Tinker

Author

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Homepage

https://dasher.wustl.edu/tinker/

Source

Source code is available in the homepage.
https://dasher.wustl.edu/tinker/

Reference

Ponder, Jay W. "TINKER: Software tools for molecular design." *Washington University School of Medicine, Saint Louis, MO* 3 (2004).

Description & Use

TINKER currently consists of 61 separate programs, which description is provided in the original documentation (included in the distribution).

Quick start

Each program has ist own syntax for batch use, the following list is (a very incomplete) illustration of input information sequence required by each from them. For more details, please refer to the original manual.

ALCHEMY

```
Enter Cartesian Coordinate File Name :  a.xyz
Numbers of First and Last File to Analyze :  1 2
Enter the Lambda Increment for FEP :  0.01
Enter the System Temperature [300 K] :  300
Enter Number of Blocks for Sub-Averages [1] :  1
Consider only Intermolecular Perturbation Energy [N] :  N
```

ANALYZE

```
Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Energy Analysis Utility Can :

 General System and Force Field Information [G]
 Force Field Parameters for Interactions [P]
 Total Potential Energy and its Components [E]
 Energy Breakdown over Each of the Atoms [A]
 List of the Large Individual Interactions [L]
 Details for All Individual Interactions [D]
 Electrostatic Moments and Principle Axes [M]
 Internal Virial, dE/dV Values & Pressure [V]
 Connectivity Lists for Each of the Atoms [C]

 Enter the Desired Analysis Types [G,P,E,A,L,D,M,V,C] :  g

Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Energy Analysis Utility Can :

 General System and Force Field Information [G]
 Force Field Parameters for Interactions [P]
 Total Potential Energy and its Components [E]
 Energy Breakdown over Each of the Atoms [A]
 List of the Large Individual Interactions [L]
 Details for All Individual Interactions [D]
 Electrostatic Moments and Principle Axes [M]
 Internal Virial, dE/dV Values & Pressure [V]
 Connectivity Lists for Each of the Atoms [C]

 Enter the Desired Analysis Types [G,P,E,A,L,D,M,V,C] :  p

 List Atoms for which Output is Desired [ALL] :
    >  ALL

Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Energy Analysis Utility Can :

 General System and Force Field Information [G]
 Force Field Parameters for Interactions [P]
 Total Potential Energy and its Components [E]
 Energy Breakdown over Each of the Atoms [A]
 List of the Large Individual Interactions [L]
 Details for All Individual Interactions [D]
 Electrostatic Moments and Principle Axes [M]
 Internal Virial, dE/dV Values & Pressure [V]
 Connectivity Lists for Each of the Atoms [C]

 Enter the Desired Analysis Types [G,P,E,A,L,D,M,V,C] :  e
```

```
Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Energy Analysis Utility Can :

 General System and Force Field Information [G]
 Force Field Parameters for Interactions [P]
 Total Potential Energy and its Components [E]
 Energy Breakdown over Each of the Atoms [A]
 List of the Large Individual Interactions [L]
 Details for All Individual Interactions [D]
 Electrostatic Moments and Principle Axes [M]
 Internal Virial, dE/dV Values & Pressure [V]
 Connectivity Lists for Each of the Atoms [C]

 Enter the Desired Analysis Types [G,P,E,A,L,D,M,V,C] :  a

 List Atoms for which Output is Desired [ALL] :
    >  ALL

Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Energy Analysis Utility Can :

 General System and Force Field Information [G]
 Force Field Parameters for Interactions [P]
 Total Potential Energy and its Components [E]
 Energy Breakdown over Each of the Atoms [A]
 List of the Large Individual Interactions [L]
 Details for All Individual Interactions [D]
 Electrostatic Moments and Principle Axes [M]
 Internal Virial, dE/dV Values & Pressure [V]
 Connectivity Lists for Each of the Atoms [C]

 Enter the Desired Analysis Types [G,P,E,A,L,D,M,V,C] :  l

Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Energy Analysis Utility Can :

 General System and Force Field Information [G]
 Force Field Parameters for Interactions [P]
 Total Potential Energy and its Components [E]
 Energy Breakdown over Each of the Atoms [A]
 List of the Large Individual Interactions [L]
 Details for All Individual Interactions [D]
 Electrostatic Moments and Principle Axes [M]
 Internal Virial, dE/dV Values & Pressure [V]
 Connectivity Lists for Each of the Atoms [C]

 Enter the Desired Analysis Types [G,P,E,A,L,D,M,V,C] :  d
```

```
Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Energy Analysis Utility Can :

 General System and Force Field Information [G]
 Force Field Parameters for Interactions [P]
 Total Potential Energy and its Components [E]
 Energy Breakdown over Each of the Atoms [A]
 List of the Large Individual Interactions [L]
 Details for All Individual Interactions [D]
 Electrostatic Moments and Principle Axes [M]
 Internal Virial, dE/dV Values & Pressure [V]
 Connectivity Lists for Each of the Atoms [C]

 Enter the Desired Analysis Types [G,P,E,A,L,D,M,V,C] :  m

Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Energy Analysis Utility Can :

 General System and Force Field Information [G]
 Force Field Parameters for Interactions [P]
 Total Potential Energy and its Components [E]
 Energy Breakdown over Each of the Atoms [A]
 List of the Large Individual Interactions [L]
 Details for All Individual Interactions [D]
 Electrostatic Moments and Principle Axes [M]
 Internal Virial, dE/dV Values & Pressure [V]
 Connectivity Lists for Each of the Atoms [C]

 Enter the Desired Analysis Types [G,P,E,A,L,D,M,V,C] :  v

Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Energy Analysis Utility Can :

 General System and Force Field Information [G]
 Force Field Parameters for Interactions [P]
 Total Potential Energy and its Components [E]
 Energy Breakdown over Each of the Atoms [A]
 List of the Large Individual Interactions [L]
 Details for All Individual Interactions [D]
 Electrostatic Moments and Principle Axes [M]
 Internal Virial, dE/dV Values & Pressure [V]
 Connectivity Lists for Each of the Atoms [C]

 Enter the Desired Analysis Types [G,P,E,A,L,D,M,V,C] :  c

 List Atoms for which Output is Desired [ALL] :
    >  ALL
```

ANNEAL

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter the Initial and Final Temperatures in Degrees K [1000,0] :
1000,0
Enter the Number of Equilibration Steps [0] :  0
Enter the Number of Cooling Protocol Steps [2000] :  100
Use Linear, Sigmoidal or Exponential Cooling Protocol ([L], S or E)
:  L
Enter the Time Step Length in Femtoseconds [1.0] :  1.0
Enter Time between Dumps in Picoseconds [0.1] :  0.1
Increase Atomic Weights by a Factor of 10^x [x=0.0] :  0

