

Materials Science 142

Applications of Diffraction Techniques in Materials Science

Assigned: 1/18/12

Homework Assignment 2

Due: 1/25/12, 5pm

Plane Group Symmetry

Goal: Determine the symmetries present in a 2-dimensional pattern; identify an appropriate unit cell. Seven patterns are to be analyzed.

1. Identify all (unique) symmetry operations: rotation axes, mirror planes and glide planes.
2. Identify the unit cell (more than one choice may be possible).
3. Draw the unit cell outline in black and show all of the symmetry operations within this cell.
 - Indicate the rotation axes using the appropriate symbol.
 - Draw the mirror planes as solid blue lines.
 - Draw the glide planes as dotted red lines.

Details:

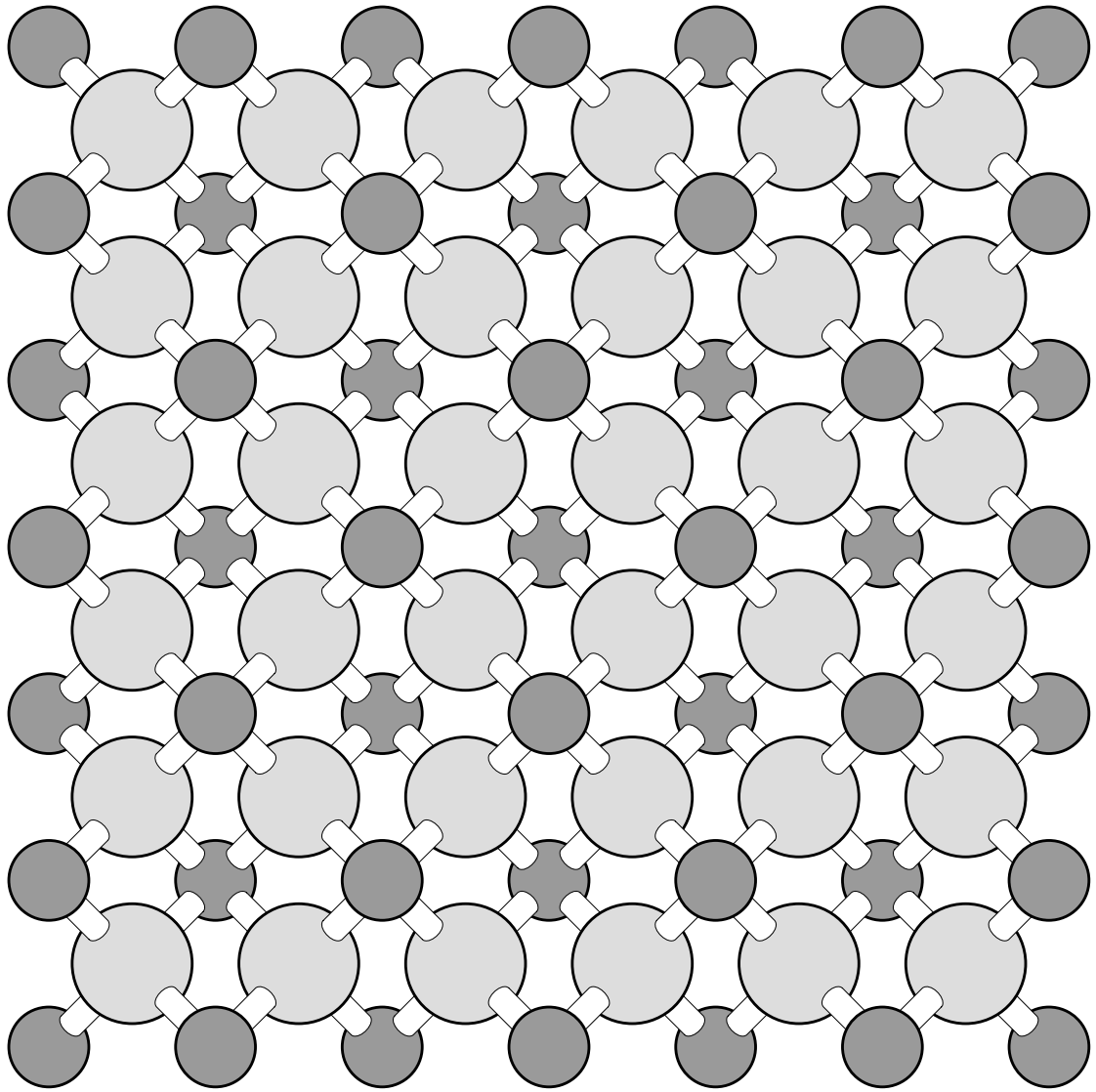
Make sure your patterns are relatively neat and legible. The seven patterns are appended.

