Directions for downloading and using the Mercury 2.2 software and crystal structure visualizations in the science classroom

For Mac users

1. Go to *www.ccdc.cam.ac.uk/free_services/mercury/downloads.*
2. Click on the "Mercury 2.2" link.
3. Read the license agreement and click the "Accept" button at bottom of page.
4. Scroll down and click on "Mac OS X - 130 MB" link.
5. Allow the "mercury_2.2.dmg" to download.
6. Click "Agree" to accept the Mercury software conditions of use.
7. Move the "Hg" application icon into the "Applications" folder.
8. Double click on the "Hg" icon in the "Applications" folder to open the program.
9. When asked "Do you want to register to access advanced Mercury features?," click "No."
10. Go to *http://web.me.com/dsmithenry/WCI/CIFs.html* and click on "Teaching CIFs.zip" to download a folder of CIFs that are useful to science teachers.
11. Open up the downloaded "Teaching CIFs" folder and choose one of the subfolders within to access a CIF file.
12. Drag a CIF into the black window of the Mercury program.
13. In the upper left hand corner of the Mercury program screen, you can change the Style of how the atoms are displayed. To begin, select the Style as "Ball and Stick."
14. Click on the "packing" button to see unit cell.
15. To increase the number of atoms displayed on the screen, go to Calculate -->Packing/Slicing. For "a" change the first "0.0" to "-1.0". Do the same for "b" and "c". By doing so, you can allow students to clearly see how the particles are packed together in three dimensions.
16. Click and drag displayed structure to rotate it.
17. Play with features of the Mercury program.
18. Drag another CIF into Mercury program to view a different crystal structure.

For Windows users

1. Go to *www.ccdc.cam.ac.uk/free_services/mercury/downloads.*

2. Click on the “Mercury 2.2” link.

3. Read the license agreement and click the “Accept” button at bottom of page.

4. Scroll down and click on “Windows - 60 MB”, then click “Save File”.

5. Allow the “mercury_2.2.exe” (Windows) to download.

6. Double click on the “mercury_2.2.exe” icon (likely downloaded to the Desktop) and click “run”.

7. Follow the instructions of the “Welcome to the Mercury 2.2 Installation Wizard” to install the program. Once the installation is finished, a “Hg” shortcut icon should appear on your desktop.

8. Double click on the “Hg” shortcut icon to open the Mercury 2.2 program. If asked “Do you want to register to access advanced Mercury features?,” click “No.”

9. Go to *http://web.me.com/dsmithenry/WCI/CIFs.html* and click on “Teaching CIFs.zip” to download a folder of CIFs that are useful to science teachers.

10. Double click on the “Teaching CIFs” zipped folder on the Desktop. Either (a) simply drag the “Teaching CIFs” folder onto the Desktop or (b) highlight the “Teaching CIFs” folder that appears and click “Extract all files” (and follow subsequent directions).

11. Open up the unzipped “Teaching CIFs” folder (on Desktop) and choose one of the subfolders within to access a CIF file.

12. Drag a CIF into the black window of the Mercury program.

13. In the upper left hand corner of the Mercury program screen, you can change the Style of how the atoms are displayed. To begin, select the Style as “Ball and Stick.”

14. Then click on the “packing” button to see the particles packed in the unit cell.

15. To increase the number of atoms displayed on the screen, go to Calculate -->Packing/Slicing. For “a” change the first “0.0” to “-1.0”. Do the same for “b” and “c”. By doing so, you can allow students to clearly see how the particles are packed together in three dimensions.

16. Click and drag displayed structure to rotate it.

17. Play with features of the Mercury program.

18. Drag another CIF into Mercury program to view a different crystal structure.