion van der Waals interaction energy and partitions the energy among the atoms using a pairwise double loop

EGBSA0A Subroutine

"egbsa0a" calculates the generalized Born polarization energy for the GB/SA solvation models

EGBSA0B Subroutine

"egbsa0b" calculates the generalized Born polarization energy for the GB/SA solvation models for use with potential smoothing methods via analogy to the smoothing of Coulomb's law

EGBSA1A Subroutine

"egbsa1a" calculates the generalized Born energy and first derivatives of the GB/SA solvation models

EGBSA1B Subroutine

"egbsa1b" calculates the generalized Born energy and first derivatives of the GB/SA solvation models for use with potential smoothing methods

EGBSA2A Subroutine

"egbsa2a" calculates second derivatives of the generalized Born energy term for the GB/SA solvation models

EGBSA2B Subroutine

"egbsa2b" calculates second derivatives of the generalized Born energy term for the GB/SA solvation models for use with potential smoothing methods

EGBSA3A Subroutine

"egbsa3a" calculates the generalized Born energy term for the GB/SA solvation models; also partitions the energy among the atoms

EGBSA3B Subroutine

"egbsa3b" calculates the generalized Born polarization energy for the GB/SA solvation models for use with potential smoothing methods via analogy to the smoothing of Coulomb's law; also partitions the energy among the atoms

EGEOM Subroutine

"egeom" calculates the energy due to restraints on positions, distances, angles and torsions as well as Gaussian basin and spherical droplet restraints

EGEOM1 Subroutine

"egeom1" calculates the energy and first derivatives with respect to Cartesian coordinates due to restraints on positions, distances, angles and torsions as well as Gaussian basin and spherical droplet restraints

EGEOM2 Subroutine

"egeom2" calculates second derivatives of restraints on positions, distances, angles and torsions as well as Gaussian basin and spherical droplet restraints

EGEOM3 Subroutine

"egeom3" calculates the energy due to restraints on positions, distances, angles and torsions as well as Gaussian basin and droplet restraints; also partitions energy among the atoms

EHAL Subroutine

"ehal" calculates the buffered 14-7 van der Waals energy

EHAL0A Subroutine

"ehal0a" calculates the buffered 14-7 van der Waals energy using a pairwise double loop

EHAL0B Subroutine

"ehal0a" calculates the buffered 14-7 van der Waals energy using the method of lights to locate neighboring atoms

EHAL1 Subroutine

"ehal1" calculates the buffered 14-7 van der Waals energy and its first derivatives with respect to Cartesian coordinates

EHAL1A Subroutine

"ehal1a" calculates the buffered 14-7 van der Waals energy and its first derivatives with respect to Cartesian coordinates using a pairwise double loop

EHAL1B Subroutine

"ehal1b" calculates the buffered 14-7 van der Waals energy and its first derivatives with respect to Cartesian coordinates using the method of lights to locate neighboring atoms

EHAL2 Subroutine

"ehal2" calculates the buffered 14-7 van der Waals second derivatives for a single atom at a time

EHAL3 Subroutine

"ehal3" calculates the buffered 14-7 van der Waals energy and partitions the energy among the atoms

EHAL3A Subroutine

"ehal3a" calculates the buffered 14-7 van der Waals energy and partitions the energy among the atoms using a pairwise double loop

EHAL3B Subroutine

"ehal3b" calculates the buffered 14-7 van der Waals energy and also partitions the energy among the atoms using the method of lights to locate neighboring atoms

EIGEN Subroutine

"eigen" uses the power method to compute the largest eigenvalues and eigenvectors of the metric matrix, "valid" is set true if the first three eigenvalues are positive

EIGENRGD Subroutine

EIGENROT Subroutine

EIGENROT Subroutine

EIGENTOR Subroutine

EIGENXYZ Subroutine

EIMPROP Subroutine

"eimprop" calculates the improper dihedral potential energy

EIMPROP1 Subroutine

"eimprop1" calculates improper dihedral energy and its first derivatives with respect to Cartesian coordinates

EIMPROP2 Subroutine

"eimprop2" calculates second derivatives of the improper dihedral angle energy for a single atom

EIMPROP3 Subroutine

"eimprop3" calculates the improper dihedral potential energy; also partitions the energy terms among the atoms

EIMPTOR Subroutine

"eimptor" calculates the improper torsion potential energy

EIMPTOR1 Subroutine

"eimptor1" calculates improper torsion energy and its first derivatives with respect to Cartesian coordinates

EIMPTOR2 Subroutine

"eimptor2" calculates second derivatives of the improper torsion energy for a single atom

EIMPTOR3 Subroutine

"eimptor3" calculates the improper torsion potential energy; also partitions the energy terms among the atoms

ELJ Subroutine

"elj" calculates the Lennard-Jones 6-12 van der Waals energy

ELJ0A Subroutine

"elj0a" calculates the Lennard-Jones 6-12 van der Waals energy using a pairwise double loop

ELJ0B Subroutine

"elj0b" calculates the Lennard-Jones 6-12 van der Waals energy using the method of lights to locate neighboring atoms

ELJ0C Subroutine

"elj0c" calculates the Lennard-Jones 6-12 van der Waals energy via a Gaussian approximation for potential energy smoothing

ELJ0D Subroutine

"elj0d" calculates the Lennard-Jones 6-12 van der Waals energy for use with stophat potential energy smoothing

ELJ1 Subroutine

"elj1" calculates the Lennard-Jones 6-12 van der Waals energy and its first derivatives with respect to Cartesian coordinates

ELJ1A Subroutine

"elj1a" calculates the Lennard-Jones 6-12 van der Waals energy and its first derivatives using a pairwise double loop

ELJ1B Subroutine

"elj1b" calculates the Lennard-Jones 6-12 van der Waals energy and its first derivatives using the method of lights to locate neighboring atoms

ELJ1C Subroutine

"elj1c" calculates the Lennard-Jones 6-12 van der Waals energy and its first derivatives via a Gaussian approximation for potential energy smoothing

ELJ1D Subroutine

"elj1d" calculates the van der Waals interaction energy and its first derivatives for use with stophat potential energy smoothing

ELJ2 Subroutine

"elj2" calculates the Lennard-Jones 6-12 van der Waals second derivatives for a single atom at a time

ELJ2A Subroutine

"elj2a" calculates the Lennard-Jones 6-12 van der Waals second derivatives using a double loop over relevant atom pairs

ELJ2B Subroutine

"elj2b" calculates the Lennard-Jones 6-12 van der Waals second derivatives via a Gaussian approximation for use with potential energy smoothing

ELJ2C Subroutine

"elj2c" calculates the Lennard-Jones 6-12 van der Waals second derivatives for use with stophat potential energy smoothing

ELJ3 Subroutine

"elj3" calculates the Lennard-Jones 6-12 van der Waals energy and also partitions the energy among the atoms

ELJ3A Subroutine

"elj3a" calculates the Lennard-Jones 6-12 van der Waals energy and also partitions the energy among the atoms using a pairwise double loop

ELJ3B Subroutine

"elj3b" calculates the Lennard-Jones 6-12 van der Waals energy and also partitions the energy among the atoms using the method of lights to locate neighboring atoms

ELJ3C Subroutine

"elj3c" calculates the Lennard-Jones 6-12 van der Waals energy and also partitions the energy among the atoms via a Gaussian approximation for potential energy smoothing

ELJ3D Subroutine

"elj3d" calculates the Lennard-Jones 6-12 van der Waals energy and also partitions the energy among the atoms for use with stophat potential energy smoothing

EMBED Subroutine

"embed" is a distance geometry routine patterned after the ideas of Gordon Crippen, Irwin Kuntz and Tim Havel; it takes as input a set of upper and lower bounds on the interpoint distances, chirality restraints and torsional restraints, and attempts to generate a set of coordinates that satisfy the input bounds and restraints

EMETAL Subroutine

"emetal" calculates the transition metal ligand field energy

EMETAL1 Subroutine

"emetal1" calculates the transition metal ligand field energy and its first derivatives with respect to Cartesian coordinates

EMETAL2 Subroutine

"emetal2" calculates the transition metal ligand field second derivatives for a single atom at a time

EMETAL3 Subroutine

"emetal3" calculates the transition metal ligand field energy and also partitions the energy among the atoms

EMM3HB Subroutine

"emm3hb" calculates the MM3 exp-6 van der Waals and directional charge transfer hydrogen bonding energy

EMM3HB0A Subroutine

"emm3hb0a" calculates the MM3 exp-6 van der Waals and directional charge transfer hydrogen bonding energy using a pairwise double loop

EMM3HB0B Subroutine

"emm3hb0b" calculates the MM3 exp-6 van der Waals and directional charge transfer hydrogen bonding energy using the method of lights to locate neighboring atoms

EMM3HB1 Subroutine

"emm3hb1" calculates the MM3 exp-6 van der Waals and directional charge transfer hydrogen bonding energy with respect to Cartesian coordinates

EMM3HB1A Subroutine

"emm3hb1a" calculates the MM3 exp-6 van der Waals and directional charge transfer hydrogen bonding energy with respect to Cartesian coordinates using a pairwise double loop

EMM3HB1B Subroutine

"emm3hb1b" calculates the MM3 exp-6 van der Waals and directional charge transfer hydrogen bonding energy with respect to Cartesian coordinates using the method of lights to locate neighboring atoms

EMM3HB2 Subroutine

"emm3hb2" calculates the MM3 exp-6 van der Waals and directional charge transfer hydrogen bonding second derivatives for a single atom at a time

EMM3HB3 Subroutine

"emm3hb3" calculates the MM3 exp-6 van der Waals and directional charge transfer hydrogen bonding energy, and partitions the energy among the atoms

EMM3HB3A Subroutine

"emm3hb3" calculates the MM3 exp-6 van der Waals and directional charge transfer hydrogen bonding energy, and partitions the energy among the atoms

EMM3HB3B Subroutine

"emm3hb3b" calculates the MM3 exp-6 van der Waals and directional charge transfer hydrogen bonding energy using the method of lights to locate neighboring atoms

EMPOLE Subroutine

"empole" calculates the electrostatic energy due to atomic multipole interactions and dipole polarizability

EMPOLE0A Subroutine

"empole0a" calculates the electrostatic energy due to atomic multipole interactions and dipole polarizability using a pairwise double loop

EMPOLE0B Subroutine

"empole0b" calculates the electrostatic energy due to atomic multipole interactions and dipole polarizability using a regular Ewald summation

EMPOLE1 Subroutine

"empole1" calculates the multipole and dipole polarization energy and derivatives with respect to Cartesian coordinates

EMPOLE1A Subroutine

"empole1a" calculates the multipole and dipole polarization energy and derivatives with respect to Cartesian coordinates using a pairwise double loop

EMPOLE1B Subroutine

"empole1b" calculates the multipole and dipole polarization energy and derivatives with respect to Cartesian coordinates using a regular Ewald summation

EMPOLE2 Subroutine

"empole2" calculates second derivatives of the multipole and dipole polarization energy for a single atom at a time

EMPOLE2A Subroutine

"empole2a" computes multipole and dipole polarization first derivatives for a single atom with respect to Cartesian coordinates; used to get finite difference second derivatives

EMPOLE3 Subroutine

"empole3" calculates the electrostatic energy due to atomic multipole interactions and dipole polarizability, and partitions the energy among the atoms

EMPOLE3A Subroutine

"empole3a" calculates the electrostatic energy due to atomic multipole interactions and dipole polarizability, and partitions the energy among the atoms using a double loop

EMPOLE3B Subroutine

"empole3b" calculates the electrostatic energy due to atomic multipole interactions and dipole polarizability, and partitions the energy among the atoms using a regular Ewald summation

ENERGY Function

"energy" calls the subroutines to calculate the potential energy terms and sums up to form the total energy

ENRGYZE Subroutine

"energyze" is an auxiliary routine for the analyze program that performs the energy analysis and prints the total and intermolecular energies

EOPBEND Subroutine

"eopbend" computes the out-of-plane bend potential energy at trigonal centers via a Wilson-Decius-Cross angle bend

EOPBEND1 Subroutine

"eopbend1" computes the out-of-plane bend potential energy and first derivatives at trigonal centers via a Wilson-Decius-Cross angle bend

EOPBEND2 Subroutine

"eopbend2" calculates second derivatives of the out-of-plane bend energy via a Wilson-Decius-Cross angle bend for a single atom using finite difference methods

EOPBEND2A Subroutine

"eopbend2a" calculates out-of-plane bending first derivatives at a trigonal center via a Wilson-Decius-Cross angle bend; used in computation of finite difference second derivatives

EOPBEND3 Subroutine

"eopbend3" computes the out-of-plane bend potential energy at trigonal centers via a Wilson-Decius-Cross angle bend; also partitions the energy among the atoms

EOPDIST Subroutine

"eopdist" computes the out-of-plane distance potential energy at trigonal centers via the central atom height

EOPDIST1 Subroutine

"eopdist1" computes the out-of-plane distance potential energy and first derivatives at trigonal centers via the central atom height

EOPDIST2 Subroutine

"eopdist2" calculates second derivatives of the out-of-plane distance energy for a single atom via the central atom height

EOPDIST3 Subroutine

"eopdist3" computes the out-of-plane distance potential energy at trigonal centers via the central atom height; also partitions the energy among the atoms

EPITORS Subroutine

"epitors" calculates the pi-orbital torsion potential energy

EPITORS1 Subroutine

"epitors1" calculates the pi-orbital torsion potential energy and first derivatives with respect to Cartesian coordinates

EPITORS2 Subroutine

"epitors2" calculates the second derivatives of the pi-orbital torsion energy for a single atom using finite difference methods

EPITORS2A Subroutine

"epitors2a" calculates the pi-orbital torsion first derivatives; used in computation of finite difference second derivatives

EPITORS3 Subroutine

"epitors3" calculates the pi-orbital torsion potential energy; also partitions the energy terms among the atoms

EPME Subroutine

"epme" computes the reciprocal space energy for a particle mesh Ewald summation over partial charges

EPME1 Subroutine

"epme1" computes the reciprocal space energy and first derivatives for a particle mesh Ewald summation

EPME3 Subroutine

"epme3" computes the reciprocal space energy for a particle mesh Ewald summation over partial charges and prints information about the energy over the charge grid points

EPUCLC Subroutine

EREAL Subroutine

"ereal" evaluates the real space portion of the regular Ewald summation energy due to atomic multipole interactions and dipole polarizability

EREAL1 Subroutine

"ereal1" evaluates the real space portion of the regular Ewald summation energy and gradient due to atomic multipole interactions and dipole polarizability

EREAL3 Subroutine

"ereal3" evaluates the real space portion of the regular Ewald summation energy due to atomic multipole interactions and dipole polarizability and partitions the energy among the atoms

ERECIP Subroutine

"erecip" evaluates the reciprocal space portion of the regular Ewald summation energy due to atomic multipole interactions and dipole polarizability

ERECIP1 Subroutine

"erecip1" evaluates the reciprocal space portion of the regular Ewald summation energy and gradient due to atomic multipole interactions and dipole polarizability

ERECIP3 Subroutine

"erecip3" evaluates the reciprocal space portion of the regular Ewald summation energy due to atomic multipole interactions and dipole polarizability, and prints information about the energy over the reciprocal lattice vectors

ERF Function

"erf" computes a numerical approximation to the value of the error function via a Chebyshev approximation

ERFC Function

"erfc" computes a numerical approximation to the value of the complementary error function via a Chebyshev approximation

ERFCORE Subroutine

"erfcore" evaluates erf(x) or erfc(x) for a real argument x; when called with mode set to 0 it returns erf, a mode of 1 returns erfc; uses rational functions that approximate erf(x) and erfc(x) to at least 18 significant decimal digits

ERFIK Subroutine

"erfik" compute the reaction field energy due to a single pair of atomic multipoles

ERFINV Function

"erfinv" evaluates the inverse of the error function erf for a real argument in the range (-1,1) using a rational function approximation followed by cycles of Newton-Raphson correction

ERXNFLD Subroutine

"erxnfld" calculates the macroscopic reaction field energy arising from a set of atomic multipoles

ERXNFLD1 Subroutine

"erxnfld1" calculates the macroscopic reaction field energy and derivatives with respect to Cartesian coordinates

ERXNFLD2 Subroutine

"erxnfld2" calculates second derivatives of the macroscopic reaction field energy for a single atom at a time

ERXNFLD3 Subroutine

"erxnfld3" calculates the macroscopic reaction field energy, and also partitions the energy among the atoms

ESOLV Subroutine

"esolv" calculates the continuum solvation energy via either the Eisenberg-McLachlan ASP model, Ooi-Scheraga SASA model, various GB/SA methods or the ACE model

ESOLV1 Subroutine

"esolv1" calculates the continuum solvation energy and first derivatives with respect to Cartesian coordinates using either the Eisenberg-McLachlan ASP, Ooi-Scheraga SASA or various GB/SA solvation models

ESOLV2 Subroutine

"esolv2" calculates second derivatives of the continuum solvation energy using either the Eisenberg-McLachlan ASP, Ooi-Scheraga SASA or various GB/SA solvation models