Preparation for X-ray Data Analysis:

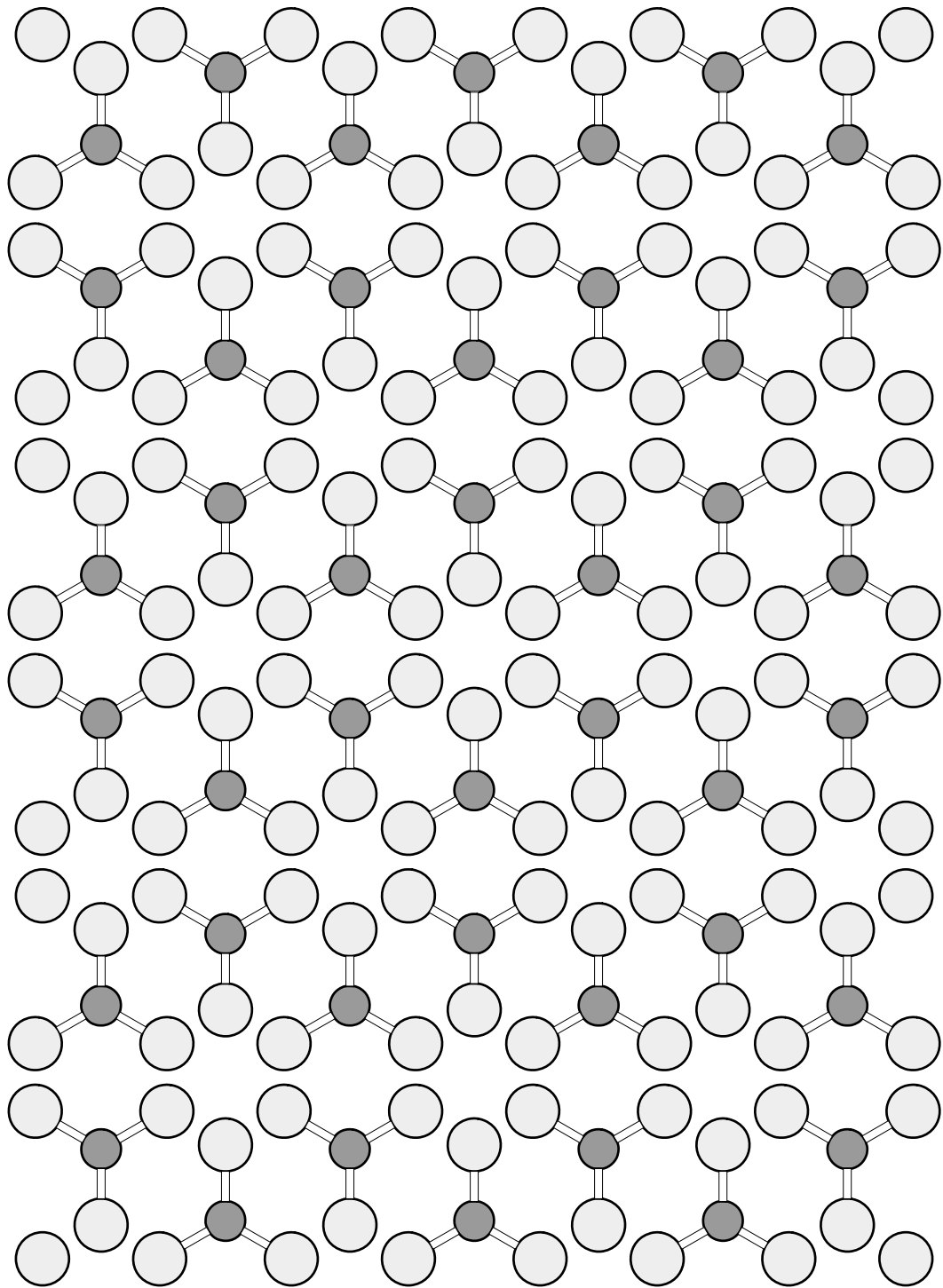
X-ray data analysis will be performed in this class using XPert HighScore and XPert Plus Software from Panalytical. You are permitted to install these packages on your personal computer on the condition that you uninstall them at the end of the term. If you cannot abide by this condition, or you simply do not wish to do the installation, you can use the computers in Steele 339 (the diffractometer lab), which already have this software. In this assignment you will use the HighScore program only. It is advised, however, that if you are doing an installation, you do both packages at the same time.

