GETTING STARTED WITH WEBMO

To build molecule:
1. Touch "Build"
2. Choose atom (C, O, N, H, or Periodic Table)
3. Tap to insert atom and/or drag to insert bond
4. Choose Cleanup: Comprehensive to finish

To adjust molecular geometry:
1. Touch "Adjust"
2. Tap 2, 3, or 4 atoms
3. Choose Adjust… and specify length/angle

To import molecule:
1. Touch "Lookup"
2. Choose Import
3. Type in name
Tip: Touch microphone, speak molecule name, touch microphone

To view molecular orbitals:
1. Touch "Display"
2. Choose Orbitals
3. Select desired orbital

To view symmetry elements:
1. Touch "Display"
2. Choose Symmetry
3. If (approx.), choose Symmetrize
4. Choose Show symmetry elements

To view molecule stoichiometry, name, molar mass:
1. Touch "Lookup"
2. Choose Info

To view external database information:
1. Touch "Lookup"
2. Choose Databases
3. Select database
4. Follow web links as appropriate
5. Use back, forward, close buttons

To perform WebMO calculation:
Note: WebMO calculations requires authentication credentials on a WebMO server v14 or higher - see below to specify server location
1. Touch "WebMO"
2. Choose Submit

3. Choose Computational Engine, forward arrow, Job Options, and forward arrow
4. When job is complete, choose job Name to view computed structure
5. Choose Results to view numerical data
6. Choose links to visualize specific results
7. Choose Close to return to WebMO app

To view previous WebMO jobs:
Note: WebMO calculations requires authentication credentials on a WebMO server v14 or higher - see below to specify server location
1. Touch "WebMO"
2. Choose Job Manager
3. Choose job Name to view computer structure and results
4. Choose Results to view numerical data
5. Choose links to visualize specific results
6. Choose Close to return to WebMO app

To specify a new or different WebMO server:
1. Open Safari on your iOS device
2. Navigate to the desired WebMO server (v14 or higher)
3. Click the "Connect using WebMO app" link
        or
1. Open the Settings app
2. Under WebMO setting, specify the WebMO server URL and Authentication details

Hints:
• **Undo** and **Redo** when building are available as icons in upper left
• "Build":New **erases** molecule and starts over
• "Build":Find or "Adjust":Find **centers and scales** a molecule
• An atom can be **replaced** in "Build" by tapping with a different atom
• Atoms and bonds can be **deleted** in "Adjust" by tapping and choosing Delete (or by choosing the select box, selecting, and choosing Delete)
• In "Adjust", selecting 1, 2, 3, or 4 atoms **displays information** about hybridization, bond length, bond angle, dihedral angle
• To **save** molecule, choose Save (diskette) icon, Save or Save As, and provide name
• To **recall** saved molecules, choose Save (diskette) icon, Open, and select name
• To **capture image**, choose Save (diskette) icon, Save Image, and image is available in Photo app
• To **export** molecule as an email attachment, choose Save (diskette) icon, Export, format type, and provide email address
• To **import** molecule as an email attachment, open email in Apple Mail app (not Google Gmail), select email, touch attachment, and choose Open in WebMO

- To change the **background color**, open the Settings app, choose WebMO, and select desired background color.