Enter Cartesian Coordinate File Name :  a.xyz
Enter the Initial and Final Temperatures in Degrees K [1000,0] :
1000,0
Enter the Number of Equilibration Steps [0] :  0
Enter the Number of Cooling Protocol Steps [2000] :  100
Use Linear, Sigmoidal or Exponential Cooling Protocol ([L], S or E)
:  s
Enter the Time Step Length in Femtoseconds [1.0] :  1
Enter Time between Dumps in Picoseconds [0.1] :  0.1
Increase Atomic Weights by a Factor of 10^x [x=0.0] :  0

Enter Cartesian Coordinate File Name :  a.xyz
Enter the Initial and Final Temperatures in Degrees K [1000,0] :
1000,0
Enter the Number of Equilibration Steps [0] :  0
Enter the Number of Cooling Protocol Steps [2000] :  2000
Use Linear, Sigmoidal or Exponential Cooling Protocol ([L], S or E)
:  e
Enter the Time Step Length in Femtoseconds [1.0] :  1
Enter Time between Dumps in Picoseconds [0.1] :  0.1
Increase Atomic Weights by a Factor of 10^x [x=0.0] :  0
```

ARCHIVE

```
The Tinker Archive File Utility Can :

    (1) Create an Archive from Individual Frames
    (2) Extract Individual Frames from an Archive
    (3) Trim an Archive to Remove Atoms or Frames
    (4) Enforce Periodic Boundaries for a Trajectory
    (5) Unfold Periodic Boundaries for a Trajectory
    (6) Remove Periodic Box Size from a Trajectory

 Number of the Desired Choice [<CR>=Exit] :  1
 Enter Base Name of the Individual Frames :  abc
 Numbers of First & Last File and Step Increment :  1 2 1

The Tinker Archive File Utility Can :
```

```
    (1) Create an Archive from Individual Frames
    (2) Extract Individual Frames from an Archive
    (3) Trim an Archive to Remove Atoms or Frames
    (4) Enforce Periodic Boundaries for a Trajectory
    (5) Unfold Periodic Boundaries for a Trajectory
    (6) Remove Periodic Box Size from a Trajectory

 Number of the Desired Choice [<CR>=Exit] :  2
 Enter the Coordinate Archive File Name :  abcd
 Enter the Coordinate Archive File Name :  a.xyz
 Numbers of First & Last File and Step [<CR>=Exit] :  1 2 3
 Numbers of First & Last File and Step [<CR>=Exit] :  1 2 3
 Numbers of First & Last File and Step [<CR>=Exit] :
...

The Tinker Archive File Utility Can :

    (1) Create an Archive from Individual Frames
    (2) Extract Individual Frames from an Archive
    (3) Trim an Archive to Remove Atoms or Frames
    (4) Enforce Periodic Boundaries for a Trajectory
    (5) Unfold Periodic Boundaries for a Trajectory
    (6) Remove Periodic Box Size from a Trajectory

 Number of the Desired Choice [<CR>=Exit] :  3
 Enter the Coordinate Archive File Name :  a.xyz
 Numbers of the Atoms to be Removed :  1
 Numbers of First & Last File and Step [<CR>=Exit] :
...

The Tinker Archive File Utility Can :

    (1) Create an Archive from Individual Frames
    (2) Extract Individual Frames from an Archive
    (3) Trim an Archive to Remove Atoms or Frames
    (4) Enforce Periodic Boundaries for a Trajectory
    (5) Unfold Periodic Boundaries for a Trajectory
    (6) Remove Periodic Box Size from a Trajectory

 Number of the Desired Choice [<CR>=Exit] :  3
 Enter the Coordinate Archive File Name :  a.xyz
 Numbers of the Atoms to be Removed :  1
 Numbers of First & Last File and Step [<CR>=Exit] :  1 2 3
 Numbers of First & Last File and Step [<CR>=Exit] :  1 2 0.1
 Numbers of First & Last File and Step [<CR>=Exit] :
...

The Tinker Archive File Utility Can :

    (1) Create an Archive from Individual Frames
    (2) Extract Individual Frames from an Archive
    (3) Trim an Archive to Remove Atoms or Frames
```

```
    (4) Enforce Periodic Boundaries for a Trajectory
    (5) Unfold Periodic Boundaries for a Trajectory
    (6) Remove Periodic Box Size from a Trajectory

 Number of the Desired Choice [<CR>=Exit] :  4
 Enter the Coordinate Archive File Name :  a.xyz
 Numbers of First & Last File and Step [<CR>=Exit] :  1 2 3
 Numbers of First & Last File and Step [<CR>=Exit] :
...

The Tinker Archive File Utility Can :

    (1) Create an Archive from Individual Frames
    (2) Extract Individual Frames from an Archive
    (3) Trim an Archive to Remove Atoms or Frames
    (4) Enforce Periodic Boundaries for a Trajectory
    (5) Unfold Periodic Boundaries for a Trajectory
    (6) Remove Periodic Box Size from a Trajectory

 Number of the Desired Choice [<CR>=Exit] :  5
 Enter the Coordinate Archive File Name :  a.xyz
 Numbers of First & Last File and Step [<CR>=Exit] :  1 2 3
 Numbers of First & Last File and Step [<CR>=Exit] :
...

The Tinker Archive File Utility Can :

    (1) Create an Archive from Individual Frames
    (2) Extract Individual Frames from an Archive
    (3) Trim an Archive to Remove Atoms or Frames
    (4) Enforce Periodic Boundaries for a Trajectory
    (5) Unfold Periodic Boundaries for a Trajectory
    (6) Remove Periodic Box Size from a Trajectory

 Number of the Desired Choice [<CR>=Exit] :  6
 Enter the Coordinate Archive File Name :  a.xyz
 Numbers of First & Last File and Step [<CR>=Exit] :  1 2 3
 Numbers of First & Last File and Step [<CR>=Exit] :
...
```

BAR

```
The Tinker Thermodynamic Perturbation Utility Can :

    (1) Create BAR File with Perturbed Potential Energies
    (2) Compute Thermodynamic Values from Tinker BAR File

 Enter the Number of the Desired Choice :  1
 Enter the Coordinate Archive File Name :  a.xyz
 Enter Trajectory A Temperature in Degrees K [298] :  298
 Enter the Coordinate Archive File Name :  a.xyz
 Enter Trajectory B Temperature in Degrees K [298] :  298
```

```
The Tinker Thermodynamic Perturbation Utility Can :

    (1) Create BAR File with Perturbed Potential Energies
    (2) Compute Thermodynamic Values from Tinker BAR File

