

Note: In the following, words/phrases in bold font imply left-mouse click that particular function. Indented texts indicate subcommands of the previous function. In all, if some thing that you typed/clicked does not work, try some thing different and experiment it with other options.

### 1. Structure Building and Optimization.

Your computer should have been set up so that you can simply type <insightII> followed by the [enter] or [return] key. This will initiate the program insightII to give you the main view of the program. If insightII is not found, you probably need to initialize the program yourselves by typing

```
source /usr/local/accelrys/accelrys.csh
```

We now try to build an ethane molecule, and perform energy minimization.

Click and hold down left-mouse key on the [MSI] icon, select

**Builder** (try **Biopolymer** later to find out what is available there)

**Fragment**

**Get**

**Fragment Libraries** to select fragments. Choose common.

Select **Ethyl**

**Execute**

**Cancel**

You have just created an ethane with insightII.

Note: you can use the middle and right-mouse button to move and rotate the molecule.

**Forcefield**

**Select**

Choose **cvff.frc**, followed by **execute**

**Potentials**

Select **fix** under *potential action*, **fix** under *partial charge action*,

**fix** under *partial charge action*

**execute**

**Optimize**, followed by **execute** (you do not have to change other options).

There are more advanced options, which are available from the Discover package. To initiate that package at the main manual, click the [MSI] icon again, and select Discover or Discover-3. Then, the Builder manual will disappear, only being replaced by Discover options. From this manual, you can select various options such as optimization methods, cutoff distances, dielectric constants, molecular dynamics, etc. You are

encouraged to experiment all these options, and you will need to know all these as we start doing additional experiments using insightII. Wait and observe. After finishing, you have optimized the structure of ethane using the cvff.frc force field. In the next segment, we'll practice some basic functions for molecular display.

## 2. Basic graphics and display functions.

From the main manual, select:

### **Molecule**

#### **Color**

Under *parameters*, select **atom**

Under *color method*, choose **specification**, click the blank area

Select a **color**

Click on one atom of the molecule on display (e.g., ethane)

Now the color of that atom is replaced by the one you selected.

Try some other options and see what happens.

#### **Render**

**CPK**, under *parameter* select **molecule**, then **execute**

Now, change CPK scale to **0.5** (from 1.0 originally)

**Execute**, now the size of the CPK models will decrease.

**Lines**, followed by **execute**

Try other options, e.g., **ball\_and\_stick**.

## 3. Geometrical information.

From main manual, select

### **Measure**

#### **Distance**

Click on **any two atoms** of the molecule on display.

The distance in Angstroms is displayed between the two atoms.

Try another pair, and more. **Cancel** to exit.

#### **Angle**

Click on any **three atoms**, it gives you the angle formed by the three atoms. Try more, **cancel** to exit.

#### **Dihedral**

Click on **four atoms** in sequence to show the dihedral angle.

### **Transform**

#### **Torsion**

Under *specification style*, click on **2-Atom**, but select **4-Atom**.

Click on **4 sequential atoms** to define a dihedral angle.

### Execute

#### Hold middle mouse key & move left and right

Use this method to change the HCCH dihedral angle of ethane to about 5 degrees (initially it should be 60, 180, or -60 degrees).

### Torsion

Under *torsion operation*, **clear**, followed by **execute**.

This completes the change of a dihedral angle, and the rotation of the fragment that is dependent on this dihedral angle.

Go back to [MSI]-**Builder**

**Optimize**, followed by **execute**.

Observe the change of the ethane molecule as it is being reoptimized. It will return to the trans conformation after it is finished.

To delete the molecule on display, or to hide it, do the following

### Object

**Delete**, click on the object name, **execute**.

**Blank**, click on the object name, **execute**.

4. Exercise: Build a butane molecule and optimize its geometry.

### Fragment

#### Get

Select **ethyl**, **execute**, then (1) click on **one hydrogen**, it should appear in the "A atom" box. (2) click on a **H** of the ethyl group in the *fragment libraries* box.

#### Cancel

You have created a butane molecule. Run minimization following previous steps.

5. Read in a protein structure from a protein data bank (pdb) file.

- format
- color
- display [backbone, hydrogen, sidechain, etc.]
- render [ribbon, ball\_and\_stick for selected atoms]

6. Build a transition metal complex with ligands

Use *esff.frc* force field for the iron octahedral complex in energy minimization.



