#### CHEN **Molecular Models Report Sheet:** 110 \_\_\_\_\_ SEC # \_\_\_\_ LOCKER # \_ LAST NAME: UNIVERSITY **Department of Chemistry** FIRST NAME:

- Go to the website www.molview.org
- At the search window in the upper-left, enter in the compound name for questions below. In all cases, you can just copy/paste the name directly from this PDF file into the website.
- Rotate the 3D model onscreen if necessary. Answer the **questions** on the report sheet. All blue-purple shaded boxes are places to write answers or checkmark (☑) choices.

## Part 1 – Bond Rotation and Conformers

1. Ethane Select the correct name for each conformation. Check  $( \square )$  the conformation of lower energy. Which conformation did the website generate?

#### 2. 1,2-Dichloroethane

Complete the three Newman projections for the staggered conformations by writing in the **second chlorine atoms** in the correct spot. **Check** ( $\boxtimes$ ) **the conformation** of lower energy.

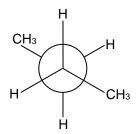
anti

gauche

Which conformation did the website generate, anti or gauche?

What colour spheres did the website use to represent chlorine atoms?

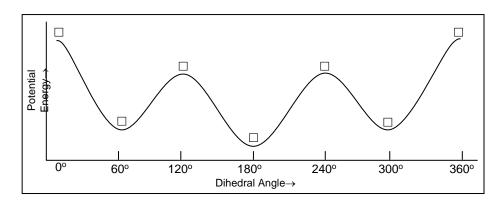
3. **Butane** The website generates a specific conformer. Rotate the 3D model to look straight down the C-C bond between carbon 2 and 3, as shown in the diagram below. Fill out the blank with the **correct name for this conformation**. The four choices are:



- anti
- gauche
- eclipsed
- staggered

Conformation is:

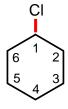
**Check** ( $\square$ ) the position(s) where the above conformation would be on this energy curve:

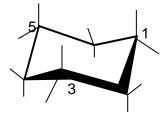


- 5. Cyclohexane Rotate the 3D model online.

  Is this the boat or chair conformation? \_\_\_\_\_\_
- 6. Now rotate the 3D model online so that 3 hydrogens are pointing up in axial positions and 3 hydrogens are pointing axially down. Notice how they are located around the carbon-ring in alternating up-down positions. This is due to the sp3 hybridization. In a similar manner, you should see 6 hydogrens located in equatorial positions around the ring, alternating up and down.
- 7. Chlorocyclohexane The website will show the top-down diagram given below at left. Rotate the model into an edge-on position, with the chlorine-atom **above** the plane of the carbon ring. Show on the edge-on diagram where the chlorine is located.

Is this an axial or equatorial postion?





For the top-down diagram, should the website use a "dash" or "wedge" to show the correct spatial-orientation of the C-Cl bond (shown in red here):

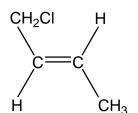
\_\_\_\_

 $\Box E$ 

or

## Part 2 - Geometrical Isomerism

- 1. **Check (☑) the correct name** of the compound drawn below. You can use the website if you want, but it is not required here.
  - $\square$  1-chloro-*cis*-2-butene  $\square$  1-chloro-*trans*-2-butene



Specify the configuration (**E or Z**) of the compound: \_\_\_\_\_

Is it possible to convert this to the other isomer without breaking any bonds? (yes or no)

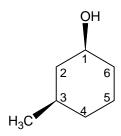
3. **Check (☑)** whether the geometry of each alkene is E or Z. **First**, determine which group (or atom) on each C of the double bond has the higher priority. Show this by **clicking on 2 of the 4 round buttons** for **each** molecule. If you want to use the website, the names are given in blue.