 Enter the Number of the Desired Choice :  2
 Enter Potential Energy BAR File Name :  a.xyz
 First & Last Frame and Step Increment for Trajectory A :  1,2,1
 First & Last Frame and Step Increment for Trajectory B :  1,2,1
```

CORRELATE

```
The Tinker Correlation Function Utility Can :

    (1) Find Velocity Autocorrelation Function
    (2) Find Superposition Correlation Function

 Enter the Number of the Desired Choice :  1
 Enter Base Name of Coordinate Cycle Files :  a.xyz
 Numbers of First & Last File and Step Increment :  1 2 1
 Maximum Frame Separation to be Used in Correlation [ALL] :  ALL

The Tinker Correlation Function Utility Can :

    (1) Find Velocity Autocorrelation Function
    (2) Find Superposition Correlation Function

 Enter the Number of the Desired Choice :  2
 Enter Base Name of Coordinate Cycle Files :  a.xyz
 Numbers of First & Last File and Step Increment :  1 2 1
 Maximum Frame Separation to be Used in Correlation [ALL] :  ALL
```

CRYSTAL

```
Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Crystal Structure Utility Can :

    (1) Convert Fractional to Cartesian Coords
    (2) Convert Cartesian to Fractional Coords
    (3) Move Any Stray Molecules into Unit Cell
    (4) Make a Unit Cell from Asymmetric Unit
    (5) Make a Big Block from Single Unit Cell

 Enter the Number of the Desired Choice :  1
 Enter Unit Cell Axis Lengths :  1 1 1
 Enter Unit Cell Axis Angles :   90 90 90

Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Crystal Structure Utility Can :
```

```
   (1) Convert Fractional to Cartesian Coords
   (2) Convert Cartesian to Fractional Coords
   (3) Move Any Stray Molecules into Unit Cell
   (4) Make a Unit Cell from Asymmetric Unit
   (5) Make a Big Block from Single Unit Cell

 Enter the Number of the Desired Choice :  2
 Enter Unit Cell Axis Lengths :  1 1 1
 Enter Unit Cell Axis Angles :   90 90 90

Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Crystal Structure Utility Can :

   (1) Convert Fractional to Cartesian Coords
   (2) Convert Cartesian to Fractional Coords
   (3) Move Any Stray Molecules into Unit Cell
   (4) Make a Unit Cell from Asymmetric Unit
   (5) Make a Big Block from Single Unit Cell

 Enter the Number of the Desired Choice :  3
 Enter Unit Cell Axis Lengths :  1 1 1
 Enter Unit Cell Axis Angles :   90 90 90

Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Crystal Structure Utility Can :

   (1) Convert Fractional to Cartesian Coords
   (2) Convert Cartesian to Fractional Coords
   (3) Move Any Stray Molecules into Unit Cell
   (4) Make a Unit Cell from Asymmetric Unit
   (5) Make a Big Block from Single Unit Cell

 Enter the Number of the Desired Choice :  4

 Available Crystallographic Space Groups :

   (1) P1          (2) P2          (3) P1(-)       (4) P21
   (5) C2          (6) Pm          (7) Pc          (8) Cm
   (9) Cc         (10) P2/m       (11) P21/m      (12) C2/m
  (13) P2/c       (14) P21/c      (15) P21/n      (16) P21/a
  (17) C2/c       (18) P21212     (19) P212121    (20) C2221
  (21) Pca21      (22) Pmn21      (23) Pna21      (24) Pn21a
  (25) Cmc21      (26) Aba2       (27) Fdd2       (28) Pnna
  (29) Pmna       (30) Pcca       (31) Pbam       (32) Pccn
  (33) Pbcm       (34) Pnnm       (35) Pbcn       (36) Pbca
  (37) Pnma       (38) Cmcm       (39) Cmca       (40) P41
  (41) P43        (42) I4(-)      (43) P42/n      (44) I41/a
  (45) P41212     (46) P43212     (47) P4(-)21m   (48) P4(-)21c
  (49) P4(-)m2    (50) R3(-)      (51) R3c        (52) P63/m
```

```
  (53) P6(3)/mmc    (54) Pa3(-)       (55) P43m         (56) I4(-)3m
  (57) P4(-)3n      (58) Pm3(-)m      (59) Fm3(-)m      (60) Im3(-)m

 Enter the Number of the Desired Choice :  4
 Enter Unit Cell Axis Lengths :  1 1 1
 Enter Unit Cell Axis Angles :   90 90 90
 Attempt to Merge Fragments to Form Full Molecules [N] :   N
 Move Any Stray Molecules into Unit Cell [N] :   N
 Locate Center of Unit Cell at Coordinate Origin [N] :   N

Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker Crystal Structure Utility Can :

    (1) Convert Fractional to Cartesian Coords
    (2) Convert Cartesian to Fractional Coords
    (3) Move Any Stray Molecules into Unit Cell
    (4) Make a Unit Cell from Asymmetric Unit
    (5) Make a Big Block from Single Unit Cell

 Enter the Number of the Desired Choice :  5
 Enter Unit Cell Axis Lengths :  1 1 1
 Enter Unit Cell Axis Angles :   90 90 90
 Enter Number of Replicates along a-, b- and c-Axes [1 1 1] :   1 1
1
```

DIFFUSE

```
Enter the Coordinate Archive File Name :  a.xyz
Numbers of First & Last Frame and Step Increment :  1 10 1
Enter the Time Increment in Picoseconds [1.0] :  1.0
Numbers of any Atoms to be Excluded :  0
```

DISTGEOM

```
Enter Cartesian Coordinate File Name :  a.xyz
```

DYNAMIC

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter the Number of Dynamics Steps to be Taken :  100
Enter the Time Step Length in Femtoseconds [1.0] :  1.0
Enter Time between Dumps in Picoseconds [0.1] :  0.1

 Available Simulation Control Modes :

    (1) Constant Total Energy Value (E)
    (2) Constant Temperature via Thermostat (T)

 Enter the Number of the Desired Choice [1] :  1

Enter Cartesian Coordinate File Name :  a.xyz
```

```
Enter the Number of Dynamics Steps to be Taken :  100
Enter the Time Step Length in Femtoseconds [1.0] :  1.0
Enter Time between Dumps in Picoseconds [0.1] :  0.1

 Available Simulation Control Modes :

    (1) Constant Total Energy Value (E)
    (2) Constant Temperature via Thermostat (T)

 Enter the Number of the Desired Choice [1] :  2
 Enter the Desired Temperature in Degrees K [298] :  298
```

GDA

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter the Initial Mean Squared Gaussian Width [200.0] :  200.0
Enter Number of Annealing Trials [1] :  1
Use Randomized Initial Coordinates [N] :  N
Enter Initial and Final Beta [0.01, 10**10] :  0.01, 100**10
```

INTEDIT

```
Enter Internal Coordinate File Name :  a.xyz

 If a single atom number is entered, the current definition of
 the atom will be displayed.