Obtain the installation files from your TA. Instruction and data files can be accessed from the course website (or can also be obtained from your TA).

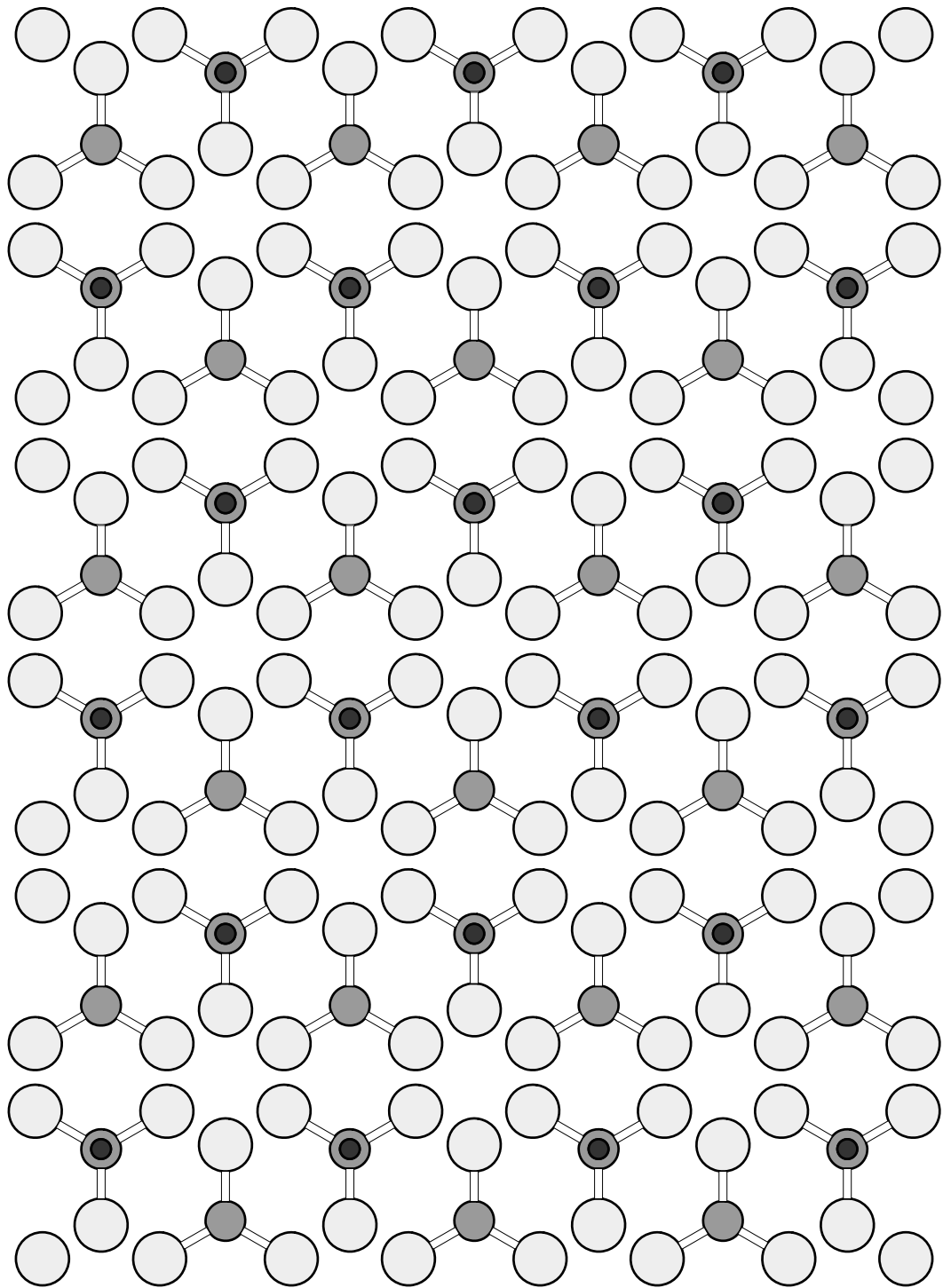
Referring to the detailed instructions provided, import the example *.xml file provided. Strip the $K\alpha$ -2 peaks using the default parameters. Perform a peak search both before and after $K\alpha$ -2 stripping. Prepare a table comparing the results and give it a meaningful title. Export the image of the diffraction pattern as a bitmap and insert it into a document (i.e. word) file. Also export the data as ascii and plot in Origin. Convince yourself that the data conversion to ascii was carried out properly by comparing to the two plots. Properly label axes and provide a meaningful figure caption. Data are collected at room temperature from the compound $Rb_3H(SeO_4)_2$.



