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| **1.** | **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.