3.26 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 type, a color for the spheres (atoms), and specify an atom size. Let us enter "Sn" as the name of the atom type (since "Sn" the symbol for tin). Next it is necessary to choose a color from the selections that appear in the pull-down menu—for example, "LtBlue" (light blue). In the "Atom Size" window, it is necessary to enter an atom size. In the instructions for this step, it is suggested that the atom diameter in nanometers be used. From the table found inside the front cover of the textbook, the atomic radius for tin is 0.151 nm, and, therefore, the atomic diameter is twice this value (i.e., 0.302 nm); therefore, we enter the value "0.302". 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 atoms 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 atoms in the unit cell. For example, let us name the first atom "Sn1". 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 "Sn", our only choice, and the name we specified in Step 1. For the next atom, which has point coordinates of 100, let us name it "Sn2"; since it is located a distance of a units along the x-axis the value of "0.583" 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 13 of the point coordinates specified in the problem statement. For the atom having point coordinates of "111" respective values of "0.583", "0.583", and "0.318" 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 (0.583) and c (0.318 nm), respectively. For fractional point coordinates, the appropriate a or c value is multiplied by the fraction. For example, the second point coordinate set in the right-hand column, $\frac{1}{2}0\frac{3}{4}$, the x, y, and z atom positions are $\frac{1}{2}$(0.583) = 0.2915, 0, and $\frac{3}{4}$(0.318) = 0.2385, respectively. The x, y, and z atom position entries for all 13 sets of point coordinates are as follows:

0, 0, and 0	0, 0.583, and 0.318
0.583, 0, and 0	0.2915, 0, and 0.2385
0.583, 0.583, and 0	0.2915, 0.583, and 0.2385
0, 0.583, and 0	0.583, 0.2915, and 0.0795
0, 0, and 0.318	0, 0.2915, 0.0795
0.583, 0, and 0.318	0.2915, 0.2915, and 0.159
0.583, 0.583, and 0.318	

In Step 3, we may specify which atoms are to be represented as being bonded to one another, and which type of bond(s) to use (single solid, single dashed, double, and triple are possibilities), or we may elect to not