12.12 First of all, open the "Molecular Definition Utility"; it may be found in either of "Metallic Crystal Structures and Crystallography" or "Ceramic Crystal Structures" modules.

In the "Step 1" window, it is necessary to define the atom types, colors for the spheres (atoms/ions), and specify atom/ion sizes. Let us enter "Pb" as the name for the lead ions (since "Pb" the symbol for lead), and "O" as the name for the oxygen ions. Next it is necessary to choose a color for each ion type from the selections that appear in the pull-down menu—for example, "LtBlue" (light blue) for Pb and LtRed (light red) for O. In the "Atom Size" window, it is necessary to enter an atom/ion size. In the instructions for this step, it is suggested that the atom/ion diameter in nanometers be used. From the table found inside the front cover of the textbook, the ionic radii for lead and oxygen are 0.120 nm and 0.140 nm, respectively, and, therefore, their ionic diameters are twice these values (i.e., 0.240 nm and 0.280 nm); therefore, we enter the values "0.240" and "0.280" for the two atom types. Now click on the "Register" button, followed by clicking on the "Go to Step 2" button.

In the "Step 2" window we specify positions for all of the ions within the unit cell; their point coordinates are specified in the problem statement. Now we must enter a name in the box provided for each of the ions in the unit cell. For example, for oxygen let us name the first ion "O1". Its point coordinates are 000, and, therefore, we enter a "0" (zero) in each of the "x", "y", and "z" atom position boxes. Next, in the "Atom Type" pull-down menu we select "O", the name we specified in Step 1. For the next oxygen ion, which has point coordinates of 100, let us name it "O2"; since it is located a distance of a units along the x-axis the value of "0.397" is entered in the "x" atom position box (since this is the value of a given in the problem statement); zeros are entered in each of the "y" and "z" position boxes. We next click on the "Register" button. This same procedure is repeated for all 10 the point coordinates for the oxygen ions, as well as the four coordinates for lead ions; these values are specified in the problem statement. For the oxygen ion having point coordinates of "111" respective values of "0.397", "0.397", and "0.502" are entered in the x, y, and z atom position boxes, since the unit cell edge length along the y and z axes are a (0.397) and c (0.502 nm), respectively. For fractional point coordinates, the appropriate a or c value is multiplied by the fraction. For example, for oxygen ions, the last point coordinate set in the left-hand column, $\frac{1}{2}\frac{1}{2}0$, the x, y, and z atom positions are $\frac{1}{2}(0.397) = 0.1985$, $\frac{1}{2}(0.397) = 0.1985$, and 0, respectively. The x, y, and z position entries for the 10 sets of point coordinates for the oxygen ions are as follows:

0, 0, and 0	0, 0, and 0.502
0.397, 0, and 0	0.397, 0, and 0.502
0, 0.397, and 0	0, 0.397, and 0.502
0.397, 0.397, and 0	0.397, 0.397, and 0.502
0.1985, 0.1985, and 0	0.1985, 0.1985, and 0.502

Likewise, for the lead ions, x, y, and z position entries for the four sets of points coordinates are the following:

0.1985, 0, and 0.383	0, 0.1985, and 0.1190
0.1985, 0.397, and 0.383	0.397, 0.1985, and 0.1190