 If two atom numbers are entered, the output gives the distance
 between the atoms, and asks for a new bond length if applicable;
 Entry of three atoms shows the angle, and entry of four atoms
 will display the corresponding dihedral angle.

 To change the chirality at an atom, enter its number and -1.
 To change the type of an atom, enter its number, -1, and the
 new atom type number.

 A carriage return at the prompt will display the atom last
 changed or the next atom after the one just examined.

 Typing SHOW will display the contents of the current Z-matrix.

 Entering EXIT writes a new file then stops, while QUIT aborts.

 INTEDIT>  EXIT
...
```

INTXYZ

```
Enter Internal Coordinate File Name :  a.xyz
```

MINIMIZE

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter RMS Gradient per Atom Criterion [0.01] :  0.01
```

MINIROT

```
Enter Internal Coordinate File Name :  a.xyz
```

MINIRIGID

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter RMS Gradient per Rigid Body Criterion [0.01] :  0.01
```

MOL2XYZ

```
Enter a Tripos MOL2 File Name :  a.xyz
```

MOLXYZ

```
Enter a MDL MOL File Name :  a.xyz
```

MONTE

```
Enter Cartesian Coordinate File Name :  a.xyz
Number of Monte Carlo Steps [1000] :  1000
Use [C]artesian or [T]orsional Moves [C] :  C
Enter Maximum Step in Angstroms [3.0] :  3.0
Enter the Desired Temperature in Degrees K [500] :  500
Enter RMS Gradient Criterion [0.01] :  0.01

Enter Cartesian Coordinate File Name :  a.xyz
Number of Monte Carlo Steps [1000] :  1000
Use [C]artesian or [T]orsional Moves [C] :  T

 Selection of Torsional Angles for Rotation :

    0  - Automatic Selection of Torsional Angles
    1  - Manual Selection of Angles to Rotate
    2  - Manual Selection of Angles to Freeze

 Enter the Method of Choice [0] :  0
 Number of Torsions Used in Derivative Computation :     1
 Enter Maximum Step in Degrees [180] :  180
 Enter the Desired Temperature in Degrees K [500] :  500
 Enter RMS Gradient Criterion [0.01] :  0.1

Enter Cartesian Coordinate File Name :  a.xyz
Number of Monte Carlo Steps [1000] :  100
Use [C]artesian or [T]orsional Moves [C] :  T

 Selection of Torsional Angles for Rotation :
```

```
    0  - Automatic Selection of Torsional Angles
    1  - Manual Selection of Angles to Rotate
    2  - Manual Selection of Angles to Freeze

 Enter the Method of Choice [0] :  1
 Enter Atoms in Rotatable Bond    1 :  1
...
```

NEWTON

```
Enter Cartesian Coordinate File Name :  a.xyz
Choose Automatic, Newton, TNCG or DTNCG Method [A] :  a
Precondition via Auto/None/Diag/Block/SSOR/ICCG [A] :  a
Enter RMS Gradient per Atom Criterion [0.01] :  0.1
```

NEWTROT

```
Enter Internal Coordinate File Name :  a.xyz
```

NUCLEIC

```
Enter Name to be Used for Output Files :  test
 Enter Title :  test
 Enter Potential Parameter File Name :  amoeba94
 Enter Potential Parameter File Name :  ../../params/amoeba04
 Enter A-, B- or Z-Form Helix for the Structure [B] :  B

 Enter One Nucleotide per Line, 5' to 3':  Give PDB Residue Code,
 followed by Backbone Torsions (6F) and Glycosidic Torsion (1F)

 Use Residue=MOL to Begin a New Strand, Residue=<CR> to End Input

 Enter Residue   1 :  G
 Enter Residue   2 :  G
 Enter Residue   3 :  A
 Enter Residue   4 :  G
 Enter Residue   5 :  C
 Enter Residue   6 :  G
...
 Enter Residue   7 :
 Build a Double Helix using Complimentary Bases [N] :  N
```

OPTIMIZE

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter RMS Gradient per Atom Criterion [0.01] :  0.1
```

OPTIROT

```
Enter Internal Coordinate File Name :  a.xyz
```

OPTIRIGID

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter RMS Gradient per Rigid Body Criterion [0.01] :  0.1
```

PATH

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter Cartesian Coordinate File Name :  a.xyz
Enter Number of Path Points to Generate [9] :  9
Enter RMS Gradient per Atom Criterion [0.1] :  0.1
```

PDBXYZ

```
Enter Protein Data Bank File Name :  a.xyz
```

POLARIZE

```
Enter Cartesian Coordinate File Name :  a.xyz
```

POLEDIT

```
The Tinker Multipole Editing Utility Can :

    (1) Multipole Parameters from GDMA Output
    (2) Alter Local Coordinate Frame Definitions
    (3) Removal of Intramolecular Polarization

 Enter the Number of the Desired Choice :  1
 Enter GDMA Output File Name :  a.xyz
 Average the Multipole Moments of Equivalent Atoms [N] :  N
 Remove Multipole Components Zeroed by Symmetry [N] :  N

The Tinker Multipole Editing Utility Can :

    (1) Multipole Parameters from GDMA Output
    (2) Alter Local Coordinate Frame Definitions
    (3) Removal of Intramolecular Polarization

 Enter the Number of the Desired Choice :  2
 Enter Cartesian Coordinate File Name :  a.xyz

The Tinker Multipole Editing Utility Can :

    (1) Multipole Parameters from GDMA Output
    (2) Alter Local Coordinate Frame Definitions
    (3) Removal of Intramolecular Polarization

 Enter the Number of the Desired Choice :  3
 Enter Cartesian Coordinate File Name :  a.xyz
 Average the Multipole Moments of Equivalent Atoms [N] :  N
```

```
 Remove Multipole Components Zeroed by Symmetry [N] :  N
```