ESOLV3 Subroutine

"esolv3" calculates the continuum solvation energy using either the Eisenberg-McLachlan ASP model, Ooi-Scheraga SASA model, various GB/SA methods or the ACE model; also partitions the energy among the atoms

ESTRBND Subroutine

"estrbnd" calculates the stretch-bend potential energy

ESTRBND1 Subroutine

"estrbnd1" calculates the stretch-bend potential energy and first derivatives with respect to Cartesian coordinates

ESTRBND2 Subroutine

"estrbnd2" calculates the stretch-bend potential energy second derivatives with respect to Cartesian coordinates

ESTRBND3 Subroutine

"estrbnd3" calculates the stretch-bend potential energy; also partitions the energy among the atoms

ESTRTOR Subroutine

"estrtor" calculates the stretch-torsion potential energy

ESTRTOR1 Subroutine

"estrtor1" calculates the stretch-torsion energy and first derivatives with respect to Cartesian coordinates

ESTRTOR2 Subroutine

"estrtor2" calculates the stretch-torsion potential energy second derivatives with respect to Cartesian coordinates

ESTRTOR3 Subroutine

"estrtor3" calculates the stretch-torsion potential energy; also partitions the energy terms among the atoms

ETORS Subroutine

"etors" calculates the torsional potential energy

ETORS0A Subroutine

"etors0a" calculates the torsional potential energy using a standard sum of Fourier terms

ETORS0B Subroutine

"etors0b" calculates the torsional potential energy for use with potential energy smoothing methods

ETORS1 Subroutine

"etors1" calculates the torsional potential energy and first derivatives with respect to Cartesian coordinates

ETORS1A Subroutine

"etors1a" calculates the torsional potential energy and first derivatives with respect to Cartesian coordinates using a standard sum of Fourier terms

ETORS1B Subroutine

"etors1b" calculates the torsional potential energy and first derivatives with respect to Cartesian coordinates for use with potential energy smoothing methods

ETORS2 Subroutine

"etors2" calculates the second derivatives of the torsional energy for a single atom

ETORS2A Subroutine

"etors2a" calculates the second derivatives of the torsional energy for a single atom using a standard sum of Fourier terms

ETORS2B Subroutine

"etors2b" calculates the second derivatives of the torsional energy for a single atom for use with potential energy smoothing methods

ETORS3 Subroutine

"etors3" calculates the torsional potential energy; also partitions the energy among the atoms

ETORS3A Subroutine

"etors3a" calculates the torsional potential energy using a standard sum of Fourier terms and partitions the energy among the atoms

ETORS3B Subroutine

"etors3b" calculates the torsional potential energy for use with potential energy smoothing methods and partitions the energy among the atoms

ETORTOR Subroutine

"etortor" calculates the torsion-torsion potential energy

ETORTOR1 Subroutine

"etortor1" calculates the torsion-torsion energy and first derivatives with respect to Cartesian coordinates

ETORTOR2 Subroutine

"etortor2" calculates the torsion-torsion potential energy second derivatives with respect to Cartesian coordinates

ETORTOR3 Subroutine

"etortor3" calculates the torsion-torsion potential energy; also partitions the energy terms among the atoms

EUREY Subroutine

"eurey" calculates the Urey-Bradley 1-3 interaction energy

EUREY1 Subroutine

"eurey1" calculates the Urey-Bradley interaction energy and its first derivatives with respect to Cartesian coordinates

EUREY2 Subroutine

"eurey2" calculates second derivatives of the Urey-Bradley interaction energy for a single atom at a time

EUREY3 Subroutine

"eurey3" calculates the Urey-Bradley energy; also partitions the energy among the atoms

EWALDCOF Subroutine

"ewaldcof" finds a value of the Ewald coefficient such that all terms beyond the specified cutoff distance will have an value less than a specified tolerance

EXPLORE Subroutine

"explore" uses simulated annealing on an initial crude embedded distance geoemtry structure to refine versus the bound, chirality, planarity and torsional error functions

EXTRA Subroutine

"extra" calculates any additional user defined potential energy contribution

EXTRA1 Subroutine

"extra1" calculates any additional user defined potential energy contribution and its first derivatives

EXTRA2 Subroutine

"extra2" calculates second derivatives of any additional user defined potential energy contribution for a single atom at a time

EXTRA3 Subroutine

"extra3" calculates any additional user defined potential contribution and also partitions the energy among the atoms

FATAL Subroutine

"fatal" terminates execution due to a user request, a severe error or some other nonstandard condition

FFTBACK Subroutine

FFTFRONT Subroutine

FFTSETUP Subroutine

FIELD Subroutine

"field" sets the force field potential energy functions from a parameter file and modifications specified in a keyfile

FINAL Subroutine

"final" performs any final program actions, prints a status message, and then pauses if necessary to avoid closing the execution window

FINDATM Subroutine

"findatm" locates a specific PDB atom name type within a range of atoms from the PDB file, returns zero if the name type was not found

FIXPDB Subroutine

"fixpdb" corrects problems with PDB files by converting residue and atom names to the forms used by TINKER

FRACDIST Subroutine

"fracdist" computes a normalized distribution of the pairwise fractional distances between the smoothed upper and lower bounds

FREEUNIT Function

"freeunit" finds an unopened Fortran I/O unit and returns its numerical value from 1 to 99; the units already assigned to "input" and "iout" (usually 5 and 6) are skipped since they have special meaning as the default I/O units

GAMMLN Function

"gammln" uses a series expansion due to Lanczos to compute the natural logarithm of the Gamma function at "x" in [0,1]

GDA Program

"gda" implements Gaussian Density Annealing (GDA) algorithm for global optimization via simulated annealing

GDA1 Subroutine

GDA2 Function

GDA3 Subroutine

GDASTAT Subroutine

GENDOT Subroutine

"gendot" finds the coordinates of a specified number of surface points for a sphere with the input radius and coordinate center

GEODESIC Subroutine

"geodesic" smooths the upper and lower distance bounds via the triangle inequality using a sparse matrix version of a shortest path algorithm

GEOMETRY Function

"geometry" finds the value of the interatomic distance, angle or dihedral angle defined by two to four input atoms

GETBASE Subroutine

"getbase" finds the base heavy atoms for a single nucleotide residue and copies the names and coordinates to the Protein Data Bank file

GETIME Subroutine

"getime" gets elapsed CPU time in seconds for an interval

GETINT Subroutine

"getint" asks for an internal coordinate file name, then reads the internal coordinates and computes Cartesian coordinates

GETKEY Subroutine

"getkey" finds a valid keyfile and stores its contents as line images for subsequent keyword parameter searching

GETMOL2 Subroutine

"getmol2" asks for a Sybyl MOL2 molecule file name, then reads the coordinates from the file

GETMONITOR Subroutine

GETNUCH Subroutine

"getnuch" finds the nucleotide hydrogen atoms for a single residue and copies the names and coordinates to the Protein Data Bank file

GETNUMB Subroutine

"getnumb" searchs an input string from left to right for an integer and puts the numeric value in "number"; returns zero with "next" unchanged if no integer value is found

GETPDB Subroutine

"getpdb" asks for a Protein Data Bank file name, then reads in the coordinates file

GETPRB Subroutine

"getprb" tests for a possible probe position at the interface between three neighboring atoms

GETPRM Subroutine

"getprm" finds the potential energy parameter file and then opens and reads the parameters

GETPROH Subroutine

"getproh" finds the hydrogen atoms for a single amino acid residue and copies the names and coordinates to the Protein Data Bank file

GETREF Subroutine

"getref" copies structure information from the reference area into the standard variables for the current system structure

GETSEQ Subroutine

"getseq" asks the user for the amino acid sequence and torsional angle values needed to define a peptide

GETSEQN Subroutine

"getseqn" asks the user for the nucleotide sequence and torsional angle values needed to define a nucleic acid

GETSIDE Subroutine

"getside" finds the side chain heavy atoms for a single amino acid residue and copies the names and coordinates to the Protein Data Bank file

GETSTRING Subroutine

"getstring" searchs for a quoted text string within an input character string; the region between the first and second quotes is returned as the "text"; if the actual text is too long, only the first part is returned

GETTEXT Subroutine

"gettext" searchs an input string for the first string of non-blank characters; the region from a non-blank character to the first blank space is returned as "text"; if the actual text is too long, only the first part is returned

GETTOR Subroutine

"gettor" tests for a possible torus position at the interface between two atoms, and finds the torus radius, center and axis

GETWORD Subroutine

"getword" searchs an input string for the first alphabetic character (A-Z or a-z); the region from this first character to the first blank space or comma is returned as a "word"; if the actual word is too long, only the first part is returned

GETXYZ Subroutine

"getxyz" asks for a Cartesian coordinate file name, then reads in the coordinates file

GRADIENT Subroutine

"gradient" calls subroutines to calculate the potential energy and first derivatives with respect to Cartesian coordinates

GRADRGD Subroutine

"gradrgd" calls subroutines to calculate the potential energy and first derivatives with respect to rigid body coordinates

GRADROT Subroutine

"gradrot" calls subroutines to calculate the potential energy and its torsional first derivatives

GRAFIC Subroutine

"grafic" outputs the upper & lower triangles and diagonal of a square matrix in a schematic form for visual inspection

GROUPS Subroutine

"groups" tests a set of atoms to see if all are members of a single atom group or a pair of atom groups; if so, then the correct intra- or intergroup weight is assigned

GRPLINE Subroutine

"grpline" tests each atom group for linearity of the sites contained in the group

GYRATE Subroutine

"gyrate" computes the radius of gyration of a molecular system from its atomic coordinates

HANGLE Subroutine

"hangle" constructs hybrid angle bending parameters given an initial state, final state and "lambda" value

HATOM Subroutine

"hatom" assigns a new atom type to each hybrid site

HBOND Subroutine

"hbond" constructs hybrid bond stretch parameters given an initial state, final state and "lambda" value

HCHARGE Subroutine

"hcharge" constructs hybrid charge interaction parameters given an initial state, final state and "lambda" value

HDIPOLE Subroutine

"hdipole" constructs hybrid dipole interaction parameters given an initial state, final state and "lambda" value

HESSIAN Subroutine

"hessian" calls subroutines to calculate the Hessian elements for each atom in turn with respect to Cartesian coordinates

HESSRGD Subroutine

"hessrgd" computes the numerical Hessian elements with respect to rigid body coordinates via 6*ngroup+1 gradient evaluations

HESSROT Subroutine

"hessrot" computes the numerical Hessian elements with respect to torsional angles; either the full matrix or just the diagonal can be calculated; the full matrix needs nomega+1 gradient evaluations while the diagonal requires just two gradient calls

HIMPTOR Subroutine

"himptor" constructs hybrid improper torsional parameters given an initial state, final state and "lambda" value

HSTRBND Subroutine

"hstrbnd" constructs hybrid stretch-bend parameters given an initial state, final state and "lambda" value

HSTRTOR Subroutine

"hstrtor" constructs hybrid stretch-torsion parameters given an initial state, final state and "lambda" value

HTORS Subroutine

"htors" constructs hybrid torsional parameters for a given initial state, final state and "lambda" value

HVDW Subroutine

"hvdw" constructs hybrid van der Waals parameters given an initial state, final state and "lambda" value

HYBRID Subroutine

"hybrid" constructs the hybrid hamiltonian for a specified initial state, final state and mutation parameter "lambda"

IJKPTS Subroutine

"ijkpts" stores a set of indices used during calculation of macroscopic reaction field energetics

IMAGE Subroutine

"image" takes the components of pairwise distance between two points in the same or neighboring periodic boxes and converts to the components of the minimum image distance

IMPOSE Subroutine

"impose" performs the least squares best superposition of two atomic coordinate sets via a quaternion method; upon return, the first coordinate set is unchanged while the second set is translated and rotated to give best fit; the final root mean square fit is returned in "rmsvalue"

INDUCE Subroutine

"induce" computes the induced dipole moment at each polarizable site due to direct or mutual polarization; assumes that multipole components have already been rotated into the global coordinate frame

INDUCE0A Subroutine

"induce0a" computes the induced dipole moment at each polarizable site using a pairwise double loop

INDUCE0B Subroutine

"induce0b" computes the induced dipole moment at each polarizable site using a regular Ewald summation

INEDGE Subroutine

"inedge" inserts a concave edge into the linked list for its temporary torus

INERTIA Subroutine

"inertia" computes the principal moments of inertia for the system, and optionally translates the center of mass to the origin and rotates the principal axes onto the global axes

INITERR Function

"initerr" is the initial error function and derivatives for a distance geometry embedding; it includes components from the local geometry and torsional restraint errors

INITIAL Subroutine

"initial" sets up original values for some parameters and variables that might not otherwise get initialized

INITPRM Subroutine

"initprm" completely initializes a force field by setting all parameters to zero and using defaults for control values

INITRES Subroutine

"initres" sets names for biopolymer residue types used in PDB file conversion and automated generation of structures

INITROT Subroutine

"initrot" sets the torsional angles which are to be rotated in subsequent computation, by default automatically selects all rotatable single bonds; assumes internal coordinates have already been setup

INSERT Subroutine

"insert" adds the specified atom to the Cartesian coordinates list and shifts the remaining atoms

INTEDIT Program

"intedit" allows the user to extract information from or alter the values within an internal coordinates file

INTXYZ Program

"intxyz" takes as input an internal coordinates file, converts to and then writes out Cartesian coordinates

INVBETA Function

"invbeta" computes the inverse Beta distribution function via a combination of Newton iteration and bisection search

INVERT Subroutine

"invert" inverts a matrix using the Gauss-Jordan method

IPEDGE Subroutine

"ipedge" inserts convex edge into linked list for atom

ISPLPE Subroutine

"isplpe" computes the coefficients for a cubic periodic interpolating spline

JACOBI Subroutine

"jacobi" performs a matrix diagonalization of a real symmetric matrix by the method of Jacobi rotations

KANGANG Subroutine

"kangang" assigns the parameters for angle-angle cross term interactions and processes new or changed parameter values

KANGLE Subroutine

"kangle" assigns the force constants and ideal angles for the bond angles; also processes new or changed parameters

KATOM Subroutine

"katom" assigns an atom type definitions to each atom in the structure and processes any new or changed values

KBOND Subroutine

"kbond" assigns a force constant and ideal bond length to each bond in the structure and processes any new or changed parameter values

KCHARGE Subroutine

"kcharge" assigns partial charges to the atoms within the structure and processes any new or changed values

KCHIRAL Subroutine

"kchiral" determines the target value for each chirality and planarity restraint as the signed volume of the parallelpiped spanned by vectors from a common atom to each of three other atoms

KDIPOLE Subroutine

"kdipole" assigns bond dipoles to the bonds within the structure and processes any new or changed values

KENEG Subroutine

"keneg" applies primary and secondary electronegativity bond length corrections to applicable bond parameters

KEWALD Subroutine

"kewald" assigns both regular Ewald summation and particle mesh Ewald parameters for a periodic box

KGEOM Subroutine

"kgeom" asisgns parameters for geometric restraint terms to be included in the potential energy calculation

KIMPROP Subroutine

"kimprop" assigns potential parameters to each improper dihedral in the structure and processes any changed values

KIMPTOR Subroutine

"kimptor" assigns torsional parameters to each improper torsion in the structure and processes any changed values

KINETIC Subroutine

"kinetic" computes the total kinetic energy and kinetic energy contributions to the pressure tensor by summing over velocities

KMETAL Subroutine

"kmetal" assigns ligand field parameters to transition metal atoms and processes any new or changed parameter values

KMPOLE Subroutine

"kmpole" assigns atomic multipole moments to the atoms of the structure and processes any new or changed values

KOPBEND Subroutine

"kopbend" assigns the force constants for out-of-plane bending at trigonal centers via Wilson-Decius-Cross angle bends; also processes any new or changed parameter values

KOPDIST Subroutine

"kopdist" assigns the force constants for out-of-plane distance at trigonal centers via the central atom height; also processes any new or changed parameter values

KORBIT Subroutine

"korbit" assigns pi-orbital parameters to conjugated systems and processes any new or changed parameters

KPITORS Subroutine

"kpitors" assigns pi-orbital torsion parameters to torsions needing them, and processes any new or changed values

KPOLAR Subroutine

"kpolar" assigns atomic dipole polarizabilities to the atoms within the structure and processes any new or changed values

KSOLV Subroutine

"ksolv" assigns continuum solvation energy parameters for the Eisenberg-McLachlan ASP, Ooi-Scheraga SASA or various GB/SA solvation models

KSTRBND Subroutine

"kstrbnd" assigns the parameters for the stretch-bend interactions and processes new or changed parameter values

KSTRTOR Subroutine

"kstrtor" assigns stretch-torsion parameters to torsions needing them, and processes any new or changed values

KTORS Subroutine

"ktors" assigns torsional parameters to each torsion in the structure and processes any new or changed values

KTORTOR Subroutine

"ktortor" assigns torsion-torsion parameters to adjacent torsion pairs and processes any new or changed values

KUREY Subroutine

"kurey" assigns the force constants and ideal distances for the Urey-Bradley 1-3 interactions; also processes any new or changed parameter values

KVDW Subroutine

"kvdw" assigns the parameters to be used in computing the van der Waals interactions and processes any new or changed values for these parameters