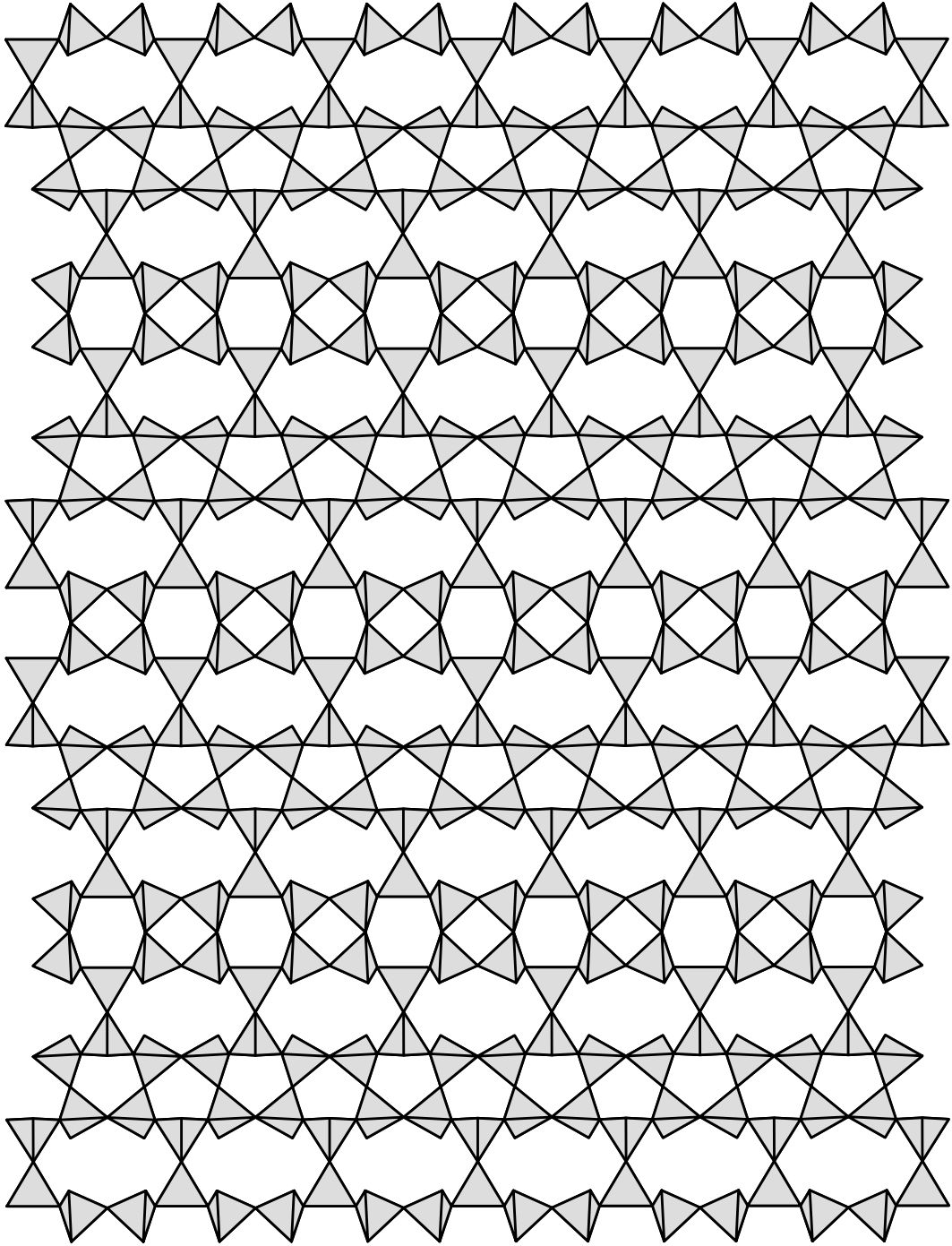
Pattern 1