POTENTIAL

```
The Tinker Electrostatic Potential Utility Can :

    (1) Create an Input File for Gaussian CUBEGEN
    (2) Get QM Potential from a Gaussian CUBE File
    (3) Calculate the Model Potential for a System
    (4) Compare Two Model Potentials for a System
    (5) Compare a Model Potential to a Target Grid
    (6) Fit Electrostatic Parameters to Target Grid

 Enter the Number of the Desired Choice :  1
 Enter Cartesian Coordinate File Name :  a.xyz

The Tinker Electrostatic Potential Utility Can :

    (1) Create an Input File for Gaussian CUBEGEN
    (2) Get QM Potential from a Gaussian CUBE File
    (3) Calculate the Model Potential for a System
    (4) Compare Two Model Potentials for a System
    (5) Compare a Model Potential to a Target Grid
    (6) Fit Electrostatic Parameters to Target Grid

 Enter the Number of the Desired Choice :  2
 Enter the Gaussian CUBE File Name :  a.xyz

The Tinker Electrostatic Potential Utility Can :

    (1) Create an Input File for Gaussian CUBEGEN
    (2) Get QM Potential from a Gaussian CUBE File
    (3) Calculate the Model Potential for a System
    (4) Compare Two Model Potentials for a System
    (5) Compare a Model Potential to a Target Grid
    (6) Fit Electrostatic Parameters to Target Grid

 Enter the Number of the Desired Choice :  3
 Enter Cartesian Coordinate File Name :  a.xyz

The Tinker Electrostatic Potential Utility Can :

    (1) Create an Input File for Gaussian CUBEGEN
    (2) Get QM Potential from a Gaussian CUBE File
    (3) Calculate the Model Potential for a System
    (4) Compare Two Model Potentials for a System
    (5) Compare a Model Potential to a Target Grid
    (6) Fit Electrostatic Parameters to Target Grid

 Enter the Number of the Desired Choice :  4
 Enter Cartesian Coordinate File Name :  a.xyz
```

```
The Tinker Electrostatic Potential Utility Can :

    (1) Create an Input File for Gaussian CUBEGEN
    (2) Get QM Potential from a Gaussian CUBE File
    (3) Calculate the Model Potential for a System
    (4) Compare Two Model Potentials for a System
    (5) Compare a Model Potential to a Target Grid
    (6) Fit Electrostatic Parameters to Target Grid

 Enter the Number of the Desired Choice :  5
 Enter Cartesian Coordinate File Name :  a.xyz

The Tinker Electrostatic Potential Utility Can :

    (1) Create an Input File for Gaussian CUBEGEN
    (2) Get QM Potential from a Gaussian CUBE File
    (3) Calculate the Model Potential for a System
    (4) Compare Two Model Potentials for a System
    (5) Compare a Model Potential to a Target Grid
    (6) Fit Electrostatic Parameters to Target Grid

 Enter the Number of the Desired Choice :  6
 Enter Cartesian Coordinate File Name :  a.xyz
```

PRMEDIT

```
Enter Potential Parameter File Name :  a.xyz

 The Parameter Editing Facility can Provide :

    (1) Format Individual Parameter Records
    (2) Reorder Individual Parameter Records
    (3) Renumber the Atom Types, and Reorder
    (4) Renumber the Atom Classes, and Reorder
    (5) Renumber Types and Classes, and Reorder
    (6) Sort and Format Multipole Parameters
    (7) Renumber and Format Biotype Parameters

 Enter the Number of the Desired Choice :  1
 Reformated Parameter File Written To:  parameter.prm

Enter Potential Parameter File Name :  a.xyz

 The Parameter Editing Facility can Provide :

    (1) Format Individual Parameter Records
    (2) Reorder Individual Parameter Records
    (3) Renumber the Atom Types, and Reorder
    (4) Renumber the Atom Classes, and Reorder
    (5) Renumber Types and Classes, and Reorder
    (6) Sort and Format Multipole Parameters
    (7) Renumber and Format Biotype Parameters
```

```
 Enter the Number of the Desired Choice :  2
 Renumbered Parameter File Written To:  parameter.prm_2

Enter Potential Parameter File Name :  a.xyz

 The Parameter Editing Facility can Provide :

    (1) Format Individual Parameter Records
    (2) Reorder Individual Parameter Records
    (3) Renumber the Atom Types, and Reorder
    (4) Renumber the Atom Classes, and Reorder
    (5) Renumber Types and Classes, and Reorder
    (6) Sort and Format Multipole Parameters
    (7) Renumber and Format Biotype Parameters

 Enter the Number of the Desired Choice :  3
 Enter Starting Number for Atom Types [1] :  1
 Renumbered Parameter File Written To:  parameter.prm_3

Enter Potential Parameter File Name :  a.xyz

 The Parameter Editing Facility can Provide :

    (1) Format Individual Parameter Records
    (2) Reorder Individual Parameter Records
    (3) Renumber the Atom Types, and Reorder
    (4) Renumber the Atom Classes, and Reorder
    (5) Renumber Types and Classes, and Reorder
    (6) Sort and Format Multipole Parameters
    (7) Renumber and Format Biotype Parameters

 Enter the Number of the Desired Choice :  4
 Enter Starting Number for Atom Classes [1] :  1
 Renumbered Parameter File Written To:  parameter.prm_4

Enter Potential Parameter File Name :  a.xyz

 The Parameter Editing Facility can Provide :

    (1) Format Individual Parameter Records
    (2) Reorder Individual Parameter Records
    (3) Renumber the Atom Types, and Reorder
    (4) Renumber the Atom Classes, and Reorder
    (5) Renumber Types and Classes, and Reorder
    (6) Sort and Format Multipole Parameters
    (7) Renumber and Format Biotype Parameters

 Enter the Number of the Desired Choice :  5
 Enter Starting Number for Atom Types [1] :  1
 Enter Starting Number for Atom Classes [1] :  2
 Renumbered Parameter File Written To:  parameter.prm_5
```

```
Enter Potential Parameter File Name :  a.xyz

 The Parameter Editing Facility can Provide :

    (1) Format Individual Parameter Records
    (2) Reorder Individual Parameter Records
    (3) Renumber the Atom Types, and Reorder
    (4) Renumber the Atom Classes, and Reorder
    (5) Renumber Types and Classes, and Reorder
    (6) Sort and Format Multipole Parameters
    (7) Renumber and Format Biotype Parameters

 Enter the Number of the Desired Choice :  6
 Sorted Multipole Values Written To:  multipole.prm

Enter Potential Parameter File Name :  a.xyz

 The Parameter Editing Facility can Provide :

    (1) Format Individual Parameter Records
    (2) Reorder Individual Parameter Records
    (3) Renumber the Atom Types, and Reorder
    (4) Renumber the Atom Classes, and Reorder
    (5) Renumber Types and Classes, and Reorder
    (6) Sort and Format Multipole Parameters
    (7) Renumber and Format Biotype Parameters

 Enter the Number of the Desired Choice :  7
 Renumbered Biotype Values Written To:  biotype.prm
```