LATTICE Subroutine

"lattice" stores the periodic box dimensions and sets angle values to be used in computing fractional coordinates

LBFGS Subroutine

"lbfgs" is a limited memory BFGS quasi-newton nonlinear optimization routine

LIGASE Subroutine

"ligase" translates a nucleic acid structure in Protein Data Bank format to a Cartesian coordinate file and sequence file

LIGHTS Subroutine

"lights" computes the set of nearest neighbor interactions using the method of lights algorithm

LINBODY Subroutine

"linbody" finds the angular velocity of a linear rigid body given the inertia tensor and angular momentum

LMSTEP Subroutine

"lmstep" computes the Levenberg-Marquardt step during a nonlinear least squares calculation; this version is based upon ideas from the Minpack routine LMPAR together with with the internal doubling strategy of Dennis and Schnabel

LOCALMIN Subroutine

"localmin" is used during normal mode local search to perform a Cartesian coordinate energy minimization

LOCALRGD Subroutine

"localrgd" is used during the PSS local search procedure to perform a rigid body energy minimization

LOCALROT Subroutine

"localrot" is used during the PSS local search procedure to perform a torsional space energy minimization

LOCALXYZ Subroutine

"localxyz" is used during the potential smoothing and search procedure to perform a local optimization at the current smoothing level

LOCERR Function

"locerr" is the local geometry error function and derivatives including the 1-2, 1-3 and 1-4 distance bound restraints

LOWCASE Subroutine

"lowcase" converts a text string to all lower case letters

MAJORIZE Subroutine

"majorize" refines the projected coordinates by attempting to minimize the least square residual between the trial distance matrix and the distances computed from the coordinates

MAKEINT Subroutine

"makeint" converts Cartesian to internal coordinates where selection of internal coordinates is controlled by "mode"

MAKEPDB Subroutine

"makexyz" converts a set of Cartesian coordinates to Protein Data Bank format with special handling for systems consisting of polypeptide chains, ligands and water molecules

MAKEREF Subroutine

"makeref" copies the information contained in the "xyz" file of the current structure into corresponding reference areas

MAKEXYZ Subroutine

"makexyz" generates a complete set of Cartesian coordinates for a full structure from the internal coordinate values

MAPCHECK Subroutine

"mapcheck" checks the current minimum energy structure for possible addition to the master list of local minima

MAXWELL Function

"maxwell" returns a speed in Angstroms/picosecond randomly selected from a 3-D Maxwell-Boltzmann distribution for the specified particle mass and system temperature

MCM1 Function

"mcm1" is a service routine that computes the energy and gradient for truncated Newton optimization in Cartesian coordinate space

MCM2 Subroutine

"mcm2" is a service routine that computes the sparse matrix Hessian elements for truncated Newton optimization in Cartesian coordinate space

MCMSTEP Function

"mcmstep" implements the minimization phase of an MCM step via Cartesian minimization following a Monte Carlo step

MDINIT Subroutine

"mdinit" initializes the velocities and accelerations for a molecular dynamics trajectory, including restarts

MDREST Subroutine

"mdrest" finds and removes any translational or rotational kinetic energy of the overall system center of mass

MDSAVE Subroutine

"mdsave" writes molecular dynamics trajectory snapshots and auxiliary files with velocity and induced dipole information; also checks for user requested termination of a simulation

MDSTAT Subroutine

"mdstat" is called at each molecular dynamics time step to form statistics on various average values and fluctuations, and to periodically save the state of the trajectory

MEASFN Subroutine

MEASFP Subroutine

MEASFS Subroutine

MEASPM Subroutine

"measpm" computes the volume of a single prism section of the full interior polyhedron

MECHANIC Subroutine

"mechanic" sets up needed parameters for the potential energy calculation and reads in many of the user selectable options

MERGE Subroutine

"merge" combines the reference and current structures into a single new "current" structure containing the reference atoms followed by the atoms of the current structure

METRIC Subroutine

"metric" takes as input the trial distance matrix and computes the metric matrix of all possible dot products between the atomic vectors and the center of mass using the law of cosines and the following formula for the distances to the center of mass:

MIDERR Function

"miderr" is the secondary error function and derivatives for a distance geometry embedding; it includes components from the distance bounds, local geometry, chirality and torsional restraint errors

MINIMIZ1 Function

"minimiz1" is a service routine that computes the energy and gradient for a low storage BFGS optimization in Cartesian coordinate space

MINIMIZE Program

"minimize" performs energy minimization in Cartesian coordinate space using a low storage BFGS nonlinear optimization

MINIROT Program

"minirot" performs an energy minimization in torsional angle space using a low storage BFGS nonlinear optimization

MINIROT1 Function

"minirot1" is a service routine that computes the energy and gradient for a low storage BFGS nonlinear optimization in torsional angle space

MINPATH Subroutine

"minpath" is a routine for finding the triangle smoothed upper and lower bounds of each atom to a specified root atom using a sparse variant of the Bellman-Ford shortest path algorithm

MINRIGID Program

"minrigid" performs an energy minimization of rigid body atom groups using a low storage BFGS nonlinear optimization

MINRIGID1 Function

"minrigid1" is a service routine that computes the energy and gradient for a low storage BFGS nonlinear optimization of rigid bodies

MMID Subroutine

"mmid" implements a modified midpoint method to advance the integration of a set of first order differential equations

MODECART Subroutine

MODEROT Subroutine

MODESRCH Subroutine

MODETORS Subroutine

MODULI Subroutine

"moduli" sets the moduli of the inverse discrete Fourier transform of the B-splines; bsmod[1-3] hold these values, nfft[1-3] are the grid dimensions, bsorder is the order of B-spline approximation

MOLECULE Subroutine

"molecule" counts the molecules, assigns each atom to its molecule and computes the mass of each molecule

MOLUIND Subroutine

"moluind" computes the molecular induced dipole components in the presence of an external electric field

MOMENTS Subroutine

"moments" computes the total electric charge, dipole and quadrupole moments for the entire system as a sum over the partial charges, bond dipoles and atomic multipole moments

MONTE Program

"monte" performs a Monte Carlo/MCM conformational search using either Cartesian single atom or torsional move sets

MUTATE Subroutine

"mutate" constructs the hybrid hamiltonian for a specified initial state, final state and mutation parameter "lambda"

NEEDUPDATE Subroutine

NEIGHBOR Subroutine

"neighbor" finds all of the neighbors of each atom

NEWATM Subroutine

"newatm" creates and defines an atom needed for the Cartesian coordinates file, but which may not present in the original Protein Data Bank file

NEWTON Program

"newton" performs an energy minimization in Cartesian coordinate space using a truncated Newton method

NEWTON1 Function

"newton1" is a service routine that computes the energy and gradient for truncated Newton optimization in Cartesian coordinate space

NEWTON2 Subroutine

"newton2" is a service routine that computes the sparse matrix Hessian elements for truncated Newton optimization in Cartesian coordinate space

NEWTROT Program

"newtrot" performs an energy minimization in torsional angle space using a truncated Newton conjugate gradient method

NEWTROT1 Function

"newtrot1" is a service routine that computes the energy and gradient for truncated Newton conjugate gradient optimization in torsional angle space

NEWTROT2 Subroutine

"newtrot2" is a service routine that computes the sparse matrix Hessian elements for truncated Newton optimization in torsional angle space

NEXTARG Subroutine

"nextarg" finds the next unused command line argument and returns it in the input character string

NEXTTEXT Function

"nexttext" finds and returns the location of the first non-blank character within an input text string; zero is returned if no such character is found

NORMAL Function

"normal" generates a random number from a normal Gaussian distribution with a mean of zero and a variance of one

NUCBASE Subroutine

"nucbase" builds the side chain for a single nucleotide base in terms of internal coordinates

NUCCHAIN Subroutine

"nucchain" builds up the internal coordinates for a nucleic acid sequence from the sugar type, backbone and glycosidic torsional values

NUCLEIC Program

"nucleic" builds the internal and Cartesian coordinates of a polynucleotide from nucleic acid sequence and torsional angle values for the nucleic acid backbone and side chains

NUMBER Function

"number" converts a text numeral into an integer value; the input string must contain only numeric characters

NUMERAL Subroutine

"numeral" converts an input integer number into the corresponding right- or left-justified text numeral

NUMGRAD Subroutine

"numgrad" computes the gradient of the objective function "fvalue" with respect to Cartesian coordinates of the atoms via a two-sided numerical differentiation

OCVM Subroutine

"ocvm" is an optimally conditioned variable metric nonlinear optimization routine without line searches

OLDATM Subroutine

"oldatm" get the Cartesian coordinates for an atom from the Protein Data Bank file, then assigns the atom type and atomic connectivities

OPENEND Subroutine

"openend" opens a file on a Fortran unit such that the position is set to the bottom for appending to the end of the file

OPTIMIZ1 Function

"optimiz1" is a service routine that computes the energy and gradient for optimally conditioned variable metric optimization in Cartesian coordinate space

OPTIMIZE Program

"optimize" performs energy minimization in Cartesian coordinate space using an optimally conditioned variable metric method

OPTIROT Program

"optirot" performs an energy minimization in torsional angle space using an optimally conditioned variable metric method

OPTIROT1 Function

"optirot1" is a service routine that computes the energy and gradient for optimally conditioned variable metric optimization in torsional angle space

OPTRIGID Program

"optrigid" performs an energy minimization of rigid body atom groups using an optimally conditioned variable metric method

OPTRIGID1 Function

"optrigid1" is a service routine that computes the energy and gradient for optimally conditioned variable metric optimization of rigid bodies

OPTSAVE Subroutine

"optsave" is used by the optimizers to write imtermediate coordinates and other relevant information; also checks for user requested termination of an optimization

ORBITAL Subroutine

"orbital" finds and organizes lists of atoms in a pisystem, bonds connecting pisystem atoms and torsions whose two central atoms are both pisystem atoms

ORIENT Subroutine

"orient" computes a set of reference Cartesian coordinates in standard orientation for each rigid body atom group

ORTHOG Subroutine

"orthog" performs an orthogonalization of an input matrix via the modified Gram-Schmidt algorithm

OVERLAP Subroutine

"overlap" computes the overlap for two parallel p-orbitals given the atomic numbers and distance of separation

PARAMYZE Subroutine

"paramyze" prints the force field parameters used in the computation of each of the potential energy terms

PASSB Subroutine

PASSB2 Subroutine

PASSB3 Subroutine

PASSB4 Subroutine

PASSB5 Subroutine

PASSF Subroutine

PASSF2 Subroutine

PASSF3 Subroutine

PASSF4 Subroutine

PASSF5 Subroutine

PATH Program

"path" locates a series of structures equally spaced along a conformational pathway connecting the input reactant and product structures; a series of constrained optimizations orthogonal to the path is done via Lagrangian multipliers

PATH1 Function

PATHPNT Subroutine

"pathpnt" finds a structure on the synchronous transit path with the specified path value "t"

PATHSCAN Subroutine

"pathscan" makes a scan of a synchronous transit pathway by computing structures and energies for specific path values

PATHVAL Subroutine

"pathval" computes the synchronous transit path value for the specified structure

PDBATM Subroutine

"pdbatm" adds an atom to the Protein Data Bank file

PDBXYZ Program

"pdbxyz" takes as input a Protein Data Bank file and then converts to and writes out a Cartesian coordinates file and, for biopolymers, a sequence file

PIALTER Subroutine

"pialter" first modifies bond lengths and force constants according to the standard bond slope parameters and the bond order values stored in "pnpl"; also alters some 2-fold torsional parameters based on the bond-order * beta matrix

PIMOVE Subroutine

"pimove" rotates the vector between atoms "list(1)" and "list(2)" so that atom 1 is at the origin and atom 2 along the x-axis; the atoms defining the respective planes are also moved and their bond lengths normalized

PIPLANE Subroutine

"piplane" selects the three atoms which specify the plane perpendicular to each p-orbital; the current version will fail in certain situations, including ketenes, allenes, and isolated or adjacent triple bonds

PISCF Subroutine

"piscf" performs an scf molecular orbital calculation for the pisystem using a modified Pariser-Parr-Pople method

PITILT Subroutine

"pitilt" calculates for each pibond the ratio of the actual p-orbital overlap integral to the ideal overlap if the same orbitals were perfectly parallel

PLACE Subroutine

"place" finds the probe sites by putting the probe sphere tangent to each triple of neighboring atoms

POLARGRP Subroutine

"polargrp" generates members of the polarization group of each atom and separate lists of the 1-2, 1-3 and 1-4 group connectivities

POLARIZE Program

"polarize" computes the molecular polarizability by applying an external field along each axis followed by diagonalization of the resulting polarizability tensor

POLYMER Subroutine

"polymer" tests for the presence of an infinite polymer extending across periodic boundaries

POLYP Subroutine

"polyp" is a polynomial product routine that multiplies two algebraic forms

POTNRG Function

POTOFF Subroutine

"potoff" clears the forcefield definition by turning off the use of each of the potential energy functions

POWER Subroutine

"power" uses the power method with deflation to compute the few largest eigenvalues and eigenvectors of a symmetric matrix

PRECISE Function

"precise" finds a machine precision value as selected by the input argument: (1) the smallest positive floating point value, (2) the smallest relative floating point spacing, (3) the largest relative floating point spacing

PRECOND Subroutine

"precond" solves a simplified version of the Newton equations Ms = r, and uses the result to precondition linear conjugate gradient iterations on the full Newton equations in "tnsolve"

PRESSURE Subroutine

"pressure" uses the internal virial to find the pressure in a periodic box and maintains a constant desired pressure by scaling the coordinates via coupling to an external constant pressure bath

PRMKEY Subroutine

"field" parses a text string to extract keywords related to force field potential energy functional forms and constants

PROCHAIN Subroutine

"prochain" builds up the internal coordinates for an amino acid sequence from the phi, psi, omega and chi values

PROJCT Subroutine

PROMO Subroutine

"promo" writes a short message containing information about the TINKER version number and the copyright notice

PROPERTY Function

"property" takes two input snapshot frames and computes the value of the property for which the correlation function is being accumulated

PROPYZE Subroutine

"propyze" finds and prints the total charge, dipole moment components, radius of gyration and moments of inertia

PROSIDE Subroutine

"proside" builds the side chain for a single amino acid residue in terms of internal coordinates

PROTEIN Program

"protein" builds the internal and Cartesian coordinates of a polypeptide from amino acid sequence and torsional angle values for the peptide backbone and side chains

PRTARC Subroutine

"prtarc" writes out a set of Cartesian coordinates for all active atoms in the TINKER XYZ archive format

PRTCAR Subroutine

"prtcar" writes out a set of Cartesian coordinates for all active atoms in the Accelerys InsightII .car format

PRTDYN Subroutine

"prtdyn" writes out the information needed to restart a molecular dynamics trajectory to an external disk file

PRTERR Subroutine

"prterr" writes out a set of coordinates to a disk file prior to aborting on a serious error

PRTINT Subroutine

"prtint" writes out a set of Z-matrix internal coordinates to an external disk file

PRTMOL2 Program

"prtmol2" writes out a set of coordinates in Sybyl MOL2 format to an external disk file

PRTPDB Subroutine

"prtpdb" writes out a set of Protein Data Bank coordinates to an external disk file

PRTPRM Subroutine

"prtprm" writes out a formatted listing of the default set of potential energy parameters for a force field

PRTSEQ Subroutine

"prtseq" writes out a biopolymer sequence to an external disk file with 15 residues per line and distinct chains separated by blank lines

PRTXMOL Subroutine

"prtxmol" writes out a set of Cartesian coordinates for all active atoms in a simple, generic XYZ format originally used by the XMOL program

PRTXYZ Subroutine

"prtxyz" writes out a set of Cartesian coordinates to an external disk file

PSS Program

"pss" implements the potential smoothing plus search method for global optimization in Cartesian coordinate space with local searches performed in Cartesian or torsional space

PSS1 Function

"pss1" is a service routine that computes the energy and gradient during PSS global optimization in Cartesian coordinate space

PSS2 Subroutine

"pss2" is a service routine that computes the sparse matrix Hessian elements during PSS global optimization in Cartesian coordinate space

PSSRGD1 Function

"pssrgd1" is a service routine that computes the energy and gradient during PSS global optimization over rigid bodies

PSSRIGID Program

"pssrigid" implements the potential smoothing plus search method for global optimization for a set of rigid bodies

PSSROT Program

"pssrot" implements the potential smoothing plus search method for global optimization in torsional space

PSSROT1 Function

"pssrot1" is a service routine that computes the energy and gradient during PSS global optimization in torsional space

PSSWRITE Subroutine

PTINCY Function

PZEXTR Subroutine

"pzextr" is a polynomial extrapolation routine used during Bulirsch-Stoer integration of ordinary differential equations

QRFACT Subroutine

"qrfact" performs Householder transformations with column pivoting (optional) to compute a QR factorization of the m by n matrix a; the routine determines an orthogonal matrix q, a permutation matrix p, and an upper trapezoidal matrix r with diagonal elements of nonincreasing magnitude, such that a*p = q*r; the Householder transformation for column k, k = 1,2,...,min(m,n), is of the form