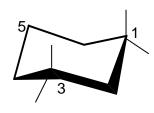
## 2-isopropyl-2-butene

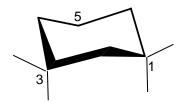
$$C = C$$
 $C + C$ 
 $C + C$ 
 $C + C$ 
 $C + C$ 
 $C + C$ 

$$CH_2-CH_3$$
 $C=C$ 
 $CH_3$ 

5. **cis-3-methylcyclohexanol** The diagram at left below matches the website. Complete the two chair conformations, **showing the position of the hydroxyl and methyl groups only**. Do **not** include the hydrogens. Are the groups in **axial or equatorial** positions? **Fill in the blanks**.







-OH and -CH<sub>3</sub> located in: \_\_\_\_\_ positions

\_\_\_\_\_ positions

axial or equatorial

## Part 3 – Optical Isomerism

#### 1. Bromochloromethane

Does the online model have a plane of symmetry? (yes or no)

CH<sub>2</sub>CIBr

Would a second molecule of CH₂ClBr be superimposable on the first? (yes or no) \_\_\_\_\_

Is CH<sub>2</sub>ClBr chiral or achiral?

#### 2. Bromochlorofluoromethane CHCIBrF

The online model will likely be positioned with the C-H bond going behind the screen, and the Br, Cl, and F atoms coming towards the viewer.

Is the online model showing the **R** or **S** enantiomer?

**Check (**☑**)** which one diagram shown below matches the online model:



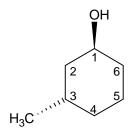
Would a second molecule of CHClBrF be superimposable on the first? (yes or no)

Part 3 – Optical Isomerism – continues on the next page.

# Use models of the following compounds and then complete the table:

|  |  | Sketch of the<br>Mirror Image   | je<br>ble?  | of of                                   | iral                        |
|--|--|---|---|---|-----------------------------|
| Compound                               | Online Model  Rotate it to match the         | Fill out the diagrams below showing the mirror images.  The red line is the mirror plane. | Is Mirror Image<br>Superimposable?<br>( <i>yes/no</i> ) | Internal Plane<br>Symmetry?<br>(yes/no) | Number of Chiral<br>Centres |
| 2.1 Chroine                            | diagram shown below                          | ,   | S S   | 7 S S                                   | 20                          |
| 3.1 Glycine COOH means:                | H<br>C///COOH<br>NH <sub>2</sub>             | IIIIIIIC  |   |   |                             |
|  | The model shows how planar this molecule is. | This compound is achiral.   |   |   |                             |
| 3.2 Alanine  This compound is chiral.  | H <sub>3</sub> C COOH                        | nnno-C  |   |   |                             |
|  | Is this R or S?                              | Is this R or S?   |   |   |                             |
| 4.1 cis-1,2-dichloro-cyclopropane      | 3 CI 1                                       | 1 2 3   |   |   |                             |
|  | Is carbon atom 1<br>R or S ?                 | Is carbon atom 1<br>R or S ?  |   |   |                             |
| 4.2  trans-1,2- dichloro- cyclopropane | 3 CI   | 1 2 3   |   |   |                             |
|  | Is carbon atom 1<br>R or S ?                 | Is carbon atom 1<br>R or S ?  |   |   |                             |

#### 5. trans-3-methylcyclohexanol



How many chiral centres does it have?

Is there a plane of symmetry? (yes/no)

What is the R/S configuration at carbon 1? \_\_\_\_\_

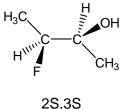
## 6. 3-fluorobutan-2-ol

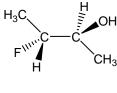
Fill in the blanks below:

The online model will likely match stereoisomer (d) shown below. Answer that one first.

In all diagrams, the -OH group is attached to carbon 2 and the -F group is on carbon 3.

Show the configuration (R or S) at carbons 2 & 3 on stereoisomers (b), (c) & (d) below:





Refer to the bottom of page 172 of the lab manual for these questions:

Give the letter (b, c or d) of one enantiomer of conformer (a):

Give the letters (a, b, d) of two diastereomers of conformer (c):

Please save this PDF and submit to your lab instructor as per their instructions.