PROTEIN

```
Enter Name to be Used for Output Files :  test2
Enter Title :  test2
Enter Potential Parameter File Name :  ../../params/amoeba04

 Enter One Residue Name per Line as the Standard Three-Letter Code,
then
 Phi Psi Omega (3F), Chi Angles (4F), then Disulfide Partner if CYX
(I),
 and D/L Chirality as Desired (A1)

 If Only Residue Names are Entered, the Default is to Build an
Extended
 Conformation Using L-Amino Acids and Zwitterionic Termini

 Regular Amino Acids:  GLY, ALA, VAL, LEU, ILE, SER, THR, CYS, CYX,
PRO,
 PHE, TYR, TRP, HIS, ASP, ASN, GLU, GLN, MET, LYS, ARG, ORN, AIB

 Alternative Protonation States:  CYD, TYD, HID, HIE, ASH, GLH, LYD
```

```
 N-Terminal Cap Residues:  H2N=Deprotonated, FOR=Formyl, ACE=Acetyl,
                           PCA=Pyroglutamic Acid
 C-Terminal Cap Residues:  COH=Protonated, NH2=Amide, NME=N-
MethylAmide

 Use Residue Name=MOL to Start a New Chain, and Use <CR> to End
Input

 Enter Residue   1 :  ALA
 Enter Residue   2 :  GLY
 Enter Residue   3 :

 Cyclize the Polypeptide Chain [N] :  N
```

PSS

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter the Potential Surface Smoothing Parameter [0.0] :  0.0
Enter the Number of Steps for Smoothing Schedule [100] :  10
Perform Forward Smoothing from Input Structure [Y] :  Y
Use Quadratic, Cubic or Sigmoidal Schedule (Q [C] or S) :  Q
Local Search Type - Cartesian, Torsional or None (C T or [N]) :  C
Enter the Range of Local Search Directions (1=Highest Freq) :  1
```

PSSRIGID

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter the Potential Surface Smoothing Parameter [0.0] :  0
```

PSSROT

```
Enter Internal Coordinate File Name :  a.xyz
Enter the Potential Surface Smoothing Parameter [0.0] :  0.1
```

RADIAL

```
Enter the Coordinate Archive File Name :  a.xyz
Numbers of First & Last Frame and Step Increment :  1 3 1
Enter 1st & 2nd Atom Names or Type Numbers :  N H H H
Enter Maximum Distance to Accumulate [10.0 Ang] :  10
Enter Width of Distance Bins [0.01 Ang] :  0.1
Include Intramolecular Pairs in Distribution [N] :  Y
```

SADDLE

```
Enter Cartesian Coordinate File Name :  a.xyz
Selection of Torsional Angles for Rotation :

    0  - Automatic Selection of Torsional Angles
    1  - Manual Selection of Angles to Rotate
    2  - Manual Selection of Angles to Freeze
```

```
 Enter the Method of Choice [0] :  0
 Number of Torsions Used in Derivative Computation :     1
 Enter the Number Search Directions for Local Search [5] :  5
 Enter the Energy Threshold for Local Minima [100.0] :  100
 Enter RMS Gradient per Atom Criterion [0.0001] :  0.1

Enter Cartesian Coordinate File Name :  a.xyz
Selection of Torsional Angles for Rotation :

    0  - Automatic Selection of Torsional Angles
    1  - Manual Selection of Angles to Rotate
    2  - Manual Selection of Angles to Freeze

 Enter the Method of Choice [0] :  1
 Enter Atoms in Rotatable Bond    1 :  1 2
 Enter Atoms in Rotatable Bond    1 :
...

Enter Cartesian Coordinate File Name :  a.xyz
Selection of Torsional Angles for Rotation :

    0  - Automatic Selection of Torsional Angles
    1  - Manual Selection of Angles to Rotate
    2  - Manual Selection of Angles to Freeze

 Enter the Method of Choice [0] :  2
 Enter Atoms in Frozen Bond    1 :  1 2
 Enter Atoms in Frozen Bond    2 :
 Number of Torsions Used in Derivative Computation :     1
 Enter the Number Search Directions for Local Search [5] :  5
 Enter the Energy Threshold for Local Minima [100.0] :  0.02
 Enter RMS Gradient per Atom Criterion [0.0001] :  0.1
```

SCAN

```
Enter Cartesian Coordinate File Name :  a.xyz
Selection of Torsional Angles for Rotation :

    0  - Automatic Selection of Torsional Angles
    1  - Manual Selection of Angles to Rotate
    2  - Manual Selection of Angles to Freeze

 Enter the Method of Choice [0] :  0
 Number of Torsions Used in Derivative Computation :     1
 Enter the Number Search Directions for Local Search [5] :  5
 Enter the Energy Threshold for Local Minima [100.0] :  100
 Enter RMS Gradient per Atom Criterion [0.0001] :  0.1


Enter Cartesian Coordinate File Name :  a.xyz
Selection of Torsional Angles for Rotation :
```

```
    0  - Automatic Selection of Torsional Angles
    1  - Manual Selection of Angles to Rotate
    2  - Manual Selection of Angles to Freeze

 Enter the Method of Choice [0] :  1
 Enter Atoms in Rotatable Bond    1 :  1 2
 Enter Atoms in Rotatable Bond    1 :
 ...

Enter Cartesian Coordinate File Name :  a.xyz
Selection of Torsional Angles for Rotation :

    0  - Automatic Selection of Torsional Angles
    1  - Manual Selection of Angles to Rotate
    2  - Manual Selection of Angles to Freeze

 Enter the Method of Choice [0] :  2
 Enter Atoms in Frozen Bond    1 :  1 2
 Enter Atoms in Frozen Bond    2 :
 Number of Torsions Used in Derivative Computation :     1
 Enter the Number Search Directions for Local Search [5] :  5
 Enter the Energy Threshold for Local Minima [100.0] :  0.02
 Enter RMS Gradient per Atom Criterion [0.0001] :  0.1
```

SNIFFER

```
Enter Cartesian Coordinate File Name :  a.xyz
```

SPACEFILL

```
 Enter Cartesian Coordinate File Name :  a.xyz

 Three Types of Area and Volume can be Computed :

    (1) Van der Waals Area and Volume
    (2) Accessible Area and Excluded Volume
    (3) Contact-Reentrant Area and Volume

 Enter the Number of your Choice [1] :  1
 Include the Hydrogen Atoms in Computation [N] :  Y


 Enter Cartesian Coordinate File Name :  a.xyz

 Three Types of Area and Volume can be Computed :

    (1) Van der Waals Area and Volume
    (2) Accessible Area and Excluded Volume
    (3) Contact-Reentrant Area and Volume

 Enter the Number of your Choice [1] :  2
```

```
 Enter a Value for the Probe Radius [1.4 Ang] :  1.4
 Include the Hydrogen Atoms in Computation [N] :  Y


 Enter Cartesian Coordinate File Name :  a.xyz

 Three Types of Area and Volume can be Computed :

    (1) Van der Waals Area and Volume
    (2) Accessible Area and Excluded Volume
    (3) Contact-Reentrant Area and Volume

 Enter the Number of your Choice [1] :  3
 Enter a Value for the Probe Radius [1.4 Ang] :  1.5
 Include the Hydrogen Atoms in Computation [N] :  Y
```