QRSOLVE Subroutine

"qrsolve" solves a*x=b and d*x=0 in the least squares sense; normally used in combination with routine "qrfact" to solve least squares problems

QUATFIT Subroutine

"quatfit" uses a quaternion-based method to achieve the best fit superposition of two sets of coordinates

RADIAL Program

"radial" finds the radial distribution function for a specified pair of atom types via analysis of a set of coordinate frames

RANDOM Function

"random" generates a random number on [0,1] via a long period generator due to L'Ecuyer with Bays-Durham shuffle

RANVEC Subroutine

"ranvec" generates a unit vector in 3-dimensional space with uniformly distributed random orientation

RATTLE Subroutine

"rattle" implements the first portion of the rattle algorithm by correcting atomic positions and half-step velocities to maintain interatomic distance and absolute spatial constraints

RATTLE2 Subroutine

"rattle2" implements the second portion of the rattle algorithm by correcting the full-step velocities in order to maintain interatomic distance constraints

READBLK Subroutine

"readblk" reads in a set of snapshot frames and transfers the values to internal arrays for use in the computation of time correlation functions

READDYN Subroutine

"readdyn" get the positions, velocities and accelerations for a molecular dynamics restart from an external disk file

READINT Subroutine

"readint" gets a set of Z-matrix internal coordinates from an external file

READMOL2 Subroutine

"readmol2" gets a set of Sybyl MOL2 coordinates from an external disk file

READPDB Subroutine

"readpdb" gets a set of Protein Data Bank coordinates from an external disk file

READPRM Subroutine

"readprm" processes the potential energy parameter file in order to define the default force field parameters

READSEQ Subroutine

"readseq" gets a biopolymer sequence containing one or more separate chains from an external file; all lines containing sequence must begin with the starting sequence number, the actual sequence is read from subsequent nonblank characters

READXYZ Subroutine

"readxyz" gets a set of Cartesian coordinates from an external disk file

REFINE Subroutine

"refine" performs minimization of the atomic coordinates of an initial crude embedded distance geometry structure versus the bound, chirality, planarity and torsional error functions

RELEASEMONITOR Subroutine

REPLICA Subroutine

"replica" decides between images and replicates for generation of periodic boundary conditions, and sets the cell replicate list if the replicates method is to be used

RFINDEX Subroutine

"rfindex" finds indices for each multipole site for use in computing reaction field energetics

RGDSRCH Subroutine

RGDSTEP Subroutine

"rgdstep" performs a single molecular dynamics time step for a rigid body calculation

RIBOSOME Subroutine

"ribosome" translates a polypeptide structure in Protein Data Bank format to a Cartesian coordinate file and sequence file

RIGIDXYZ Subroutine

"rigidxyz" computes Cartesian coordinates for a rigid body group via rotation and translation of reference coordinates

RINGS Subroutine

"rings" searches the structure for small rings and stores their constituent atoms

RMSERROR Subroutine

"rmserror" computes the maximum absolute deviation and the rms deviation from the distance bounds, and the number and rms value of the distance restraint violations

RMSFIT Function

"rmsfit" computes the rms fit of two coordinate sets

ROTANG Function

ROTCHECK Function

"rotcheck" tests a specified candidate rotatable bond for the disallowed case where inactive atoms are found on both sides of the candidate bond

ROTEULER Subroutine

"roteuler" computes a set of Euler angle values consistent with an input rotation matrix

ROTLIST Subroutine

"rotlist" generates the minimum list of all the atoms lying to one side of a pair of directly bonded atoms; optionally finds the minimal list by choosing the side with fewer atoms

ROTMAT Subroutine

"rotmat" finds the rotation matrix that converts from the local coordinate system to the global frame at a multipole site

ROTPOLE Subroutine

"rotpole" constructs the set of atomic multipoles in the global frame by applying the correct rotation matrix for each site

ROTRGD Subroutine

"rotrgd" finds the rotation matrix for a rigid body due to a single step of dynamics

ROTSITE Subroutine

"rotsite" computes the atomic multipoles at a specified site in the global coordinate frame by applying a rotation matrix

SADDLE Program

"saddle" finds a transition state between two conformational minima using a combination of ideas from the synchronous transit (Halgren-Lipscomb) and quadratic path (Bell-Crighton) methods

SADDLE1 Function

"saddle1" is a service routine that computes the energy and gradient for transition state optimization

SADDLES Subroutine

"saddles" constructs circles, convex edges and saddle faces

SCAN Program

"scan" attempts to find all the local minima on a potential energy surface via an iterative series of local searches

SCAN1 Function

"scan1" is a service routine that computes the energy and gradient during exploration of a potential energy surface via iterative local search

SCAN2 Subroutine

"scan2" is a service routine that computes the sparse matrix Hessian elements during exploration of a potential energy surface via iterative local search

SDAREA Subroutine

"sdarea" optionally scales the atomic friction coefficient of each atom based on its accessible surface area

SDSTEP Subroutine

"sdstep" performs a single stochastic dynamics time step via a velocity Verlet integration algorithm

SDTERM Subroutine

"sdterm" gets frictional and random force terms needed to update positions and velocities via stochastic dynamics

SEARCH Subroutine

"search" is a unidimensional line search based upon parabolic extrapolation and cubic interpolation using both function and gradient values; if forced to search in an uphill direction, return is after the initial step

SETACCELERATION Subroutine

SETATOMIC Subroutine

SETATOMTYPES Subroutine

SETCHARGE Subroutine

SETCONNECTIVITY Subroutine

SETCOORDINATES Subroutine

SETENERGY Subroutine

SETFILE Subroutine

SETFORCEFIELD Subroutine

SETGRADIENTS Subroutine

SETIME Subroutine

"setime" initializes the elapsed interval CPU timer

SETINDUCED Subroutine

SETKEYWORD Subroutine

SETMASS Subroutine

SETNAME Subroutine

SETSTEP Subroutine

SETSTORY Subroutine

SETTIME Subroutine

SETUPDATED Subroutine

SETVELOCITY Subroutine

SHAKEUP Subroutine

"shakeup" initializes any holonomic constraints for use with the rattle algorithm during molecular dynamics

SIGMOID Function

"sigmoid" implements a normalized sigmoidal function on the interval [0,1]; the curves connect (0,0) to (1,1) and have a cooperativity controlled by beta, they approach a straight line as beta -> 0 and get more nonlinear as beta increases

SKTDYN Subroutine

"sktdyn" sends the current dynamics info via a socket

SKTINIT Subroutine

"sktinit" sets up socket communication with the graphical user interface by starting a Java virtual machine, initiating a server, and loading an object with system information

SKTKILL Subroutine

"sktkill" closes the server and Java virtual machine

SKTOPT Subroutine

"sktopt" sends the current optimization info via a socket

SLATER Subroutine

"slater" is a general routine for computing the overlap integrals between two Slater-type orbitals

SMOOTH Subroutine

"smooth" sets the type of smoothing method and the extent of surface deformation for use with potential energy smoothing

SNIFFER Program

"sniffer" performs a global energy minimization using a discrete version of Griewank's global search trajectory

SNIFFER1 Function

"sniffer1" is a service routine that computes the energy and gradient for the Sniffer global optimization method

SOAK Subroutine

"soak" takes a currently defined solute system and places it into a solvent box, with removal of any solvent molecules that overlap the solute

SORT Subroutine

"sort" takes an input list of integers and sorts it into ascending order using the Heapsort algorithm

SORT10 Subroutine

"sort10" takes an input list of character strings and sorts it into alphabetical order using the Heapsort algorithm, duplicate values are removed from the final sorted list

SORT2 Subroutine

"sort2" takes an input list of reals and sorts it into ascending order using the Heapsort algorithm; it also returns a key into the original ordering

SORT3 Subroutine

"sort3" takes an input list of integers and sorts it into ascending order using the Heapsort algorithm; it also returns a key into the original ordering

SORT4 Subroutine

"sort4" takes an input list of integers and sorts it into ascending absolute value using the Heapsort algorithm

SORT5 Subroutine

"sort5" takes an input list of integers and sorts it into ascending order based on each value modulo "m"

SORT6 Subroutine

"sort6" takes an input list of character strings and sorts it into alphabetical order using the Heapsort algorithm

SORT7 Subroutine

"sort7" takes an input list of character strings and sorts it into alphabetical order using the Heapsort algorithm; it also returns a key into the original ordering

SORT8 Subroutine

"sort8" takes an input list of integers and sorts it into ascending order using the Heapsort algorithm, duplicate values are removed from the final sorted list

SORT9 Subroutine

"sort9" takes an input list of reals and sorts it into ascending order using the Heapsort algorithm, duplicate values are removed from the final sorted list

SPACEFILL Program

"spacefill" computes the surface area and volume of a structure; the van der Waals, accessible-excluded, and contact-reentrant definitions are available

SPECTRUM Program

"spectrum" computes a power spectrum over a wavelength range from the velocity autocorrelation as a function of time

SQUARE Subroutine

"square" is a nonlinear least squares routine derived from the IMSL routine BCLSF and More's Minpack routine LMDER; the Jacobian is estimated by finite differences and bounds can be specified for the variables to be refined

SUFFIX Subroutine

"suffix" checks a filename for the presence of an extension, and appends an extension if none is found

SUPERPOSE Program

"superpose" takes pairs of structures and superimposes them in the optimal least squares sense; it will attempt to match all atom pairs or only those specified by the user

SURFACE Subroutine

"surface" performs an analytical computation of the weighted solvent accessible surface area of each atom and the first derivatives of the area with respect to Cartesian coordinates

SURFATOM Subroutine

"surfatom" performs an analytical computation of the surface area of a specified atom; a simplified version of "surface"

SWITCH Subroutine

"switch" sets the coeffcients used by the fifth and seventh order polynomial switching functions for spherical cutoffs

SYBYLXYZ Program

"sybylxyz" takes as input a Sybyl MOL2 coordinates file, converts to and then writes out Cartesian coordinates

SYMMETRY Subroutine

"symmetry" applies symmetry operators to the fractional coordinates of the asymmetric unit in order to generate the symmetry related atoms of the full unit cell

TANGENT Subroutine

"tangent" finds the projected gradient on the synchronous transit path for a point along the transit pathway

TEMPER Subroutine

"temper" applies a velocity correction at the half time step as needed for the Nose-Hoover extended system thermostat

TEMPER2 Subroutine

"temper2" computes the instantaneous temperature and applies a thermostat via Berendsen velocity scaling, Andersen stochastic collisions, Langevin piston or Nose-Hoover extended systems

TESTGRAD Program

"testgrad" computes and compares the analytical and numerical gradient vectors of the potential energy function with respect to Cartesian coordinates

TESTHESS Program

"testhess" computes and compares the analytical and numerical Hessian matrices of the potential energy function with respect to Cartesian coordinates

TESTLIGHT Program

"testlight" performs a set of timing tests to compare the evaluation of potential energy and energy/gradient using the method of lights with a double loop over all atom pairs

TESTROT Program

"testrot" computes and compares the analytical and numerical gradient vectors of the potential energy function with respect to rotatable torsional angles

TIMER Program

"timer" measures the CPU time required for file reading and parameter assignment, potential energy computation, energy and gradient computation, and Hessian matrix evaluation

TIMEROT Program

"timerot" measures the CPU time required for file reading and parameter assignment, potential energy computation, energy and gradient over torsions, and torsional angle Hessian matrix evaluation

TNCG Subroutine

"tncg" implements a truncated Newton optimization algorithm in which a preconditioned linear conjugate gradient method is used to approximately solve Newton's equations; special features include use of an explicit sparse Hessian or finite-difference gradient-Hessian products within the PCG iteration; the exact Newton search directions can be used optionally; by default the algorithm checks for negative curvature to prevent convergence to a stationary point having negative eigenvalues; if a saddle point is desired this test can be removed by disabling "negtest"

TNSOLVE Subroutine

"tnsolve" uses a linear conjugate gradient method to find an approximate solution to the set of linear equations represented in matrix form by Hp = -g (Newton's equations)

TORPHASE Subroutine

"torphase" sets the n-fold amplitude and phase values for each torsion via sorting of the input parameters

TORQUE Subroutine

"torque" takes the torque values on sites defined by local coordinate frames and distributes thme to convert to forces on the original sites and sites specifying the local frames

TORQUE1 Subroutine

"torque1" takes the torque value on a site defined by a local coordinate frame and distributes it to convert to forces on the original site and sites specifying the local frame

TORSER Function

"torser" computes the torsional error function and its first derivatives with respect to the atomic Cartesian coordinates based on the deviation of specified torsional angles from desired values, the contained bond angles are also restrained to avoid a numerical instability

TORSIONS Subroutine

"torsions" finds the total number of dihedral angles and the numbers of the four atoms defining each dihedral angle

TORUS Subroutine

"torus" sets a list of all of the temporary torus positions by testing for a torus between each atom and its neighbors

TOTERR Function

"toterr" is the error function and derivatives for a distance geometry embedding; it includes components from the distance bounds, hard sphere contacts, local geometry, chirality and torsional restraint errors

TRANSIT Function

"transit" evaluates the synchronous transit function and gradient; linear and quadratic transit paths are available

TRIANGLE Subroutine

"triangle" smooths the upper and lower distance bounds via the triangle inequality using a full-matrix variant of the Floyd-Warshall shortest path algorithm; this routine is usually much slower than the sparse matrix shortest path methods in "geodesic" and "trifix", and should be used only for comparison with answers generated by those routines

TRIFIX Subroutine

"trifix" rebuilds both the upper and lower distance bound matrices following tightening of one or both of the bounds between a specified pair of atoms, "p" and "q", using a modification of Murchland's shortest path update algorithm

TRIMTEXT Function

"trimtext" finds and returns the location of the last non-blank character before the first null character in an input text string; the function returns zero if no such character is found

TRIPLE Function

"triple" finds the triple product of three vectors; used as a service routine by the Connolly surface area and volume computation

TRUST Subroutine

"trust" updates the model trust region for a nonlinear least squares calculation; this version is based on the ideas found in NL2SOL and in Dennis and Schnabel's book

UDIRECT1 Subroutine

"udirect1" computes the reciprocal space contribution of the permanent atomic multipole moments to the electrostatic field for use in finding the direct induced dipole moments via a regular Ewald summation

UDIRECT2 Subroutine

"udirect2" computes the real space contribution of the permanent atomic multipole moments to the electrostatic field for use in finding the direct induced dipole moments via a regular Ewald summation

UFIELD Subroutine

"ufield" finds the field at each polarizable site due to the induced dipoles at the other sites using Thole's method to damp the field at close range

UMUTUAL1 Subroutine

"umutual1" computes the reciprocal space contribution of the induced atomic dipole moments to the electrostatic field for use in iterative calculation of induced dipole moments via a regular Ewald summation

UMUTUAL2 Subroutine

"umutual2" computes the real space contribution of the induced atomic dipole moments to the electrostatic field for use in iterative calculation of induced dipole moments via a regular Ewald summation

UNITCELL Subroutine

"unitcell" gets the periodic boundary box size and related values from an external keyword file

UPCASE Subroutine

"upcase" converts a text string to all upper case letters

VAM Subroutine

"vam" takes the analytical molecular surface defined as a collection of spherical and toroidal polygons and uses it to compute the volume and surface area

VCROSS Subroutine

"vcross" finds the cross product of two vectors

VDWERR Function

"vdwerr" is the hard sphere van der Waals bound error function and derivatives that penalizes close nonbonded contacts, pairwise neighbors are generated via the method of lights

VECANG Function

"vecang" finds the angle between two vectors handed with respect to a coordinate axis; returns an angle in the range [0,2*pi]

VERLET Subroutine

"verlet" performs a single molecular dynamics time step by means of the velocity Verlet multistep recursion formula

VERSION Subroutine

"version" checks the name of a file about to be opened; if if "old" status is passed, the name of the highest current version is returned; if "new" status is passed the filename of the next available unused version is generated

VIBRATE Program

"vibrate" performs a vibrational normal mode analysis; the Hessian matrix of second derivatives is determined and then diagonalized both directly and after mass weighting; output consists of the eigenvalues of the force constant matrix as well as the vibrational frequencies and displacements

VIBRIGID Program

"vibrigid" computes the eigenvalues and eigenvectors of the Hessian matrix over rigid body degrees of freedom

VIBROT Program

"vibrot" computes the eigenvalues and eigenvectors of the torsional Hessian matrix

VNORM Subroutine

"vnorm" normalizes a vector to unit length; used as a service routine by the Connolly surface area and volume computation

VOLUME Subroutine

"volume" calculates the excluded volume via the Connolly analytical volume and surface area algorithm

VOLUME1 Subroutine

"volume1" calculates first derivatives of the total excluded volume with respect to the Cartesian coordinates of each atom

VOLUME2 Subroutine

"volume2" calculates second derivatives of the total excluded volume with respect to the Cartesian coordinates of the atoms

WATSON Subroutine

"watson" uses a rigid body optimization to approximately align the paired strands of a nucleic acid double helix

WATSON1 Function

"watson1" is a service routine that computes the energy and gradient for optimally conditioned variable metric optimization of rigid bodies