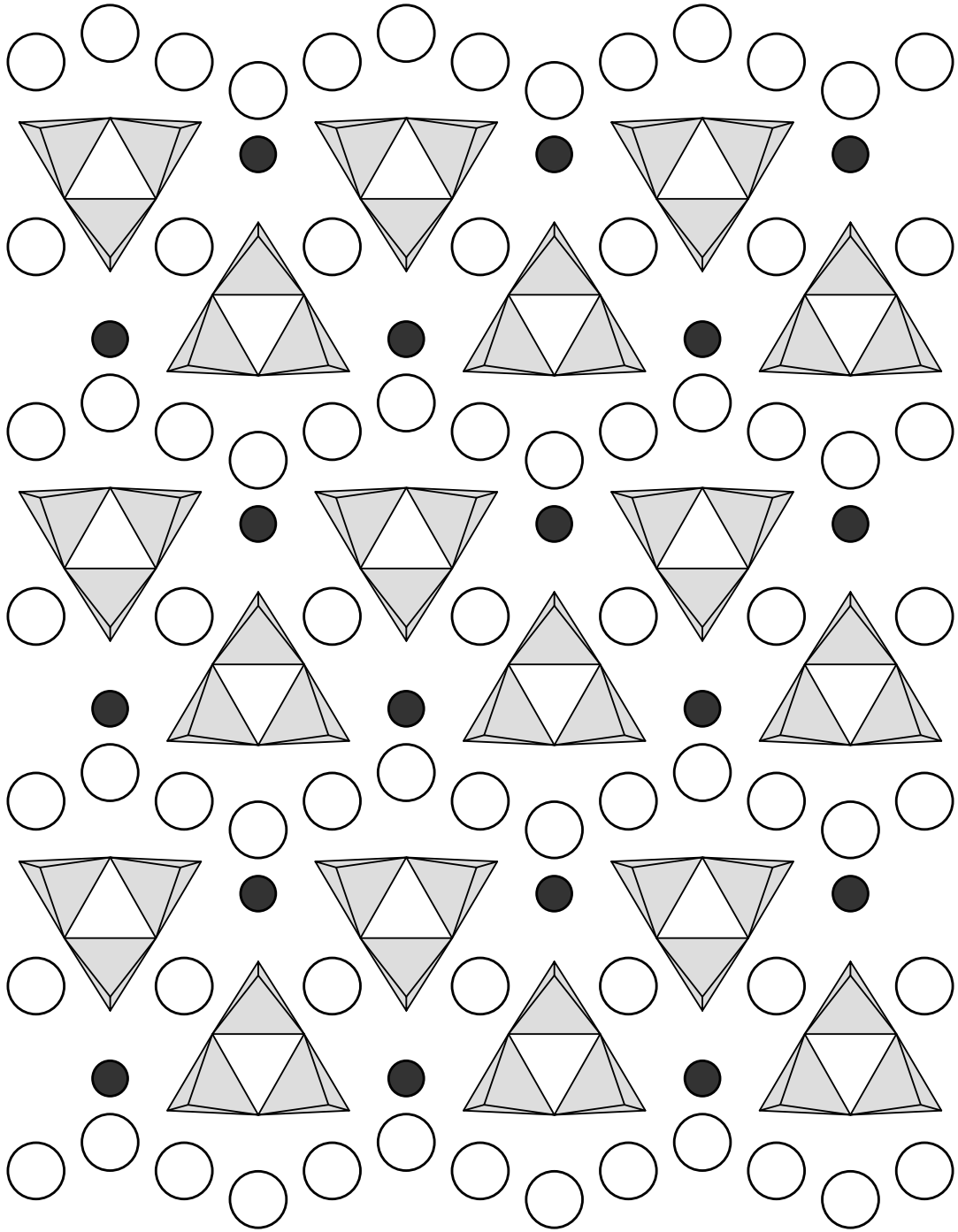
Pattern 2



