Visualizing Zeolite structure

Note: This activity was originally written as a prelab exercise to accompany synthesis of zeolites from silica gel. The introduction to the lab experiment includes a discussion of the mineral (sodalite) structure and the uses of zeolites, and could be used as background for this activity as well (see related activities).

In this activity, you will use the Database of Zeolite Structures to visualize the structure of a zeolite. The database can be found at:

http://izasc.ethz.ch/fmi/xsl/IZA-SC/ft.xsl

When you arrive at the page, make sure that the "framework type" tab is selected, and then choose "FAU" (the structure for faujasite) from the table shown. In the blue menu bar in the viewer tab, select "3D drawing" and wait for the JSmol animation to load.

1) Click and drag to rotate the view of the structure, observing how the sodalite cages are stacked together. How many connected sodalite cages are shown in the drawing?

2) Rotate the structure to the highest symmetry position you can find (the one with the most lines overlapping). What shape does the cage structure form? Take a screen shot and include it in your lab notebook.

3) Notice that the default view is set to show only the Si (or Al) atoms. Choose the ball and stick view, displaying both the Si and O atoms. Where are the oxygen atoms relative to the lines in the original view? Draw the shape of *one* facet from a sodalite cage, and show where the oxygen atoms are.

4) Switch back to the "Si-only, stick 0.15" display. Turn on the unit cell and axes labels. Rotate the structure around as necessary to get a good viewing angle. Do the unit cell axes (the lines marked a, b, and c) cut through center of the largest pores (holes) in the structure, or are the pores located between axes? Do the cell axes ever cut through atoms or bonds? Are there ever channels that go straight through the unit cell unobstructed, or does the cell structure look more like a network of interconnected pores? Explain your thinking.

5) At the bottom of the window, there is a series of boxes where you can enter a "user cell range." Set a = -0.2, **3**, b = -0.2, **3**, c = -0.2, 1.2, and click "load range." Rotate the structure around. Describe what you see, and include a screen shot of any interesting orientations in your report.

6) Turn on the unit cell and axis labels. How does the orientation of the pores/channels compare with the location of the pores that you described in #4?