XTALERR Subroutine

"xtalerr" computes an error function value derived from derivatives with respect to lattice parameters, lattice energy and monomer dipole moments

XTALFIT Program

"xtalfit" computes an optimized set of potential energy parameters for user specified van der Waals and electrostatic interactions by fitting to crystal structure, lattice energy and monomer dipole moment data

XTALLAT1 Function

"xtalmol1" is a service routine that computes the energy and numerical gradient with respect to the six lattice lengths and angles for a crystal energy minimization

XTALMIN Program

"xtalmin" performs a full crystal energy minimization by alternating cycles of truncated Newton optimization over atomic coordinates with variable metric optimization over the six lattice dimensions and angles

XTALMOL1 Function

"xtalmol1" is a service routine that computes the energy and gradient with respect to the atomic Cartesian coordinates for a crystal energy minimization

XTALMOL2 Subroutine

"xtalmol2" is a service routine that computes the sparse matrix Hessian elements with respect to the atomic Cartesian coordinates for a crystal energy minimization

XTALMOVE Subroutine

"xtalmove" converts fractional to Cartesian coordinates for rigid molecules during fitting of force field parameters to crystal structure data

XTALPRM Subroutine

"xtalprm" stores or retrieves a crystal structure; used to make a previously stored structure the currently active structure, or to store a structure for later use; only provides for the intermolecular energy terms

XTALWRT Subroutine

"xtalwrt" is a utility that prints intermediate results during fitting of force field parameters to crystal data

XYZATM Subroutine

"xyzatm" computes the Cartesian coordinates of a single atom from its defining internal coordinate values

XYZEDIT Program

"xyzedit" provides for modification and manipulation of the contents of a Cartesian coordinates file

XYZINT Program

"xyzint" takes as input a Cartesian coordinates file, then converts to and writes out an internal coordinates file

XYZPDB Program

"xyzpdb" takes as input a Cartesian coordinates file, then converts to and writes out a Protein Data Bank file

XYZRIGID Subroutine

"xyzrigid" computes the center of mass and Euler angle rigid body coordinates for each atom group in the system

XYZSYBYL Program

"xyzsybyl" takes as input a Cartesian coordinates file, converts to and then writes out a Sybyl MOL2 file

ZATOM Subroutine

"zatom" adds an atom to the end of the current Z-matrix and then increments the atom counter; atom type, defining atoms and internal coordinates are passed as arguments

ZHELP Subroutine

"zhelp" prints the general information and instructions for the Z-matrix editing program

ZVALUE Subroutine

"zvalue" gets user supplied values for selected coordinates as needed by the internal coordinate editing program

10. Descriptions of Global 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

11. Index of Function & Subroutine Calls

This section contains an alphabetical cross index listing of the routines called by each TINKER program, subroutine and function. Routines not present in this list do not make calls to any other portion of the TINKER package.

Routine	List of Source Code Units called by this Routine				
ACTIVE	GETTEXT	UPCASE			
ADDBASE	ADDBOND	FINDATM	JACOBI	NEWATM	OLDATM
	OVERLAP	PIALTER	PIMOVE	PITILT	
ADDSIDE	ADDBASE	ADDBOND	FATAL	FINDATM	FREEUNIT
	JACOBI	NEWATM	OLDATM	OVERLAP	PIALTER
	PIMOVE	PITILT	PRTSEQ	VERSION	
ALCHEMY	ENERGY	FINAL	FREEUNIT	GETTEXT	GETXYZ
	HATOM	HYBRID	INITIAL	MECHANIC	NUMERAL
	READXYZ	UPCASE	VERSION		
ANALYSIS	BOUNDS	EANGANG3	EANGLE3	EBOND3	EBUCK3
	ECHARGE3	ECHGDPL3	EGAUSS3	EGEOM3	EHAL3
	EIMPROP3	EIMPTOR3	ELJ3	EMETAL3	EMM3HB3
	EMPOLE3	EOPBEND3	EOPDIST3	EPITORS3	ERXNFLD3
	ESOLV3	ESTRBND3	ESTRTOR3	ETORS3	ETORTOR3
	EUREY3	EXTRA3	PISCF	REPLICA	
ANALYZE	ANALYZ4	ANALYZ6	ANALYZ8	ATOMYZE	ENRGYZE
	FINAL	FREEUNIT	GETXYZ	INITIAL	MECHANIC
	NEXTARG	PARAMYZE	PROPYZE	READXYZ	SUFFIX
	TRIMTEXT	UPCASE	VERSION		
ANGLES	FATAL				
ANNEAL	BEEMAN	FINAL	GETTEXT	GETXYZ	INITIAL
	MDINIT	MDREST	MECHANIC	NEXTARG	RGDSTEP
	SDSTEP	SHAKEUP	SIGMOID	UPCASE	VERLET
ARCHIVE	ACTIVE	BASEFILE	FINAL	FREEUNIT	GETTEXT
	INITIAL	NEXTARG	NUMERAL	PRTARC	PRTCAR
	PRTXMOL	PRTXYZ	READXYZ	SUFFIX	TRIMTEXT
	UPCASE	VERSION			

ATTACH	FATAL	SORT			
BASEFILE	CONTROL	GETKEY	TRIMTEXT		
BCUINT	BCUCOF				
BCUINT1	BCUCOF				
BCUINT2	BCUCOF				
BEEMAN	GRADIENT	KINETIC RATTLE	MDSAVE RATTLE2	MDSTAT TEMPER	PRESSURE TEMPER2
BETAI	BETACF	GAMMLN			
BIGBLOCK	CELLATOM				
BITORS	FATAL				
BONDS	FATAL				
BORN	SURFATOM				
BSET	BMAX				
BSSTEP	FATAL	MMID	PZEXTR		
CALENDAR	DATE_AND_TIME				
CERROR	FATAL	TRIMTEXT			
CFFTB	CFFTB1				
CFFTB1	PASSB	PASSB2	PASSB3	PASSB4	PASSB5
CFFTF	CFFTF1				
CFFTF1	PASSF	PASSF2	PASSF3	PASSF4	PASSF5
CFFTI	CFFTI1				
CHKTREE	LOCALXYZ				
CIRPLN	ANORM	DOT	VCROSS	VNORM	
CLIMBER	ENERGY	GETREF	LOCALMIN	MAKEINT	MAKEXYZ
CLIMBRGD	ENERGY	LOCALRGD	RIGIDXYZ		

CLIMBROT	ENERGY	LOCALROT	MAKEXYZ		
CLIMBTOR	CHKTREE	ENERGY MAKEXYZ	GETREF	LOCALXYZ	MAKEINT
CLIMBXYZ	CHKTREE	ENERGY	GETREF	LOCALXYZ	
CLUSTER	CUTOFFS	FATAL UPCASE	GETNUMB	GETTEXT	SORT SORT3
COMMAND	GETARG	UPCASE			
COMPRESS	CERROR	GETTOR			
CONNECT	SORT				
CONNOLLY	COMPRESS	CONTACT TORUS	NEIGHBOR VAM	PLACE	SADDLES
CONTACT	ANORM	CERROR	PTINCY		
CONTROL	GETTEXT	UPCASE			
COORDS	GYRATE	RMSERROR			
CORRELATE	FINAL	INITIAL TRIMTEXT	NEXTARG	PROPERTY	READBLK
CRYSTAL	BIGBLOCK	BOUNDS GETTEXT LATTICE SYMMETRY	FIELD GETXYZ MOLECULE UNITCELL	FINAL INITIAL NEXTARG UPCASE	FREEUNIT KATOM PRTXYZ VERSION
CUTOFFS	GETTEXT	UPCASE			
CYTSY	CYTSYP	CYTSYS			
DEPTH	DOT	VCROSS	VNORM		
DIAGQ	GETIME	SETIME			
DIFFEQ	BSSTEP	GDASTAT	GVALUE		
DIFFUSE	BASEFILE	FATAL INITIAL READXYZ	FIELD KATOM SUFFIX	FINAL MOLECULE UNITCELL	FREEUNIT NEXTARG VERSION
DISTGEOM	ACTIVE	ANGLES FATAL GETIME	ATTACH FINAL GETTEXT	BONDS FREEUNIT GETXYZ	EMBED GEODESIC GRAFIC

		IMPOSE MAKEREF SETIME VERSION	INITIAL NEXTARG TORSIONS	KCHIRAL NUMERAL TRIFIX	KGEOM PRTXYZ UPCASE
DMDUMP	GRAFIC				
DOCUMENT	FINAL	FREEUNIT INITIAL PRTPRM SUFFIX	GETPRM LOWCASE SORT10 TRIMTEXT	GETTEXT NEXTARG SORT6 UPCASE	GETWORD NEXTTEXT SORT7 VERSION
DSTMAT	GETIME	GETNUMB SETIME	GETTEXT SORT2	INVBETA TRIFIX	RANDOM UPCASE
DYNAMIC	BEEMAN	FINAL MDREST SDSTEP	GETXYZ MECHANIC SHAKEUP	INITIAL NEXTARG VERLET	MDINIT RGDSTEP
EANGANG	GROUPS	IMAGE			
EANGANG1	GROUPS	IMAGE			
EANGANG2	EANGANG2A	GROUPS			
EANGANG2A	IMAGE				
EANGANG3	GROUPS	IMAGE			
EANGLE	GROUPS	IMAGE			
EANGLE1	GROUPS	IMAGE			
EANGLE2	EANGLE2A	EANGLE2B	GROUPS		
EANGLE2A	GROUPS	IMAGE			
EANGLE2B	IMAGE				
EANGLE3	GROUPS	IMAGE			
EBOND	GROUPS	IMAGE			
EBOND1	GROUPS	IMAGE			
EBOND2	GROUPS	IMAGE			
EBOND3	GROUPS	IMAGE			
EBUCK	EBUCK0A	EBUCK0B	EBUCK0C	FATAL	

EBUCK0A	GROUPS	IMAGE	SWITCH		
EBUCK0B	GROUPS	LIGHTS	SWITCH		
EBUCK0C	EGAUSS				
EBUCK1	EBUCK1A	EBUCK1B	EBUCK1C	FATAL	
EBUCK1A	GROUPS	IMAGE	SWITCH		
EBUCK1B	GROUPS	LIGHTS	SWITCH		
EBUCK1C	EGAUSS1				
EBUCK2	EBUCK2A	EBUCK2B	FATAL		
EBUCK2A	GROUPS	IMAGE	SWITCH		
EBUCK2B	EGAUSS2				
EBUCK3	EBUCK3A	EBUCK3B	EBUCK3C	FATAL	
EBUCK3A	GROUPS	IMAGE	SWITCH		
EBUCK3B	GROUPS	LIGHTS	SWITCH		
EBUCK3C	EGAUSS3				
ECHARGE	ECHARGE0A	ECHARGE0B	ECHARGE0C	ECHARGE0D	ECHARGE0E
ECHARGE0A	GROUPS	IMAGE	SWITCH		
ECHARGE0B	GROUPS	LIGHTS	SWITCH		
ECHARGE0C	ERF	GROUPS			
ECHARGE0D	EPME	ERFC	GROUPS	IMAGE	SWITCH
ECHARGE0E	EPME	ERFC	GROUPS	LIGHTS	SWITCH
ECHARGE1	ECHARGE1A	ECHARGE1B	ECHARGE1C	ECHARGE1D	
ECHARGE1A	GROUPS	IMAGE	SWITCH		
ECHARGE1B	GROUPS	LIGHTS	SWITCH		
ECHARGE1C	ERF	GROUPS			

ECHARGE1D	EPME1	ERFC	GROUPS	IMAGE	SWITCH
ECHARGE2	ECHARGE2A	ECHARGE2B	ECHARGE2C		
ECHARGE2A	GROUPS	IMAGE	SWITCH		
ECHARGE2B	ERF	GROUPS			
ECHARGE2C	ERFC	GROUPS	IMAGE		
ECHARGE3	ECHARGE3A	ECHARGE3B	ECHARGE3C	ECHARGE3D	ECHARGE3E
ECHARGE3A	GROUPS	IMAGE	SWITCH		
ECHARGE3B	GROUPS	LIGHTS	SWITCH		
ECHARGE3C	ERF	GROUPS			
ECHARGE3D	EPME3	ERFC	GROUPS	IMAGE	SWITCH
ECHARGE3E	EPME3	ERFC	GROUPS	LIGHTS	SWITCH
ECHGDPL	GROUPS	IMAGE	SWITCH		
ECHGDPL1	GROUPS	IMAGE	SWITCH		
ECHGDPL2	GROUPS	IMAGE	SWITCH		
ECHGDPL3	GROUPS	IMAGE	SWITCH		
EDIPOLE	GROUPS	IMAGE	SWITCH		
EDIPOLE1	GROUPS	IMAGE	SWITCH		
EDIPOLE2	GROUPS	IMAGE	SWITCH		
EDIPOLE3	GROUPS	IMAGE	SWITCH		
EGAUSS	EGAUSS0A	EGAUSS0B			
EGAUSS0A	GROUPS	SWITCH			
EGAUSS0B	ERF	GROUPS			
EGAUSS1	EGAUSS1A	EGAUSS1B			
EGAUSS1A	GROUPS	SWITCH			
EGAUSS1B	ERF	GROUPS			

EGAUSS2	EGAUSS2A	EGAUSS2B	
EGAUSS2A	GROUPS	SWITCH	
EGAUSS2B	GROUPS		
EGAUSS3	EGAUSS3A	EGAUSS3B	
EGAUSS3A	GROUPS	SWITCH	
EGAUSS3B	ERF	GROUPS	
EGBSA0A	GROUPS	SWITCH	
EGBSA0B	ERF	GROUPS	
EGBSA1A	GROUPS	SWITCH	
EGBSA1B	ERF	GROUPS	
EGBSA2A	SWITCH		
EGBSA2B	ERF		
EGBSA3A	GROUPS	SWITCH	
EGBSA3B	ERF	GROUPS	
EGEOM	GROUPS	IMAGE	
EGEOM1	GROUPS	IMAGE	
EGEOM2	GROUPS	IMAGE	
EGEOM3	GROUPS	IMAGE	
EHAL	EHAL0A	EHAL0B	
EHAL0A	GROUPS	IMAGE	SWITCH
EHAL0B	GROUPS	LIGHTS	SWITCH
EHAL1	EHAL1A	EHAL1B	
EHAL1A	GROUPS	IMAGE	SWITCH
EHAL1B	GROUPS	LIGHTS	SWITCH

EHAL2	GROUPS	IMAGE	SWITCH	
EHAL3	EHAL3A	EHAL3B		
EHAL3A	GROUPS	IMAGE	SWITCH	
EHAL3B	GROUPS	LIGHTS	SWITCH	
EIGEN	GETIME	POWER	SETIME	
EIGENRGD	DIAGQ	HESSRGD		
EIGENROT	DIAGQ	HESSROT		
EIGENROT	DIAGQ	HESSROT		
EIGENTOR	DIAGQ	HESSROT		
EIGENXYZ	DIAGQ	HESSIAN		
EIMPROP	GROUPS	IMAGE		
EIMPROP1	GROUPS	IMAGE		
EIMPROP2	GROUPS	IMAGE		
EIMPROP3	GROUPS	IMAGE		
EIMPTOR	GROUPS	IMAGE		
EIMPTOR1	GROUPS	IMAGE		
EIMPTOR2	GROUPS	IMAGE		
EIMPTOR3	GROUPS	IMAGE		
ELJ	ELJ0A	ELJ0B	ELJ0C	ELJ0D
ELJ0A	GROUPS	IMAGE	SWITCH	
ELJ0B	GROUPS	LIGHTS	SWITCH	
ELJ0C	EGAUSS			
ELJ0D	GROUPS			
ELJ1	ELJ1A	ELJ1B	ELJ1C	ELJ1D
ELJ1A	GROUPS	IMAGE	SWITCH	

ELJ1B	GROUPS	LIGHTS	SWITCH		
ELJ1C	EGAUSS1				
ELJ1D	GROUPS				
ELJ2	ELJ2A	ELJ2B			
ELJ2A	GROUPS	IMAGE	SWITCH		
ELJ2B	EGAUSS2				
ELJ2C	GROUPS				
ELJ3	ELJ3A	ELJ3B	ELJ3C	ELJ3D	
ELJ3A	GROUPS	IMAGE	SWITCH		
ELJ3B	GROUPS	LIGHTS	SWITCH		
ELJ3C	EGAUSS3				
ELJ3D	GROUPS				
EMBED	BNDERR	CHIRER DSTMAT FREEUNIT LOCERR PRTXYZ TORSER	CHKSIZE EIGEN GETIME MAJORIZE REFINE VDWERR	COORDS EXPLORE GYRATE METRIC RMSERROR	DMDUMP FRACDIST IMPOSE NUMERAL SETIME
EMETAL	FATAL				
EMETAL1	FATAL				
EMETAL3	EMETAL				
EMM3HB	EMM3HB0A	EMM3HB0B			
EMM3HB0A	GROUPS	IMAGE	SWITCH		
EMM3HB0B	GROUPS	LIGHTS	SWITCH		
EMM3HB1	EMM3HB1A	EMM3HB1B			
EMM3HB1A	GROUPS	IMAGE	SWITCH		
EMM3HB1B	GROUPS	LIGHTS	SWITCH		

