Short Summary Sheet for Chem3D

- **Entering Molecules**
  - Use the **File/Open** command to input a saved ChemDraw or Chem3D structure.
  - Enter the molecular formula in the text box in the upper left-hand corner of the Model area.
    - Use capital letters
    - Use parentheses to group certain groups that are branches off the main part of the molecule.
  - Draw the molecule in the Model area using the bond tools on the Tool Palette.
  - The default atom type is C. Any unfilled atom is assumed to be a H. To change the atom type, select the atom(s) to change (select top item on Tool Palette and click on atom). Type in the new atom type in the text box.
  - Save molecule by using **File/Save** command.

- **Selecting Different Views**
  - Select **View/Preferences**. Select *Model Display* under *Model Settings*. Select the type of display you want by picking the correct *Model Type*. When finished, press *Save*.
  - Rotation
    - You can rotate molecules by selecting the rotation tool on the Tool Palette (second item) and holding down the left mouse button.
    - You can click on the rotation buttons on the outside of the Model area.
    - You can rotate about an axis by selecting Analyze and one of the spin commands.

- **Modeling**
  - Select **MM2** and either **Minimize Energy** or **Compute Properties** (for Molecular Mechanics).
  - Select **MOPAC** and either **Minimize Energy** or **Compute Properties** (for Molecular Mechanics or Semi-Empirical).
  - To select a particular Method, click on *Theory* tab after selecting **Minimize Energy** or **Compute Properties**. Pick the theory you want under *Method*.

- **Display Properties**
  - Under **Compute Properties**, click on the *Properties* tab and select the properties that you wish to calculate. One of the properties must be **Molecular Surfaces**.
  - To view the display, select **View/Molecular Surfaces** and select the required display.

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