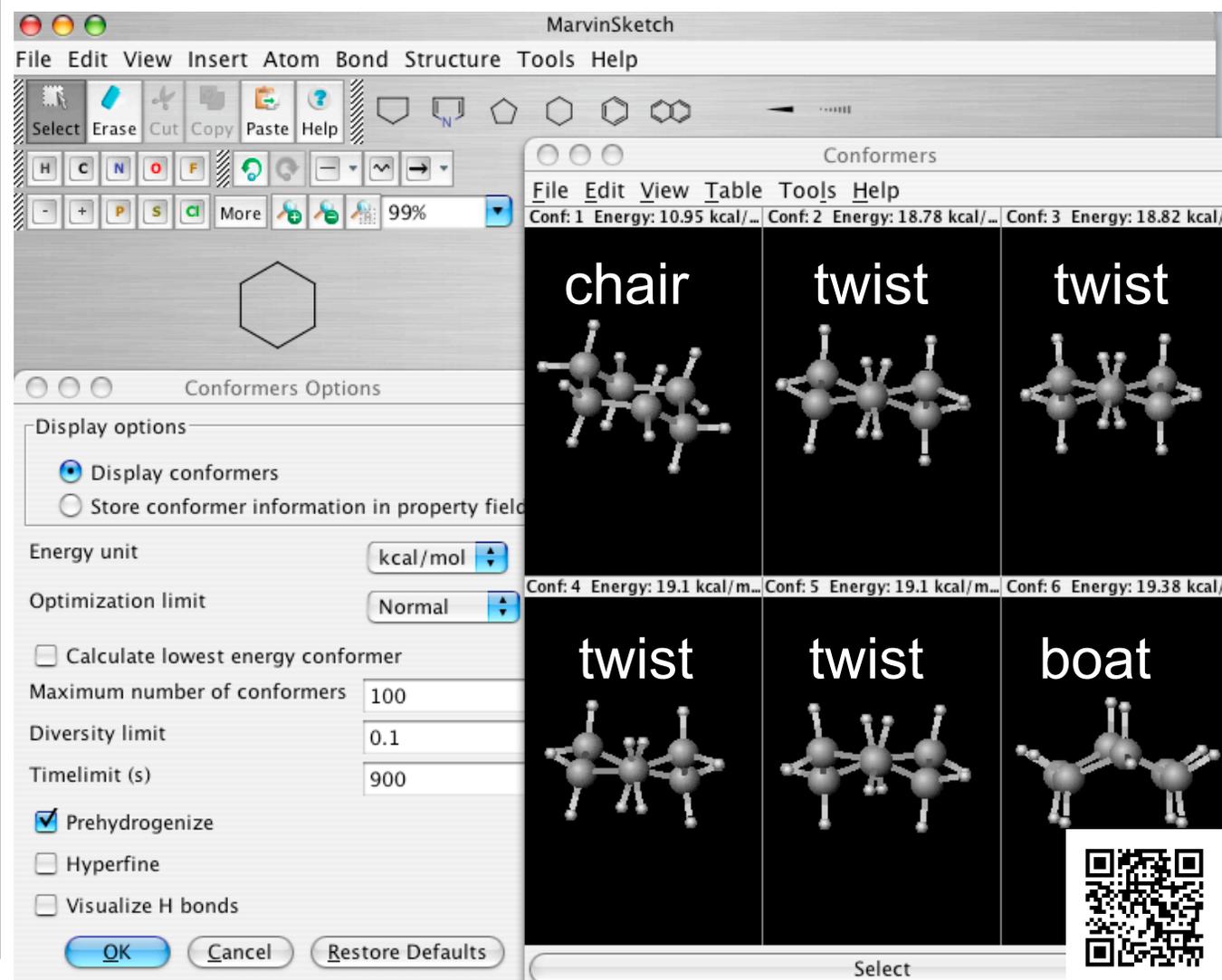


Cyclohexane's Chair, Twist and Boat Conformations

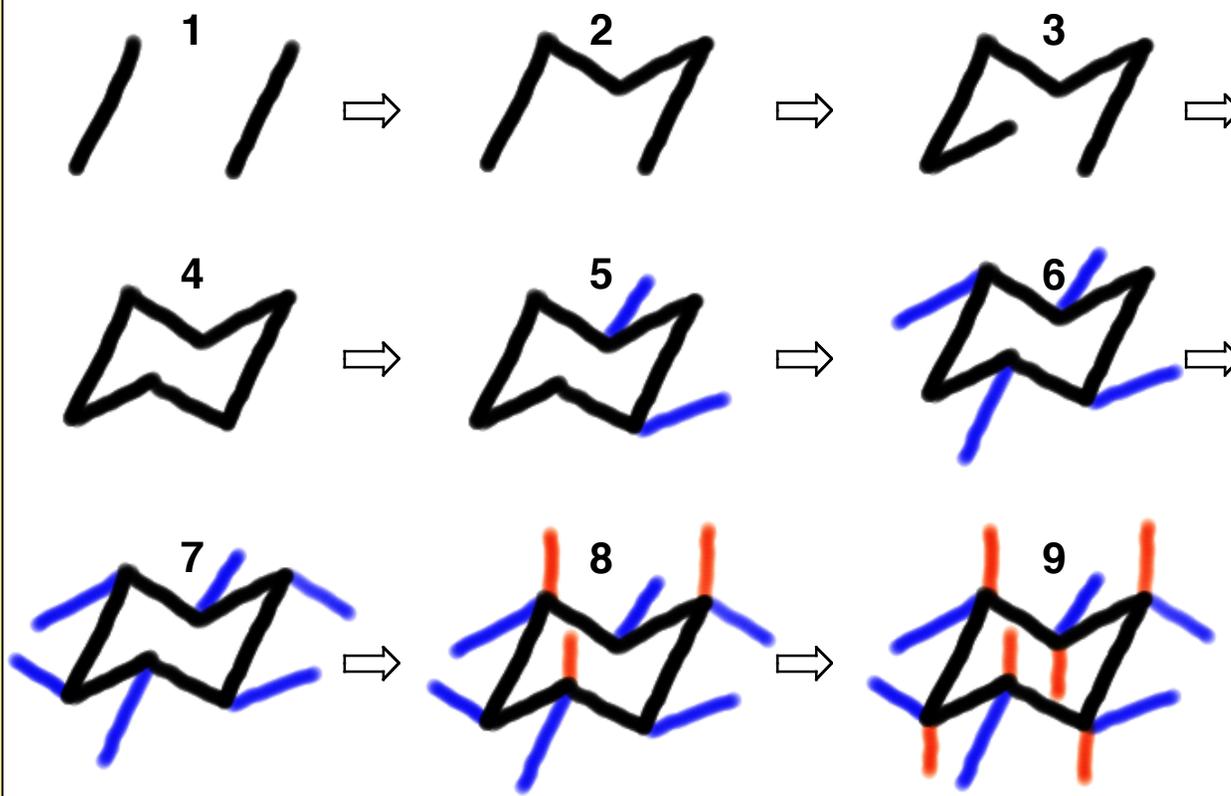
Note: The structures you generate may differ from those seen below. Don't worry; the main points will be apparent, regardless. Be inquisitive and experiment!

Repeat the process with cyclohexane, but make sure the Optimization limit is set to Normal. The greater flexibility of this molecule will be evident by the fact that MarvinSketch finds several conformations. The lowest energy form is the most important. This is the “**chair**” conformation. Carefully study this molecule by rotating it on your screen. The other conformations are known as the “**twist**” and “**boat**” forms. Run a molecular dynamics simulation in order to get a sense of the flexibility of the cyclohexane ring. Use the highest energy conformation as a starting point, as the strain energy that's present in this conformation will launch the molecule into a frenzy and provide a wider range of motion during the simulation.



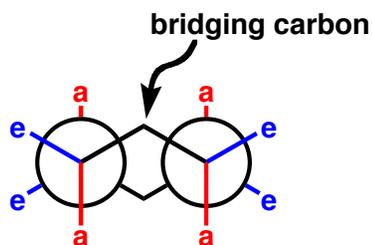
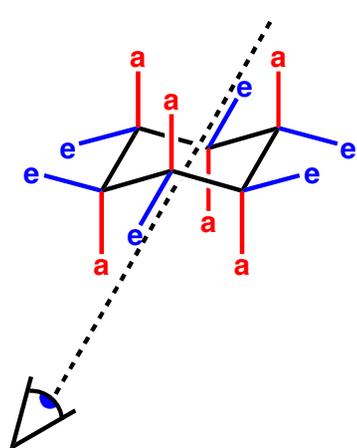
It will take some practice to learn to draw cyclohexane chair conformations. Even though we draw our structures on the computer, it is still a skill that's worth practicing. The step-by-step process is illustrated. Begin (step 1) by drawing two parallel lines slanted at the indicated angle and spaced apart in proportion to their length as shown. Next (step 2) make a "V" between the tops of the lines. The next line (step 3) should be parallel to its diagonal counterpart, ending at a point where the remaining line will be parallel to the