EMM3HB2	GROUPS	IMAGE	SWITCH		
EMM3HB3	EMM3HB3A	EMM3HB3B			
EMM3HB3A	GROUPS	IMAGE	SWITCH		
EMM3HB3B	GROUPS	LIGHTS	SWITCH		
EMPOLE	EMPOLE0A	EMPOLE0B			
EMPOLE0A	CHKPOLE	GROUPS SWITCH	IMAGE	INDUCE	ROTPOLE
EMPOLE0B	CHKPOLE	EREAL	ERECIP	INDUCE	ROTPOLE
EMPOLE1	EMPOLE1A	EMPOLE1B			
EMPOLE1A	CHKPOLE	GROUPS SWITCH	IMAGE TORQUE	INDUCE TORQUE1	ROTPOLE
EMPOLE1B	CHKPOLE	EREAL1 TORQUE	ERECIP1	INDUCE	ROTPOLE
EMPOLE2	EMPOLE2A				
EMPOLE2A	GROUPS	IMAGE	SWITCH	TORQUE	
EMPOLE3	EMPOLE3A	EMPOLE3B			
EMPOLE3A	CHKPOLE	GROUPS SWITCH	IMAGE	INDUCE	ROTPOLE
EMPOLE3B	CHKPOLE	EREAL3	ERECIP3	INDUCE	ROTPOLE
ENERGY	BOUNDS	EANGANG ECHARGE EGEOM ELJ EOPBEND ESOLV ETORTOR REPLICA	EANGLE ECHGDPL EHAL EMETAL EOPDIST ESTRBND EUREY	EBOND EDIPOLE EIMPROP EMM3HB EPITORS ESTRTOR EXTRA	EBUCK EGAUSS EIMPTOR EMPOLE ERXNFLD ETORS PISCF
ENRGYZE	ANALYSIS				
EOPBEND	GROUPS	IMAGE			
EOPBEND1	GROUPS	IMAGE			

EOPBEND2	EOPBEND2A	GROUPS			
EOPBEND2A	IMAGE				
EOPBEND3	GROUPS	IMAGE			
EOPDIST	GROUPS	IMAGE			
EOPDIST1	GROUPS	IMAGE			
EOPDIST2	GROUPS	IMAGE			
EOPDIST3	GROUPS	IMAGE			
EPITORS	GROUPS	IMAGE			
EPITORS1	GROUPS	IMAGE			
EPITORS2	EPITORS2A	GROUPS			
EPITORS2A	IMAGE				
EPITORS3	GROUPS	IMAGE			
EPME	BSPLINE	FFTFRONT			
EPME1	BSPLINE1	FFTBACK	FFTFRONT		
EPME3	BSPLINE	FFTFRONT			
EPUCLC	ANORM				
EREAL	ERFC	IMAGE	SWITCH		
EREAL1	ERFC	IMAGE	SWITCH	TORQUE	TORQUE1
EREAL3	ERFC	IMAGE	SWITCH		
ERECIP1	TORQUE				
ERF	ERFCORE				
ERFC	ERFCORE				
ERFIK	D1D2	RFINDEX			
ERFINV	ERF	FATAL			
ERXNFLD	CHKPOLE	ERFIK	IJKPTS	ROTPOLE	SWITCH

ERXNFLD3	CHKPOLE	ERFIK	IJKPTS	ROTPOLE	SWITCH
ESOLV	BORN	EGBSA0A	EGBSA0B	SURFACE	
ESOLV1	BORN	BORN1	EGBSA1A	EGBSA1B	SURFACE
ESOLV2	EGBSA2A	EGBSA2B			
ESOLV3	BORN	EGBSA3A	EGBSA3B	SURFACE	
ESTRBND	GROUPS	IMAGE			
ESTRBND1	GROUPS	IMAGE			
ESTRBND2	GROUPS	IMAGE			
ESTRBND3	GROUPS	IMAGE			
ESTRTOR	GROUPS	IMAGE			
ESTRTOR1	GROUPS	IMAGE			
ESTRTOR2	GROUPS	IMAGE			
ESTRTOR3	GROUPS	IMAGE			
ETORS	ETORS0A	ETORS0B			
ETORS0A	GROUPS	IMAGE			
ETORS0B	GROUPS				
ETORS1	ETORS1A	ETORS1B			
ETORS1A	GROUPS	IMAGE			
ETORS1B	GROUPS				
ETORS2	ETORS2A	ETORS2B			
ETORS2A	GROUPS	IMAGE			
ETORS2B	GROUPS				
ETORS3	ETORS3A	ETORS3B			
ETORS3A	GROUPS	IMAGE			

ETORS3B	GROUPS				
ETORTOR	BCUINT	GROUPS	IMAGE		
ETORTOR1	BCUINT1	GROUPS	IMAGE		
ETORTOR2	BCUINT2	GROUPS	IMAGE		
ETORTOR3	BCUINT	GROUPS	IMAGE		
EUREY	GROUPS	IMAGE			
EUREY1	GROUPS	IMAGE			
EUREY2	GROUPS	IMAGE			
EUREY3	GROUPS	IMAGE			
EWALDCOF	ERFC				
EXPLORE	INITERR	MIDERR	SIGMOID	TOTERR	
FFTBACK	CFFTB				
FFTFRONT	CFFTF				
FFTSETUP	CFFTI				
FIELD	GETPRM	PRMKEY			
FINAL	SKTKILL				
FRACDIST	DIST2	TRIMTEXT			
FREEUNIT	FATAL				
GDA	DIFFEQ	FINAL GETXYZ NUMERAL VERSION	FREEUNIT INITIAL PRTXYZ	GDASTAT MECHANIC RANDOM	GETTEXT NEXTARG TNCG UPCASE
GDA1	GRADIENT	HESSIAN			
GDA2	GRADIENT				
GDA3	HESSIAN				
GDASTAT	ENERGY	GYRATE	OPTSAVE		

GEODESIC	MINPATH	SORT3			
GETBASE	PDBATM				
GETIME	CLOCK				
GETINT	BASEFILE	CHKXYZ MAKEXYZ VERSION	CONNECT NEXTARG	FATAL READINT	FREEUNIT SUFFIX
GETKEY	FATAL	FREEUNIT UPCASE	GETTEXT	SUFFIX	TRIMTEXT
GETMOL2	BASEFILE	FREEUNIT VERSION	NEXTARG	READMOL2	SUFFIX
GETNUCH	PDBATM				
GETNUMB	TRIMTEXT				
GETPDB	BASEFILE	FREEUNIT VERSION	NEXTARG	READPDB	SUFFIX
GETPRB	DIST2	DOT	GETTOR	VCROSS	
GETPRM	FATAL	FREEUNIT READPRM VERSION	GETTEXT SUFFIX	INITPRM TRIMTEXT	NEXTARG UPCASE
GETPROH	PDBATM				
GETSEQ	GETWORD	TRIMTEXT	UPCASE		
GETSEQN	GETTEXT	GETWORD	TRIMTEXT	UPCASE	
GETSIDE	PDBATM				
GETTOR	DIST2				
GETXYZ	BASEFILE	FATAL SUFFIX	FREEUNIT VERSION	NEXTARG	READXYZ
GRADIENT	BOUNDS	EANGANG1 ECHARGE1 EGEOM1 ELJ1 EOPBEND1 ESOLV1 ETORTOR1 REPLICA	EANGLE1 ECHGDPL1 EHAL1 EMETAL1 EOPDIST1 ESTRBND1 EUREY1	EBOND1 EDIPOLE1 EIMPROP1 EMM3HB1 EPITORS1 ESTRTOR1 EXTRA1	EBUCK1 EGAUSS1 EIMPTOR1 EMPOLE1 ERXNFLD1 ETORS1 PISCF

GRADRGD	GRADIENT				
GRADROT	GRADIENT	ROTLIST			
HANGLE	NUMERAL				
HBOND	NUMERAL				
HDIPOLE	NUMERAL				
HESSIAN	BORN	BOUNDS	CHKPOLE	EANGANG2	EANGLE2
		EBOND2	EBUCK2	ECHARGE2	ECHGDPL2
		EDIPOLE2	EGAUSS2	EGEOM2	EHAL2
		EIMPROP2	EIMPTOR2	ELJ2	EMETAL2
		EMM3HB2	EMPOLE2	EOPBEND2	EOPDIST2
		EPITORS2	ERXNFLD2	ESOLV2	ESTRBND2
		ESTRTOR2	ETORS2	ETORTOR2	EUREY2
		EXTRA2	FATAL	INDUCE	PISCF
		REPLICA	ROTPOLE		
HESSRGD	GRADRGD	RIGIDXYZ			
HESSROT	GRADROT	MAKEXYZ			
HIMPTOR	NUMERAL				
HSTRTOR	NUMERAL				
HTORS	NUMERAL				
HYBRID	HANGLE	HATOM	HBOND	HCHARGE	HDIPOLE
		HIMPTOR	HSTRBND	HSTRTOR	HTORS
		HVDW			
IMPOSE	CENTER	QUATFIT	RMSFIT		
INDUCE	INDUCE0A	INDUCE0B			
INDUCE0A	FATAL	GROUPS	IMAGE	PRTERR	SWITCH
INDUCE0B	FATAL	PRTERR	UDIRECT1	UDIRECT2	UMUTUAL1
		UMUTUAL2			
INEDGE	CERROR				
INERTIA	JACOBI				
INITERR	LOCERR	TORSER			

INITIAL	COMMAND	INITRES	PRECISE	PROMO	
INITROT	FATAL	NEXTARG	ROTCHECK	ROTLIST	
INTEDIT	FIELD	FINAL GETWORD PRTINT ZHELP	FREEUNIT INITIAL TRIMTEXT ZVALUE	GEOMETRY MAKEXYZ UPCASE	GETINT NUMBER VERSION
INTXYZ	FINAL	FREEUNIT VERSION	GETINT	INITIAL	PRTXYZ
INVBETA	BETAI	GAMMLN			
INVERT	FATAL				
IPEDGE	CERROR				
ISPLPE	CYTSY	CYTSYS			
KANGANG	GETTEXT	UPCASE			
KANGLE	GETTEXT	NUMERAL	UPCASE		
KATOM	GETNUMB	GETSTRING	GETTEXT	UPCASE	
KBOND	GETTEXT	KENEG	NUMERAL	UPCASE	
KCHARGE	GETTEXT	UPCASE			
KDIPOLE	GETTEXT	NUMERAL	UPCASE		
KENEG	GETTEXT	NUMERAL	UPCASE		
KEWALD	EWALDCOF	FATAL UPCASE	FFTSETUP	GETTEXT	MODULI
KGEOM	FATAL	GEOMETRY UPCASE	GETTEXT	GETWORD	IMAGE
KIMPROP	GETTEXT	NUMERAL	UPCASE		
KIMPTOR	GETTEXT	NUMERAL	TORPHASE	UPCASE	
KMPOLE	CHKPOLE	GETTEXT SORT3	NUMBER UPCASE	NUMERAL	RANDOM
KOPBEND	GETTEXT	NUMBER	NUMERAL	UPCASE	

KOPDIST	GETTEXT	NUMERAL	UPCASE		
KORBIT	GETTEXT	NUMERAL	UPCASE		
KPITORS	GETTEXT	NUMERAL	UPCASE		
KPOLAR	CHKPOLE	GETTEXT	POLARGRP	UPCASE	
KSOLV	GETTEXT	GETWORD	KANGLE	KBOND	UPCASE
KSTRBND	GETTEXT	UPCASE			
KSTRTOR	GETTEXT	NUMERAL	UPCASE		
KTORS	GETTEXT	NUMERAL	TORPHASE	UPCASE	
KTORTOR	GETTEXT	ISPLPE	NUMERAL	SORT9	UPCASE
KUREY	GETTEXT	NUMERAL	UPCASE		
KVDW	GETTEXT	NUMBER	NUMERAL	UPCASE	
LBFGS	COMMENT'	GETTEXT	OPTSAVE	SEARCH	UPCASE
LIGASE	FINDATM				
LIGHTS	FATAL	SORT2	SORT5		
LMSTEP	PRECISE	QRSOLVE			
LOCALMIN	GRADIENT	TNCG			
LOCALRGD	OCVM				
LOCALROT	OCVM				
LOCALXYZ	TNCG				
MAJORIZE	GETIME	GYRATE	RMSERROR	SETIME	
MAKEINT	ADJACENT	FATAL	GEOMETRY	GETTEXT	UPCASE
MAKEPDB	ATTACH	FREEUNIT GETSIDE VERSION	GETBASE NUMERAL	GETNUCH PDBATM	GETPROH READSEQ
MAKEXYZ	XYZATM				
MAPCHECK	FREEUNIT	NUMERAL	PRTXYZ	VERSION	

MAXWELL	ERFINV	RANDOM			
MCM1	GRADIENT				
MCM2	HESSIAN				
MCMSTEP	TNCG				
MDINIT	FREEUNIT	GETTEXT	GETWORD	GRADIENT	GRPLINE
		LATTICE	MAXWELL	MDREST	NUMERAL
		RANVEC	READDYN	UPCASE	VERSION
MDREST	INVERT				
MDSAVE	FATAL	FREEUNIT	NUMERAL	OPENEND	PRTDYN
		PRTXYZ	SKTDYN	SUFFIX	TRIMTEXT
		VERSION			
MEASFN	CERROR	TRIPLE	VCROSS	VECANG	VNORM
MEASFP	CERROR	DOT	VCROSS	VECANG	VNORM
MEASFS	CERROR	DOT	VECANG	VNORM	
MEASPM	VCROSS				
MECHANIC	ACTIVE	ANGLES	ATTACH	BITORS	BONDS
		CLUSTER	CUTOFFS	FATAL	FIELD
		KANGANG	KANGLE	KATOM	KBOND
		KCHARGE	KDIPOLE	KEWALD	KGEOM
		KIMPROP	KIMPTOR	KMETAL	KMPOLE
		KOPBEND	KOPDIST	KORBIT	KPITORS
		KPOLAR	KSOLV	KSTRBND	KSTRTOR
		KTORS	KTORTOR	KUREY	KVDW
		LATTICE	MOLECULE	MUTATE	ORBITAL
		POLYMER	RINGS	SMOOTH	TORSIONS
		UNITCELL			
MERGE	FATAL	GETREF			
MIDERR	BNDERR	CHIRER	LOCERR	TORSER	
MINIMIZ1	GRADIENT				
MINIMIZE	FINAL	FREEUNIT	GETTEXT	GETXYZ	GRADIENT
		INITIAL	LBFGS	MECHANIC	NEXTARG
		PRTXYZ	UPCASE	VERSION	

MINIROT	FINAL	FREEUNIT INITIAL NEXTARG	GETINT INITROT PRTINT	GETTEXT LBFGS UPCASE	GRADROT MECHANIC VERSION
MINIROT1	GRADROT	MAKEXYZ			
MINRIGID	FINAL	FREEUNIT INITIAL ORIENT	GETTEXT LBFGS PRTXYZ	GETXYZ MECHANIC UPCASE	GRADRGD NEXTARG VERSION
MINRIGID1	GRADRGD	RIGIDXYZ			
MMID	GVALUE				
MODECART	CLIMBXYZ	EIGENXYZ	GETREF	IMPOSE	MAKEREF
MODEROT	CLIMBROT	EIGENROT	MAKEXYZ		
MODESRCH	CLIMBER	EIGENROT	MAKEINT	MAKEREF	MAPCHECK
MODETORS	CLIMBTOR	EIGENTOR MAKEREF	GETREF	IMPOSE	MAKEINT
MODULI	BSPLINE	DFTMOD			
MOLECULE	SORT	SORT3			
MOLUIND	UFIELD				
MOMENTS	CHKPOLE	INDUCE	JACOBI	ROTPOLE	
MONTE	CHKCLASH	FREEUNIT INITIAL MAKEXYZ PRTXYZ VERSION	GETREF INITROT MCMSTEP RANDOM	GETTEXT MAKEINT MECHANIC RANVEC	GETXYZ MAKEREF NEXTARG UPCASE
MUTATE	GETTEXT	UPCASE			
NEIGHBOR	CERROR	DIST2			
NEWATM	ADDBOND	XYZATM			
NEWTON	FINAL	FREEUNIT INITIAL TNCG	GETTEXT MECHANIC UPCASE	GETXYZ NEXTARG VERSION	GRADIENT PRTXYZ
NEWTON1	GRADIENT				
NEWTON2	HESSIAN				