SPECTRUM

```
Enter Name of Velocity Autocorrelation File :  a.xyz
Enter Time Step for Autocorrelation Data [1.0 fs] :  1.0
```

SUPERPOSE

```
 Enter Cartesian Coordinate File Name :  a.xyz
 Enter Cartesian Coordinate File Name :  a.xyz

 Two Options are Available :  (1) Fit atoms "M" through "N" from
structure 1
 to the corresponding atoms of structure 2. Enter "1,M,N" to use
this option.
 If "N" is omitted, the fit uses atoms 1 through "M". If both "M"
and "N" are
 omitted, the fit uses all atoms; or (2) Individual entry of atom
range pairs
 to be used in the fitting procedure.

 Enter an Option (either 1,M,N or 2 [<CR>=1,0,0]) :  1,2,2
 Include Hydrogen Atoms in the Fitting [Y] :  Y
 Use Mass- or Unit-Weighted Coordinates (M or [U]) :  U
 Write Best-Fit Coordinates of 2nd Molecule [N] :  N
 Cutoff Value for Listing RMS Deviations [0.0] :  0.0
 Structure File 1 :  a.xyz
 Structure File 2 :  a.xyz
```

TESTGRAD

```
Enter Cartesian Coordinate File Name :  a.xyz
Compute the Analytical Gradient Vector [Y] :  Y
Compute the Numerical Gradient Vector [Y] :   Y
Enter Finite Difference Stepsize [ 0.1D-04 Ang] :  0.1
```

TESTHESS

```
Enter Cartesian Coordinate File Name :  a.xyz
Compute Analytical Hessian Matrix [Y] :  Y
Compute Numerical Hessian Matrix [Y] :   Y
Numerical Hessian from Gradient or Function [G] :  H
Enter Finite Difference Stepsize [ 0.1D-04 Ang] :  0.1
List Individual Hessian Components [N] :   Y
```

TESTPAIR

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter Desired Number of Repetitions [1] :  1
```

TESTPOL

```
Enter Cartesian Coordinate File Name :  a.xyz
```

TESTROT

```
Enter Internal Coordinate File Name :  a.xyz
```

TIMER

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter Desired Number of Repetitions [1] :  1
Include Timing for Hessian Evaluations [N] :  Y
```

TIMEROT

```
Enter Internal Coordinate File Name :  a.xyz
```

TORSFIT

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter Central Atoms of the 1st Torsion : N
Enter Central Atoms of the 1st Torsion : N
Enter Central Atoms of the 1st Torsion : N
Enter Central Atoms of the 1st Torsion :
```

VALENCE

```
The Tinker Valence Parameter Utility Can :

    (1) Set Initial Values for Valence Parameters
    (2) Compare QM and MM Vibrational Frequencies
    (3) Force Fit of Parameters to QM Results
    (4) Structure Fit of Parameters to QM Results

 Enter the Number of the Desired Choice :  1
 Enter Cartesian Coordinate File Name :  a.xyz
 Enter the Name of the Gaussian Output File :  a.out
```

```
 Enter the Name of the Gaussian Output File :  a.out
 Enter the Name of the Gaussian Output File :  a.xyz

The Tinker Valence Parameter Utility Can :

    (1) Set Initial Values for Valence Parameters
    (2) Compare QM and MM Vibrational Frequencies
    (3) Force Fit of Parameters to QM Results
    (4) Structure Fit of Parameters to QM Results

 Enter the Number of the Desired Choice :  2
 Enter Cartesian Coordinate File Name :  a.xyz
 Enter the Name of the Gaussian Output File :  a.xyz

The Tinker Valence Parameter Utility Can :

    (1) Set Initial Values for Valence Parameters
    (2) Compare QM and MM Vibrational Frequencies
    (3) Force Fit of Parameters to QM Results
    (4) Structure Fit of Parameters to QM Results

 Enter the Number of the Desired Choice :  3
 Enter Cartesian Coordinate File Name :  a.xyz
 Enter the Name of the Gaussian Output File :  a.xyz
 Enter RMS Gradient Termination Criterion [0.01] :  0.1

 The Tinker Valence Parameter Utility Can :

    (1) Set Initial Values for Valence Parameters
    (2) Compare QM and MM Vibrational Frequencies
    (3) Force Fit of Parameters to QM Results
    (4) Structure Fit of Parameters to QM Results

 Enter the Number of the Desired Choice :  4
 Enter Cartesian Coordinate File Name :  a.xyz
 Enter the Name of the Gaussian Output File :  a.xyz
```

VIBBIG

```
Enter Cartesian Coordinate File Name :  a.xyz
Start at Lowest or Highest Frequency Normal Mode [L] :  L
Enter Desired Frequency Cutoff in cm-1 [0.0] :  0.1
```

VIBRATE

```
Enter Cartesian Coordinate File Name :  a.xyz
Enter Vibrations to Output [List, A=All or <CR>=Exit] :  A
```

VIBROT

```
Enter Internal Coordinate File Name :  a.xyz
```

XTALFIT

```
The Following Parameters can be Fit for each Atom Type :

    (1) Van der Waals Atomic Radius
    (2) Van der Waals Well Depth
    (3) Hydrogen Atom Reduction Factor
    (4) Atomic Partial Charge
    (5) Bond Dipole Moment Magnitude
    (6) Bond Dipole Moment Position
    (7) Atomic Polarizability

 Enter Parameter Type then Atom Class or Type(s) :  1
 Enter Parameter Type then Atom Class or Type(s) :  1 N
 Enter Parameter Type then Atom Class or Type(s) :  1 N
 Enter Parameter Type then Atom Class or Type(s) :
 Enter RMS Gradient Termination Criterion [0.1] :  0.1
 Enter Number of Structures to be Used [1] :  1
 Enter Cartesian Coordinate File Name :  a.xyz

The Following Parameters can be Fit for each Atom Type :

    (1) Van der Waals Atomic Radius
    (2) Van der Waals Well Depth
    (3) Hydrogen Atom Reduction Factor
    (4) Atomic Partial Charge
    (5) Bond Dipole Moment Magnitude
    (6) Bond Dipole Moment Position
    (7) Atomic Polarizability

 Enter Parameter Type then Atom Class or Type(s) :  2
 Enter Parameter Type then Atom Class or Type(s) :  N
 Enter RMS Gradient Termination Criterion [0.1] :
 Enter Number of Structures to be Used [1] :
 Enter Cartesian Coordinate File Name :  a.xyz

The Following Parameters can be Fit for each Atom Type :

