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| **1.** | **Examples using the TINKER Package** |

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.