NEWTROT	FINAL	FREEUNIT INITIAL PRTINT	GETINT INITROT TNCG	GETTEXT MECHANIC UPCASE	GRADROT NEXTARG VERSION
NEWTROT1	GRADROT	MAKEXYZ			
NEWTROT2	HESSROT	MAKEXYZ			
NORMAL	RANDOM				
NUCBASE	OCVM	ORIENT	POTOFF	ZATOM	
NUCCHAIN	NUCBASE	OCVM	ORIENT	ZATOM	
NUCLEIC	BASEFILE	CONNECT GETKEY MAKEXYZ PRTINT VERSION	DELETE GETSEQN MOLECULE PRTSEQ WATSON	FIELD INITIAL NEXTARG PRTXYZ	FREEUNIT MAKEINT NUCCHAIN TRIMTEXT
NUMBER	TRIMTEXT				
OCVM	GETTEXT	OPTSAVE	PRECISE	UPCASE	
OLDATM	ADDBOND	FATAL			
OPTIMIZ1	GRADIENT				
OPTIMIZE	FATAL	FINAL GRADIENT OCVM	FREEUNIT INITIAL PRTXYZ	GETTEXT MECHANIC UPCASE	GETXYZ NEXTARG VERSION
OPTIROT	FATAL	FINAL GRADROT NEXTARG VERSION	FREEUNIT INITIAL OCVM	GETINT INITROT PRTINT	GETTEXT MECHANIC UPCASE
OPTIROT1	GRADROT	MAKEXYZ			
OPTRIGID	FATAL	FINAL GRADRGD OCVM VERSION	FREEUNIT INITIAL ORIENT	GETTEXT MECHANIC PRTXYZ	GETXYZ NEXTARG UPCASE
OPTRIGID1	GRADRGD	RIGIDXYZ			
OPTSAVE	FATAL	FREEUNIT PRTINT VERSION	MAKEXYZ PRTXYZ	NUMERAL SKTOPT	OPENEND SUFFIX

ORBITAL	FATAL	GETTEXT	PIPLANE	UPCASE	
ORIENT	XYZRIGID				
OVERLAP	SLATER				
PATH	FINAL	GETXYZ LBFGS ORTHOG	IMPOSE MECHANIC POTNRG	INITIAL NEXTARG	INVERT OPTSAVE
PATH1	POTNRG				
PATHPNT	OCVM				
PATHSCAN	PATHPNT	SADDLE1	TANGENT		
PATHVAL	IMPOSE				
PDBXYZ	CHKXYZ	DELETE GETNUMB PRTXYZ VERSION	FIELD GETPDB RIBOSOME	FINAL INITIAL SORT	FREEUNIT LIGASE UPCASE
PIPLANE	FATAL				
PISCF	NEWATM				
PITILT	OLDATM				
PLACE	CERROR	DIST2	GETPRB	GETTOR	INEDGE
POLARGRP	SORT	SORT8			
POLARIZE	FATAL	GETXYZ MOLUIND	INITIAL	JACOBI	MECHANIC
POLYMER	FATAL	GETTEXT	IMAGE	UPCASE	
POTNRG	GRADIENT				
POWER	RANDOM				
PRECOND	CHOLESKY	COLUMN			
PRESSURE	LATTICE				
PRMKEY	GETTEXT	GETWORD	POTOFF	UPCASE	

PROCHAIN	GETTEXT	PROSIDE	UPCASE	ZATOM	
PROJCT	DOT				
PROPYZE	GRADIENT	GYRATE	INERTIA	MOMENTS	
PROSIDE	FREEUNIT	PRTINT	PRTXYZ	VERSION	ZATOM
PROTEIN	BASEFILE	CHKXYZ FREEUNIT MAKEINT PRTINT VERSION	CONNECT GETKEY MAKEXYZ PRTSEQ	DELETE GETSEQ NEXTARG PRTXYZ	FIELDFINAL INITIAL PROCHAIN TRIMTEXT
PRTARC	VERSION				
PRTCAR	VERSION				
PRTDYN	ZATOM				
PRTERR	ZATOM				
PRTINT	VERSION				
PRTMOL2	NUMBER	VERSION			
PRTPDB	VERSION				
PRTPRM	NUMBER				
PRTSEQ	VERSION				
PRTXMOL	VERSION				
PRTXYZ	VERSION				
PSS	ACTIVE	FINAL INITIAL MAKEREF NEXTARG	GETTEXT INITROT MECHANIC PSSWRITE	GETXYZ LOCALXYZ MODECART SIGMOID	IMPOSE MAKEINT MODETORS UPCASE
PSS1	GRADIENT				
PSS2	HESSIAN				
PSSRGD1	GRADRGD	RIGIDXYZ			
PSSRIGID	FINAL	FREEUNIT INITIAL NUMERAL	GETTEXT MAKEREF OCVM	GETXYZ MECHANIC ORIENT	IMPOSE NEXTARG PRTXYZ

		RGDSRCH VERSION	RIGIDXYZ	SIGMOID	UPCASE
PSSROT	FINAL	FREEUNIT INITIAL MECHANIC OCVM	GETTEXT INITROT MODEROT PRTXYZ	GETXYZ MAKEREF NEXTARG UPCASE	IMPOSE MAKEXYZ NUMERAL VERSION
PSSROT1	GRADROT	MAKEXYZ			
PSSWRITE	FREEUNIT	NUMERAL	PRTXYZ	VERSION	
PTINCY	DOT	EPUCLC	PROJCT	ROTANG	
QUATFIT	JACOBI				
RADIAL	BASEFILE	FATAL GETWORD MOLECULE UNITCELL	FINAL IMAGE NEXTARG UPCASE	FREEUNIT INITIAL READXYZ VERSION	GETTEXT LATTICE SUFFIX
RANDOM	CALENDAR	GETTEXT	UPCASE		
RANVEC	RANDOM				
RATTLE	FATAL	IMAGE	PRTERR		
RATTLE2	FATAL	IMAGE	PRTERR		
READBLK	FATAL	FREEUNIT	GETWORD	NUMERAL	
READDYN	FATAL	VERSION			
READINT	FATAL	GETTEXT VERSION	GETWORD	NEXTTEXT	TRIMTEXT
READMOL2	FATAL	GETTEXT UPCASE	GETWORD VERSION	SORT	TRIMTEXT
READPDB	FATAL	FIXPDB UPCASE	GETTEXT VERSION	NEXTARG	TRIMTEXT
READPRM	FATAL	GETNUMB NUMERAL TRIMTEXT	GETSTRING PRMKEY UPCASE	GETTEXT SORT9	GETWORD TORPHASE
READSEQ	FATAL	GETNUMB VERSION	GETTEXT	GETWORD	TRIMTEXT

READXYZ	CHKXYZ	FATAL SORT	GETTEXT TRIMTEXT	GETWORD VERSION	NEXTTEXT
REFINE	LBFGS				
REPLICA	FATAL				
RGDSRCH	CLIMBRGD	EIGENRGD	RIGIDXYZ		
RGDSTEP	CHOLESKY	GRADIENT MDSTAT	KINETIC PRESSURE	LINBODY ROTRGD	MDSAVE TEMPER2
RIBOSOME	ADDBOND	ADDSIDE NEWATM	FATAL OLDATM	FINDATM PRTSEQ	FREEUNIT VERSION
RINGS	ANGLES	BITORS	BONDS	FATAL	TORSIONS
RMSERROR	TRIMTEXT				
ROTANG	DOT	VCROSS			
ROTCHECK	ROTLIST				
ROTLIST	FATAL				
ROTPOLE	ROTMAT	ROTSITE			
SADDLE	COMMENT'	FATAL GETXYZ MAKEXYZ PATHSCAN SADDLE1 VERSION	FINAL IMPOSE MECHANIC PATHVAL SEARCH	FREEUNIT INITIAL NEXTARG PRTXYZ TANGENT	GETTEXT MAKEINT PATHPNT READXYZ UPCASE
SADDLE1	GRADIENT				
SADDLES	CERROR	IPEDGE	TRIPLE		
SCAN	ACTIVE	FINAL INITROT MECHANIC READXYZ	FREEUNIT LOCALMIN MODESRCH VERSION	GETXYZ MAKEINT NEXTARG	INITIAL MAPCHECK NUMERAL
SCAN1	GRADIENT				
SCAN2	HESSIAN				
SDAREA	SURFATOM				

SDSTEP	GRADIENT	KINETIC	MDSAVE	MDSTAT	PRESSURE
		RATTLE	RATTLE2	SDTERM	
SDTERM	NORMAL	SDAREA			
SETIME	CLOCK				
SHAKEUP	CHKRING	GETNUMB	GETTEXT	GETWORD	UPCASE
SKTDYN	CREATEUPDATE		GETMONITOR	NEEDUPDATE	
		RELEASEMONITOR		SETACCELERATION	
		SETCOORDINATES		SETENERGY	
		SETINDUCED		SETTIME	SETUPDATED
		SETVELOCITY	SKTINIT		
SKTINIT	CREATEJVM		CREATESERVER	CREATESYSTEM	SETATOMIC
		SETATOMTYPES	SETCHARGE		
		SETCONNECTIVITY		SETCOORDINATES	
		SETFILE	SETFORCEFIELD		SETKEYWORD
		SETMASS	SETNAME		SETSTORY
SKTKILL	DESTROYJVM	DESTROYSERVER		SKTDYN	SKTOPT
SKTOPT	CREATEUPDATE		GETMONITOR	NEEDUPDATE	
		RELEASEMONITOR		SETCOORDINATES	
		SETENERGY		SETGRADIENTS	SETINDUCED
		SETSTEP	SETUPDATED	SKTINIT	
SLATER	ASET	BSET	CJKM	POLYP	
SMOOTH	GETTEXT	GETWORD	NEXTARG	UPCASE	
SNIFFER	FINAL	FREEUNIT	GETREF	GETXYZ	GRADIENT
		INITIAL	MAKEREF	MECHANIC	NEXTARG
		OPTSAVE	PRTXYZ	SNIFFER1	VERSION
SNIFFER1	GRADIENT				
SOAK	DELETE	FREEUNIT	IMAGE	LATTICE	MAKEREF
		MERGE	MOLECULE	READXYZ	SUFFIX
		UNITCELL	VERSION		
SPACEFILL	ACTIVE	CONNOLLY	FIELD	FINAL	FREEUNIT
		GETTEXT	GETXYZ	INITIAL	KATOM
		KVDW	NEXTARG	READXYZ	SUFFIX
		UPCASE	VERSION		
SPECTRUM	BASEFILE	FREEUNIT	INITIAL	NEXTARG	SUFFIX
		VERSION			

SQUARE	GETTEXT	LMSTEP RSDVALUE	LSQWRITE TRUST	PRECISE UPCASE	QRFACT
SUFFIX	TRIMTEXT				
SUPERPOSE	FIELD	FINAL IMPOSE PRTXYZ UPCASE	FREEUNIT INITIAL READXYZ VERSION	GETTEXT KATOM SUFFIX	GETXYZ NEXTARG TRIMTEXT
SURFACE	FATAL	SORT2			
SURFATOM	FATAL	SORT2			
SWITCH	REPLICA				
SYBYLXYZ	FINAL	FREEUNIT VERSION	GETMOL2	INITIAL	PRTXYZ
SYMMETRY	CELLATOM				
TANGENT	PATHPNT	SADDLE1			
TEMPER	KINETIC				
TEMPER2	MAXWELL	RANDOM	RANVEC		
TESTGRAD	ENERGY	FINAL INITIAL	GETTEXT MECHANIC	GETXYZ NEXTARG	GRADIENT UPCASE
TESTHESS	FINAL	FREEUNIT HESSIAN NUMGRAD	GETTEXT INITIAL UPCASE	GETXYZ MECHANIC VERSION	GRADIENT NEXTARG
TESTLIGHT	EBUCK	EBUCK1 EGAUSS1 EMM3HB GETXYZ NEXTARG	ECHARGE EHAL EMM3HB1 INITIAL SETIME	ECHARGE1 EHAL1 FINAL LIGHTS	EGAUSS ELJ ELJ1 GETIME MECHANIC
TESTROT	ENERGY	FINAL INITROT	GETINT MAKEXYZ	GRADROT MECHANIC	INITIAL NEXTARG
TIMER	ENERGY	FINAL GRADIENT NEXTARG	GETIME HESSIAN SETIME	GETTEXT INITIAL UPCASE	GETXYZ MECHANIC
TIMEROT	ENERGY	FINAL GRADROT MECHANIC	GETIME HESSROT NEXTARG	GETINT INITIAL SETIME	GETTEXT INITROT UPCASE

TNCG	GETTEXT	HMATRIX TNSOLVE	OPTSAVE UPCASE	PISCF	SEARCH
TNSOLVE	PRECOND				
TORSIONS	FATAL				
TORUS	CERROR	GETTOR			
TOTERR	BNDERR	CHIRER	LOCERR	TORSER	VDWERR
TRIANGLE	FATAL				
TRIPLE	DOT	VCROSS			
TRUST	PRECISE	RSDVALUE			
UDIRECT2	ERFC	IMAGE	SWITCH		
UMUTUAL2	ERFC	IMAGE	SWITCH		
UNITCELL	FATAL	GETTEXT	GETWORD	UPCASE	
VAM	CERROR	CIRPLN GENDOT MEASPM	DEPTH MEASFN TRIPLE	DIST2 MEASFP VCROSS	DOT MEASFS VNORM
VDWERR	LIGHTS				
VECANG	ANORM	DOT	TRIPLE		
VERLET	GRADIENT	KINETIC RATTLE	MDSAVE RATTLE2	MDSTAT TEMPER	PRESSURE TEMPER2
VERSION	LOWCASE	NEXTARG	TRIMTEXT		
VIBRATE	DIAGQ	FATAL HESSIAN NUMERAL	FINAL INITIAL PRTXYZ	FREEUNIT MECHANIC VERSION	GETXYZ NEXTARG
VIBRIGID	DIAGQ	FINAL MECHANIC	GETXYZ ORIENT	HESSRGD	INITIAL
VIBROT	DIAGQ	FINAL INITROT	GETINT MECHANIC	HESSROT	INITIAL
VNORM	ANORM				

VOLUME	CONNOLLY				
VOLUME1	FATAL				
VOLUME2	FATAL				
WATSON	ZATOM				
WATSON1	GRADRGD	RIGIDXYZ			
XTALERR	ENERGY	XTALMOVE	XTALPRM		
XTALFIT	FINAL	GETXYZ POTOFF	INITIAL SQUARE	MECHANIC XTALPRM	NEXTARG
XTALLAT1	ENERGY	LATTICE			
XTALMIN	FINAL	FREEUNIT LATTICE TNCG	GETXYZ MECHANIC VERSION	GRADIENT NEXTARG XTALLAT1	INITIAL OCVM PRTXYZ
XTALMOL1	GRADIENT				
XTALMOL2	HESSIAN				
XTALMOVE	LATTICE				
XTALPRM	BOUNDS	LATTICE	MOLECULE		
XYZEDIT	ACTIVE	BOUNDS FREEUNIT INITIAL MAKEREF RANDOM UNITCELL	CUTOFFS GETXYZ INSERT MERGE SOAK VERSION	DELETE IMAGE KATOM MOLECULE SORT	FIELD FINAL INERTIA LATTICE PRTXYZ SORT4
XYZINT	FINAL	FREEUNIT MAKEINT UPCASE	GETTEXT NEXTARG VERSION	GETXYZ PRTINT	INITIAL READINT
XYZPDB	FIELD	FINAL KATOM VERSION	FREEUNIT MAKEPDB	GETXYZ MOLECULE	INITIAL PRTPDB
XYZRIGID	JACOBI	ROTEULER			
XYZSYBYL	BONDS	FINAL PRTMOL2	FREEUNIT VERSION	GETXYZ	INITIAL
ZATOM	FATAL				

ZVALUE MAKEXYZ TRIMTEXT

12. Test Cases & Examples

This section contains brief descriptions of the sample calculations found in the EXAMPLE subdirectory of the TINKER distribution. These examples exercise several of the current TINKER programs and are intended to provide a flavor of the capabilities of the package.

ANION Example

Computes an estimation of the free energy of hydration of Cl^- anion vs. Br^- anion via a 2 picosecond simulation on a ``hybrid'' anion in a box of water followed by a free energy perturbation calculation

ARGON Example

Performs an initial energy minimization on a periodic box containing 150 argon atoms followed by 6 picoseconds of a molecular dynamics using a modified Beeman integration algorithm and a Bersedsen thermostat

CLUSTER Example

Performs a set of 10 Gaussian density annealing (GDA) trials on a cluster of 13 argon atoms in an attempt to locate the global minimum energy structure

CRAMBIN Example

Generates a TINKER file from a PDB file, followed by a single point energy computation and determination of the molecular volume and surface area

CYCLOHEX Example

First approximately locates the transition state between chair and boat cyclohexane, followed by subsequent refinement of the transition state and a final vibrational analysis to show that a single negative frequency is associated with the saddle point

DIALANINE Example

Finds all the local minima of alanine dipeptide via a potential energy surface scan using torsional modes to jump between the minima

ENKEPHALIN Example

Produces coordinates from the met-enkephalin amino acid sequence and phi/psi angles, followed by truncated Newton energy minimization and determination of the lowest frequency normal mode

FORMAMIDE Example

Converts to a unit cell from fractional coordinates, followed by full crystal energy minimization and determination of optimal carbonyl oxygen energy parameters from a fit to lattice energy and structure

HELIX Example

Performs a rigid-body optimization of the packing of two idealized polyalanine helices using only van der Waals interactions

SALT Example

Converts a sodium chloride assymetric unit to the corresponding unit cell, then runs a crystal minimization starting from the initial diffraction structure using Ewald summation to model the long-range electrostatic interactions.