opposite side and connecting to the bottom of the first line. This provides a complete skeleton (step 4). Steps 5 – 7 show the addition of **equatorial substituents** (blue). Equatorial substituents are positioned around the ring's equator. Note that each blue line is parallel to another line of the cyclohexane skeleton. The blue lines align with the skeleton to make "W" (step 5) and "M" (step 6) arrangements. Steps 8 and 9 show the placement of **axial substituents** (red lines). All of these lines are vertical; three point up and three point down. Take special care to properly draw the orientation of the axial and equatorial substituents.

Drawing Cyclohexane



Other Ways to Represent the Chair Form

Newman projections are another way to represent cyclohexane chair conformations. The line of sight is parallel to two bonds in the chair as shown below, where axial and equatorial substituents are indicated as "a" and "e", respectively. Orient a model such that you can clearly see the view from this perspective. A MarvinSketch image is provided below.



Newman Projection
axial and equatorial substituents on the "bridging" carbon have been removed for clarity

A step-by-step procedure for drawing the chair form in Newman project follows. In step 1, two circles are drawn side-by-side. The bridging carbon at the apex of the chair is sketched in step 2. The bridging carbon in the back is drawn in step 3. Step 4 illustrates the addition of substituents to the front set of carbon atoms and step 5 shows the addition of the substituents to the back carbons. For clarity, the Newman projection doesn't display the substituents on the bridging carbons.