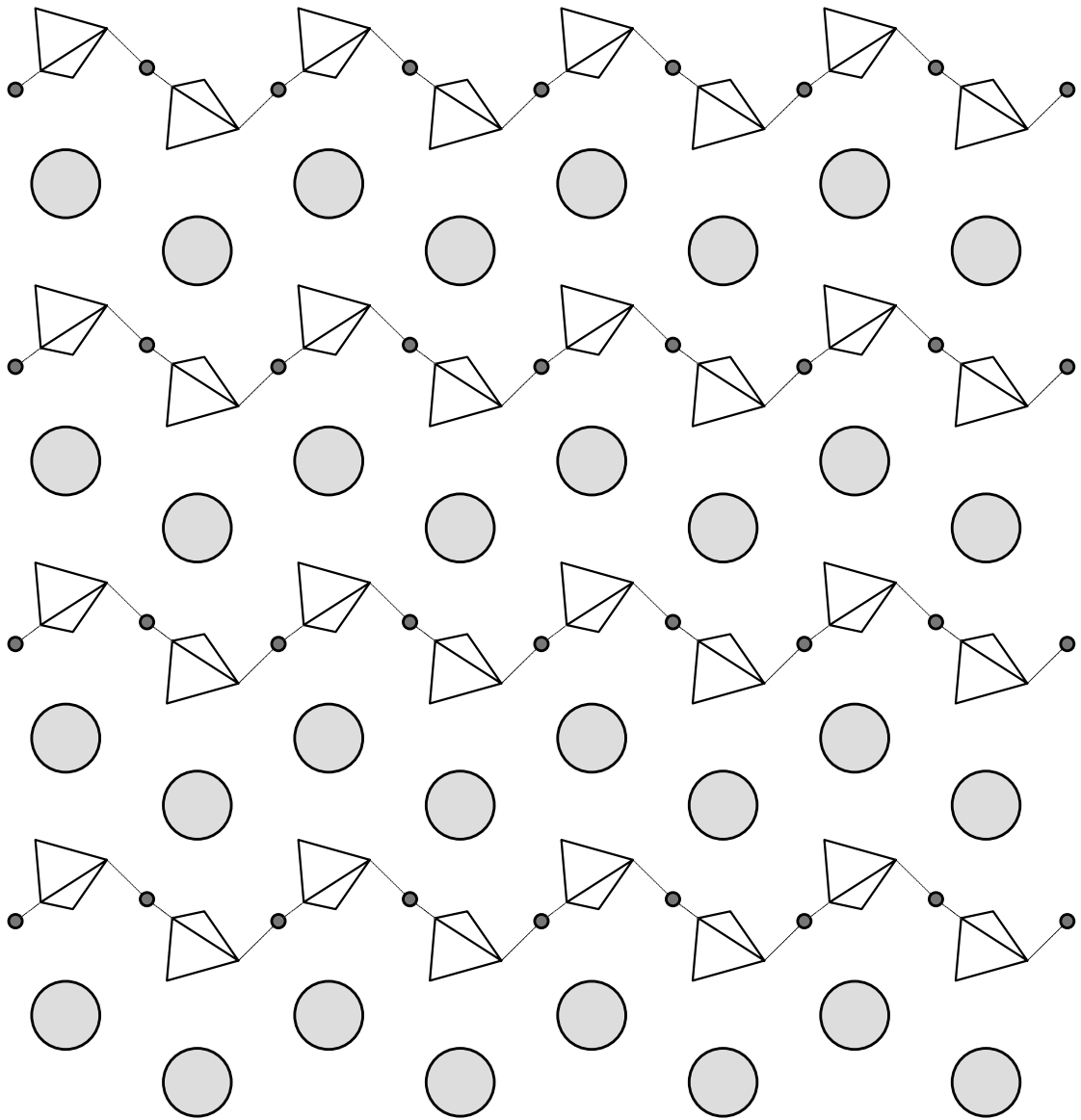
Pattern 3



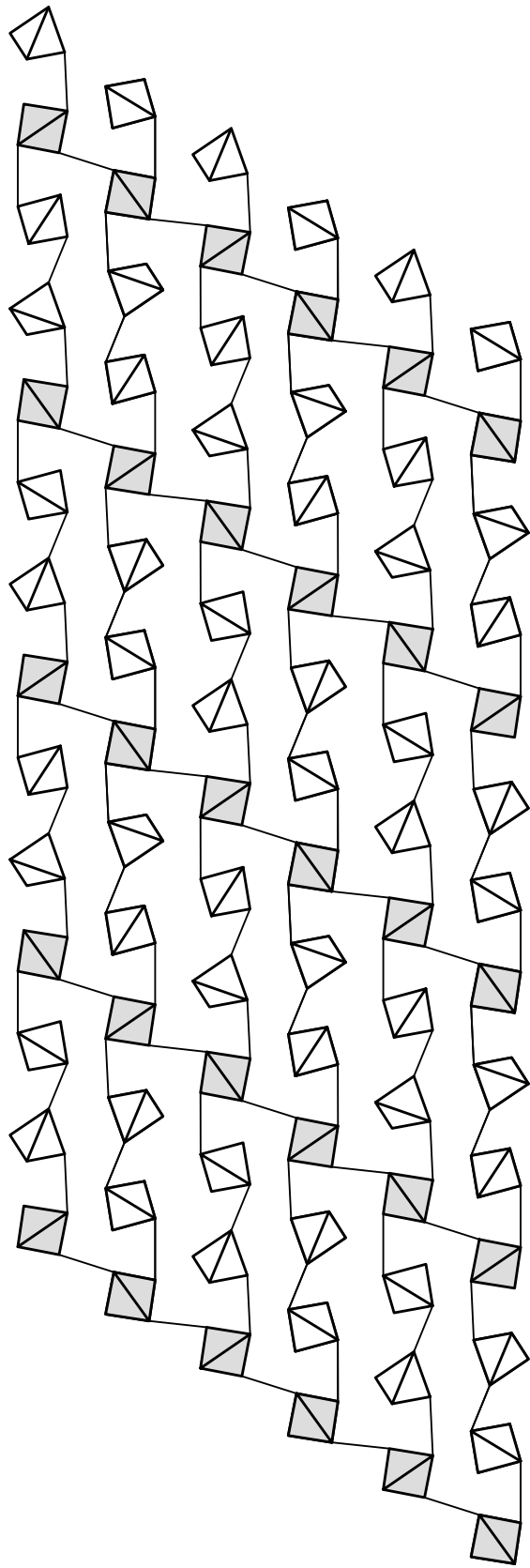
Pattern 4



Pattern 5



Pattern 6



Pattern 7