13. Benchmark Results

The tables in this section provide CPU benchmarks for basic TINKER energy and derivative evaluations, vibrational analysis and molecular dynamics. All times are in seconds and were measured with TINKER executables dimensioned to **maxatm** of 10000 and **maxhess** of 1000000 in the source file **sizes.i**. All calculations were run twice in rapid succession on a quiet machine. The times reported for each benchmark are the results from the second run. If you have built TINKER on an alternative machine type and are able to run the benchmarks on the additional machine type, please send the results for inclusion in a future listing.

BENCHMARK #1: Calmodulin Energy Evaluation

The system is an isolated molecule of the 148-residue protein calmodulin with 2264 atoms using the Amber ff94 force field. All interactions are computed with no use of cutoffs. Times listed are for calculation setup followed by a single energy, energy/gradient and Hessian evaluation.

MACHINE-OS-COMPILER TYPE	MHz	SETUP	ENERGY	GRAD	HESS
Athlon XP 2400+ (RH 8.0, Intel)	2000	0.13	0.28	0.60	2.96
Athlon XP 2400+ (RH 8.0, PGI)	2000	0.16	0.31	0.70	3.60
Athlon XP 2400+ (RH 8.0, g77 3.2)	2000	0.17	0.28	0.66	3.67
Athlon Thunderbird (RH 8.0, Intel)	1400	0.22	0.41	0.86	5.15
Athlon Thunderbird (RH 8.0, PGI)	1400	0.21	0.44	1.00	5.92
Athlon Thunderbird (RH 8.0, g77 3.2)	1400	0.19	0.40	0.94	5.81
Athlon Classic (RH 8.0, Intel)	950	0.30	0.64	1.42	7.07
Athlon Classic (RH 8.0, PGI)	950	0.30	0.69	1.65	7.96
Athlon Classic (RH 8.0, g77 3.2)	950	0.31	0.63	1.57	7.94
Compaq Evo N610c P4 (RH 8.0, Intel)	2000	0.18	0.45	0.87	3.08
Compaq Evo N610c P4 (RH 8.0, PGI)	2000	0.22	0.44	1.06	4.27
Compaq Evo N610c P4 (RH 8.0, Absoft)	2000	0.17	0.52	1.06	3.95
Compaq Evo N610c P4 (RH 8.0, g77 3.2)	2000	0.19	0.41	1.07	4.41
Compaq Evo N610c P4 (WinXP, CVF 6.6)	2000	0.16	0.38	0.98	3.54
Compaq Evo N610c P4 (WinXP, g77 3.2)	2000	0.16	0.40	1.08	4.45
Apple Power Mac G4 (OSX 10.2, Absoft)	733	0.41	2.96	5.12	17.83
Apple Power Mac G4 (OSX 10.2, g77 3.3)	733	0.37	1.98	3.79	14.48
Compaq AlphaServer DS10 (Tru64 5.0)	466	0.35	1.33	1.93	8.40
SGI IndigoII R10K (Irix 6.5, MIPS)	195	1.17	3.49	6.35	23.03

BENCHMARK #2: Crambin Crystal Energy Evaluation

The system is a unit cell of the 46-residue protein crambin containing 2 polypeptide chains, 2 ethanol and 178 water molecules for a total of 1360 atoms using the OPLS-UA force field. Periodic boundaries are used with particle mesh Ewald for electrostatics and a 9.0 ≈ cutoff for vdW interactions. Times listed are for calculation setup followed by a single energy, energy/ gradient and Hessian evaluation.

MACHINE-OS-COMPILER TYPE	MHz	SETUP	ENERGY	GRAD	HESS
Athlon XP 2400+ (RH 8.0, Intel)	2000	0.12	0.12	0.21	0.66
Athlon XP 2400+ (RH 8.0, PGI)	2000	0.13	0.14	0.24	0.63

Athlon XP 2400+ (RH 8.0, g77 3.2)	2000	0.14	0.13	0.28	0.81
Athlon Thunderbird (RH 8.0, Intel)	1400	0.19	0.17	0.30	0.91
Athlon Thunderbird (RH 8.0, PGI)	1400	0.18	0.18	0.32	0.91
Athlon Thunderbird (RH 8.0, g77 3.2)	1400	0.17	0.17	0.38	1.11
Athlon Classic (RH 8.0, Intel)	950	0.26	0.25	0.47	1.46
Athlon Classic (RH 8.0, PGI)	950	0.29	0.27	0.50	1.42
Athlon Classic (RH 8.0, g77 3.2)	950	0.27	0.27	0.56	1.70
Compaq Evo N610c P4 (RH 8.0, Intel)	2000	0.15	0.14	0.27	0.64
Compaq Evo N610c P4 (RH 8.0, PGI)	2000	0.22	0.19	0.33	0.88
Compaq Evo N610c P4 (RH 8.0, Absoft)	2000	0.14	0.22	0.39	0.84
Compaq Evo N610c P4 (RH 8.0, g77 3.2)	2000	0.15	0.20	0.45	1.13
Compaq Evo N610c P4 (WinXP, CVF 6.6)	2000	0.14	0.17	0.33	0.83
Compaq Evo N610c P4 (WinXP, g77 3.2)	2000	0.12	0.22	0.52	1.16
Apple Power Mac G4 (OSX 10.2, Absoft)	733	0.32	0.58	1.09	3.11
Apple Power Mac G4 (OSX 10.2, g77 3.3)	733	0.31	0.42	0.79	2.37
Compaq AlphaServer DS10 (Tru64 5.0)	466	0.29	0.38	0.64	1.95
SGI IndigoII R10K (Irix 6.5, MIPS)	195	0.92	0.74	1.41	3.89

BENCHMARK #3: Peptide Normal Mode Calculation

The system is a minimum energy conformation of a 20-residue peptide containing one of each of the standard amino acids for a total of 328 atoms using the OPLS-AA force field without cutoffs. The time reported is for computation of the Hessian and calculation of the normal modes of the Hessian matrix and the vibration frequencies requiring two separate matrix diagonalization steps.

MACHINE-OS-COMPILER TYPE	MHz	NORMAL MODES
Athlon XP 2400+ (RH 8.0, Intel)	2000	22
Athlon XP 2400+ (RH 8.0, PGI)	2000	26
Athlon XP 2400+ (RH 8.0, g77 3.2)	2000	24
Athlon Thunderbird (RH 8.0, Intel)	1400	31
Athlon Thunderbird (RH 8.0, PGI)	1400	34
Athlon Thunderbird (RH 8.0, g77 3.2)	1400	33
Athlon Classic (RH 8.0, Intel)	950	46
Athlon Classic (RH 8.0, PGI)	950	51
Athlon Classic (RH 8.0, g77 3.2)	950	48
Compaq Evo N610c P4 (RH 8.0, Intel)	2000	19
Compaq Evo N610c P4 (RH 8.0, PGI)	2000	19
Compaq Evo N610c P4 (RH 8.0, Absoft)	2000	20
Compaq Evo N610c P4 (RH 8.0, g77 3.2)	2000	19
Compaq Evo N610c P4 (WinXP, CVF 6.6)	2000	19
Compaq Evo N610c P4 (WinXP, g77 3.2)	2000	20
Apple Power Mac G4 (OSX 10.2, Absoft)	733	67
Apple Power Mac G4 (OSX 10.2, g77 3.3)	733	62
Compaq AlphaServer DS10 (Tru64 5.0)	466	39
SGI IndigoII R10K (Irix 6.5, MIPS)	195	144

BENCHMARK #4: TIP3P Water Box Molecular Dynamics

The system consists of 216 rigid TIP3P water molecules in a 18.643 ≈ periodic box, 9.0 ≈ shifted energy switch cutoffs for nonbonded interactions. The time reported is for 1000 dynamics steps of 1.0 fs each using the modified Beeman integrator and Rattle constraints on all bond lengths.

MACHINE-OS-COMPILER TYPE	MHz	DYNAMICS
Athlon XP 2400+ (RH 8.0, Intel)	2000	37
Athlon XP 2400+ (RH 8.0, PGI)	2000	34
Athlon XP 2400+ (RH 8.0, g77 3.2)	2000	45
Athlon Thunderbird (RH 8.0, Intel)	1400	52
Athlon Thunderbird (RH 8.0, PGI)	1400	47
Athlon Thunderbird (RH 8.0, g77 3.2)	1400	63
Athlon Classic (RH 8.0, Intel)	950	77
Athlon Classic (RH 8.0, PGI)	950	71
Athlon Classic (RH 8.0, g77 3.2)	950	96
Compaq Evo N610c P4 (RH 8.0, Intel)	2000	53
Compaq Evo N610c P4 (RH 8.0, PGI)	2000	54
Compaq Evo N610c P4 (RH 8.0, Absoft)	2000	55
Compaq Evo N610c P4 (RH 8.0, g77 3.2)	2000	91
Compaq Evo N610c P4 (WinXP, CVF 6.6)	2000	63
Compaq Evo N610c P4 (WinXP, g77 3.2)	2000	94
Apple Power Mac G4 (OSX 10.2, Absoft)	733	209
Apple Power Mac G4 (OSX 10.2, g77 3.3)	733	170
Compaq AlphaServer DS10 (Tru64 5.0)	466	106
SGI IndigoII R10K (Irix 6.5, MIPS)	195	280

BENCHMARK #5: TINKER Water Box Molecular Dynamics

The system consists of 216 AMOEBA flexible polarizable atomic multipole water molecules in a 18.643 ≈ periodic box using regular Ewald summation for the electrostatics and a 12.0 ≈ switched cutoff for vdW interactions. The time reported is for 100 dynamics steps of 1.0 fs each using the modified Beeman integrator and 0.01 Debye rms convergence for induced dipole moments.

MACHINE-OS-COMPILER TYPE	MHz	DYNAMICS
Athlon XP 2400+ (RH 8.0, Intel)	2000	108
Athlon XP 2400+ (RH 8.0, PGI)	2000	104
Athlon XP 2400+ (RH 8.0, g77 3.2)	2000	128
Athlon Thunderbird (RH 8.0, Intel)	1400	165
Athlon Thunderbird (RH 8.0, PGI)	1400	158
Athlon Thunderbird (RH 8.0, g77 3.2)	1400	183
Athlon Classic (RH 8.0, Intel)	950	282
Athlon Classic (RH 8.0, PGI)	950	261
Athlon Classic (RH 8.0, g77 3.2)	950	307
Compaq Evo N610c P4 (RH 8.0, Intel)	2000	156
Compaq Evo N610c P4 (RH 8.0, PGI)	2000	191
Compaq Evo N610c P4 (RH 8.0, Absoft)	2000	226
Compaq Evo N610c P4 (RH 8.0, g77 3.2)	2000	243
Compaq Evo N610c P4 (WinXP, CVF 6.6)	2000	176
Compaq Evo N610c P4 (WinXP, g77 3.2)	2000	263
Apple Power Mac G4 (OSX 10.2, Absoft)	733	680

Apple Power Mac G4 (OSX 10.2, g77 3.3)	733	479
Compaq AlphaServer DS10 (Tru64 5.0)	466	358
SGI IndigoII R10K (Irix 6.5, MIPS)	195	868

14. Collaborators & Acknowledgments

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Stew Rubenstein	coordinate interconversions; original optimization methods and torsional angle manipulation
Craig Kundrot	molecular surface area & volume and their derivatives
Shawn Huston	original AMBER/OPLS implementation; free energy calculations; time correlation functions
Mike Dudek	initial multipole models for peptides and proteins
Yong "Mike" Kong	multipole electrostatics; dipole polarization; reaction field treatment; TINKER water model
Reece Hart	potential smoothing methodology; Scheraga's DEM, Straub's GDA and extensions
Mike Hodsdon	extension of the TINKER distgeom program and its application to NMR NOE structure determination
Rohit Pappu	potential smoothing methodology and PSS algorithms; rigid body optimization; GB/SA solvation derivatives
Wijnand Mooij	MM3 directional hydrogen bonding term; crystal lattice minimization code
Gerald Loeffler	stochastic/Langevin dynamics implementation
Marina Vorobieva **Nina Sokolova**	nucleic acid building module and parameter translation
Peter Bagossi	AMOEBA force field parameters for alkanes and diatomics
Pengyu Ren	Ewald summation for polarizable atomic multipoles; AMOEBA force field for water, organics and peptides
Anders Carlsson	original ligand field potential energy term for transition metals
Andrey Kutepov	integrator for rigid-body dynamics trajectories
Tom Darden	Particle Mesh Ewald (PME) code, and development of PME for the AMOEBA force field

Alan Grossfield	Monte Carlo minimization; tophat potential smoothing
Michael Schnieders	Force Field Explorer GUI for TINKER; neighbor lists for nonbonded interactions
Chuanjie Wu	solvation free energy calculations; AMOEBA nucleic acid force field; parameterization tools for TINKER
Justin Xiang	angular overlap and valence bond potential models for transition metals
David Gohara	OpenMP parallelization of energy terms including PME, and parallel neighbor lists

It is critically important that TINKER's distributed force field parameter sets exactly reproduce the intent of the original force field authors. We would like to thank **Julian Tirado-Rives** (OPLS-AA), **Alex MacKerell** (CHARMM27), **Wilfred van Gunsteren** (GROMOS), and **Adrian Roitberg** and **Carlos Simmerling** (AMBER) for their help in testing TINKER's results against those given by the authentic programs and parameter sets. **Lou Allinger** provided updated parameters for MM2 and MM3 on several occasions. His very successful methods provided the original inspiration for the development of TINKER.

Still other workers have devoted considerable time in developing code that will hopefully be incorporated into future TINKER versions; for example, **Jim Kress** (UFF implementation) and **Michael Sheets** (numerous code optimizations, thermodynamic integration). Finally, we wish to thank the many users of the TINKER package for their suggestions and comments, praise and criticism, which have resulted in a variety of improvements.

15. References & Suggested Reading

This section contains a list of the references to general theory, algorithms and implementation details which have been of use during the development of the TINKER package. Methods described in some of the references have been implemented in detail within the TINKER source code. Other references contain useful background information although the algorithms themselves are now obsolete. Still other papers contain ideas or extensions planned for future inclusion in TINKER. References for specific force field parameter sets are provided in an earlier section of this User's Guide. This list is heavily skewed toward biomolecules in general and proteins in particular. This bias reflects our group's major interests; however an attempt has been made to include methods which should be generally applicable.

PARTIAL LIST OF MOLECULAR MECHANICS SOFTWARE PACKAGES

AMBER	Peter Kollman, University of California, San Francisco
AMMP	Rob Harrison, Thomas Jefferson University, Philadelphia
ARGOS	Andy McCammon, University of California, San Diego
BOSS	William Jorgensen, Yale University
BRUGEL	Shoshona Wodak, Free University of Brussels
CFF	Shneior Lifson, Weizmann Institute
CHARMM	Martin Karplus, Harvard University
CHARMM/GEMM	Bernard Brooks, National Institutes of Health, Bethesda
DELPHI	Bastian van de Graaf, Delft University of Technology
DISCOVER	Molecular Simulations Inc., San Diego
DL_POLY	W. Smith & T. Forester, CCP5, Daresbury Laboratory
ECEPP	Harold Scheraga, Cornell University
ENCAD	Michael Levitt, Stanford University
FANTOM	Werner Braun, University of Texas, Galveston
FEDER/2	Nobuhiro Go, Kyoto University
GROMACS	Herman Berendsen, University of Groningen
GROMOS	Wilfred van Gunsteren, BIOMOS and ETH, Zurich
IMPACT	Ronald Levy, Rutgers University
MACROMODEL	Schodinger, Inc., Jersey City, New Jersey
MM2/MM3/MM4	N. Lou Allinger, University of Georgia
MMC	Cliff Dykstra, Indiana Univ.≠Purdue Univ. at Indianapolis
MMFF	Tom Halgren, Merck Research Laboratories, Rahway
MMTK	Konrad Hinsen, Inst. of Structural Biology, Grenoble
MOIL	Ron Elber, Cornell University
MOLARIS	Arieh Warshal, University of Southern California
MOLDY	Keith Refson, Oxford University
MOSCITO	Dietmar Paschek & Alfons Geiger, Universit‰t Dortmund
NAMD	Klaus Schulten, University of Illinois, Urbana
OOMPAA	Andy McCammon, University of California, San Diego
ORAL	Karel Zimmerman, INRA, Jouy-en-Josas, France
ORIENT	Anthony Stone, Cambridge University
PCMODEL	Kevin Gilbert, Serena Software, Bloomington, Indiana
PEFF	Jan Dillen, University of Pretoria, South Africa
Q	Johan ≈qvist, Uppsala University
SIBFA	Nohad Gresh, INSERM, CNRS, Paris
SIGMA	Jan Hermans, University of North Carolina
SPASIBA	Gerard Vergoten, UniversitÈ de Lille
SPASMS	David Spellmeyer and the Kollman Group, UCSF

TINKER	Jay Ponder, Washington University, St. Louis
XPLOR/CNS	Axel Br¸nger, Stanford University
YAMMP	Stephen Harvey, University of Alabama, Birmingham
YASP	Florian Mueller-Plathe, ETH Zentrum, Zurich
YETI	Angelo Vedani, Biografik-Labor 3R, Basel

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