    (1) Van der Waals Atomic Radius
    (2) Van der Waals Well Depth
    (3) Hydrogen Atom Reduction Factor
    (4) Atomic Partial Charge
    (5) Bond Dipole Moment Magnitude
    (6) Bond Dipole Moment Position
    (7) Atomic Polarizability

 Enter Parameter Type then Atom Class or Type(s) :  3
 Enter Parameter Type then Atom Class or Type(s) :  N
 Enter RMS Gradient Termination Criterion [0.1] :
 Enter Number of Structures to be Used [1] :
 Enter Cartesian Coordinate File Name :  a.xyz
```

```
The Following Parameters can be Fit for each Atom Type :

    (1) Van der Waals Atomic Radius
    (2) Van der Waals Well Depth
    (3) Hydrogen Atom Reduction Factor
    (4) Atomic Partial Charge
    (5) Bond Dipole Moment Magnitude
    (6) Bond Dipole Moment Position
    (7) Atomic Polarizability

 Enter Parameter Type then Atom Class or Type(s) :  4
 Enter Parameter Type then Atom Class or Type(s) :  N
 Enter RMS Gradient Termination Criterion [0.1] :
 Enter Number of Structures to be Used [1] :
 Enter Cartesian Coordinate File Name :  a.xyz

The Following Parameters can be Fit for each Atom Type :

    (1) Van der Waals Atomic Radius
    (2) Van der Waals Well Depth
    (3) Hydrogen Atom Reduction Factor
    (4) Atomic Partial Charge
    (5) Bond Dipole Moment Magnitude
    (6) Bond Dipole Moment Position
    (7) Atomic Polarizability

 Enter Parameter Type then Atom Class or Type(s) :  5
 Enter Parameter Type then Atom Class or Type(s) :  N
 Enter RMS Gradient Termination Criterion [0.1] :
 Enter Number of Structures to be Used [1] :
 Enter Cartesian Coordinate File Name :
 Enter Cartesian Coordinate File Name :  a.xyz

The Following Parameters can be Fit for each Atom Type :

    (1) Van der Waals Atomic Radius
    (2) Van der Waals Well Depth
    (3) Hydrogen Atom Reduction Factor
    (4) Atomic Partial Charge
    (5) Bond Dipole Moment Magnitude
    (6) Bond Dipole Moment Position
    (7) Atomic Polarizability

 Enter Parameter Type then Atom Class or Type(s) :  6
 Enter Parameter Type then Atom Class or Type(s) :  N
 Enter RMS Gradient Termination Criterion [0.1] :  0.1
 Enter Number of Structures to be Used [1] :  1
 Enter Cartesian Coordinate File Name :  a.xyz

The Following Parameters can be Fit for each Atom Type :

    (1) Van der Waals Atomic Radius
```

```
    (2) Van der Waals Well Depth
    (3) Hydrogen Atom Reduction Factor
    (4) Atomic Partial Charge
    (5) Bond Dipole Moment Magnitude
    (6) Bond Dipole Moment Position
    (7) Atomic Polarizability

 Enter Parameter Type then Atom Class or Type(s) :  7
 Enter Parameter Type then Atom Class or Type(s) :  N
 Enter RMS Gradient Termination Criterion [0.1] :  0.1
 Enter Number of Structures to be Used [1] :  1
 Enter Cartesian Coordinate File Name :  a.xyz
```

XTALMIN

```
Enter Cartesian Coordinate File Name :  a.xyz
```

XYZEDIT

```
Enter Cartesian Coordinate File Name :  a.xyz

 The Tinker XYZ File Editing Utility Can :

    (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 for Linear Chain
    (8) Assign Connectivities Based on Distance
    (9) Convert Units from Bohrs to Angstroms
   (10) Invert thru Origin to Give Mirror Image
   (11) Translate All Atoms by an X,Y,Z-Vector
   (12) Translate Center of Mass to the Origin
   (13) Translate a Specified Atom to the Origin
   (14) Translate and Rotate to Inertial Frame
   (15) Move to Specified Rigid Body Coordinates
   (16) Move Stray Molecules into Periodic Box
   (17) Delete Molecules Outside of Periodic Box
   (18) Append a Second XYZ File to Current One
   (19) Create and Fill a Periodic Boundary Box
   (20) Soak Current Molecule in Box of Solvent

 Number of the Desired Choice [<CR>=Exit] :  1

 Offset used to Renumber the Atoms [0] :  0
```

XYZINT

```
Enter Cartesian Coordinate File Name :  a.xyz
```

```
Template (T), Dihedrals (D), Manual (M) or Automatic [A] :  t

Enter Cartesian Coordinate File Name :  a.xyz
Template (T), Dihedrals (D), Manual (M) or Automatic [A] :  d

Enter Cartesian Coordinate File Name :  a.xyz
Template (T), Dihedrals (D), Manual (M) or Automatic [A] :  m
Atom Number to be Defined [    1] :  1
Atom Number to be Defined [    2] :  2
Atom Number to be Defined [    3] :
Atom Number to be Defined [    4] :
Choose a Connected Atom (     2     3) :
Specify with Dihedral Angle or Second Bond Angle (D or [B]) :  d
...

Enter Cartesian Coordinate File Name :  a.xyz
Template (T), Dihedrals (D), Manual (M) or Automatic [A] :  a
```

XYZMOL2

```
Enter Cartesian Coordinate File Name :  a.xyz
```

XYZPDB

```
Enter Cartesian Coordinate File Name :  a.xyz
```

Program status

The current package contains TINKER binaries of version 8.6 compiled for x86 based Windows operating system.

License

TINKER

The distribution is published as freeware at Mobile Chemistry Portal and Google Play Store with kind permission of Jay Ponder.

MinGW

The Windows version contains few essential dynamic link libraries which are part of MinGW runtime. http://www.mingw.org/

CONNECTION WITH THE SOFTWARE OR THE USE OR OTHER DEALINGS IN THE SOFTWARE.

X11-Basic

GUI of the Windows version was built using X11-Basic (by Markus Hoffmann) framework (GPL v.3). For correct functionality, SDL library (available under GNU LGPL license) is included in package.
http://x11-basic.sourceforge.net/
https://www.libsdl.org/

Advanced Installer

The MSI installer for Windows was created using the Advanced Installer (Freeware edition).
https://www.advancedinstaller.com/
https://www.advancedinstaller.com/top-freeware-features.html

Contact

Compilation of the source code for Android/Windows as well as the Android/Windows app development was done by Alan Liška (alan.liska@jh-inst.cas.cz) and Veronika Růžičková (sucha.ver@gmail.com), J. Heyrovský Institute of Physical Chemistry of the CAS, v.v.i., Dolejškova 3/2155, 182 23 Praha 8, Czech Republic.
Website: http://www.jh-inst.cas.cz/~liska/MobileChemistry.htm