PURPOSE

To extend student understanding of how arrays produce diffraction patterns by using optical transforms that resemble various unit cells assumed by metals, ionic solids, and molecular solids. Molecular solids can be connected to predictions of molecular structure using VSEPR theory.

METHOD

To give the results obtained in Investigation 1 some chemical significance, the rows of horizontal and vertical lines could be viewed as long, highly oriented polymer chains. The square arrays of dots could be seen as several cubic structural arrangements. This investigation should build from these views and allow students to see that changing the structure from simple cubic to a body centered or a closest packed arrangement has a dramatic affect on the diffraction pattern produced. This provides a deeper understanding of the relationship between diffraction patterns and structures. The first part of this investigation uses optical transforms of different unit cells of extended solids. The second part explores optical transforms of common molecular geometries.

MATERIALS

Unit Cell and VSEPR optical transform slides (Available from ICE. See supplier information in the Appendix).

LEDs from Investigation 1

overhead transparencies of the following four pages -- ADD PG #s

stereoscope or microscope

PROCEDURE

a. Orient the Unit Cell slide provided by the instructor so that the ICE logo is on the right-hand side. With the stereoscope, look carefully at the arrays on the slide and make a sketch in the space provided in Table 1 of the Data Sheet.

b. Connect the battery snap to the red LED and place it at least a meter away from you. View the LED through the different regions of the slide and sketch the diffraction patterns that you see in the appropriate spaces in Table 2.

c. Repeat steps a and b above using the VSEPR slide provided by the instructor and record your observations in Table 3 and Table 4.

ANSWERS TO FOLLOW-UP QUESTIONS

Note: For comparison, it may be necessary to show the overheads of the following 4 pages to the class after they have completed their sketches.

1. Look at your sketches of arrays *a* and *b* on the Unit Cell slide. Array *a* is the two-dimensional projection of a body-centered cubic structure and *b* of a simple cubic arrangement. Now look in Table 2 at the diffraction patterns produced by each. What is the effect on the diffraction pattern of placing an identical atom at the center of each simple square in the array?

    Every other diffraction spot is eliminated. These are referred to as systematic absences.

2. Look at your sketches of arrays *c* and *d* in Table 1. Array *c* represents two different kinds of atoms, each surrounded by four atoms of the other type. Array *d* is is like that of array *b* above. Now look in Table 2 at the diffraction patterns produced by these arrays. What is the effect on the pattern of placing a different sized atom at the center of each simple cube?

    Every other diffraction spot has changed in intensity.

3. Look at your sketches of arrays *e* and *f* in Table 1. Array *e* represents a structure in which all angles are 90°, but the sides are of unequal length (rectangle); and *f* one in which the angles are not 90° (inclined parallelograms). Now look in Table 2 at the diffraction patterns that are produced and describe what you see.

    The diffraction patterns appear rotated. In *e*, the long direction of the rectangular array is vertical; in diffraction, the rectangle's long direction is horizontal. Note that this is a reciprocal relationship: long distances in the array become short distances in the diffraction pattern. In the array *f*, the diffraction pattern is rotated by 60° relative to the array.

4. Look at your sketches in Table 3. Each array simulates a molecule that consists of three atoms. What shape molecule is represented by array *a*? If the entire array was rotated 90°, describe what the new diffraction pattern would look like.

    Array *a* comprises linear "molecules". If the array were rotated 90°, the spots in the diffraction pattern would rotate by 90°, also.

5. The sequence of arrays (*b*, *d*, and *c*) represents an array of angular molecules. What happens to the angle as you proceed through this sequence? Why is the diffraction pattern produced by *c* similar to that produced by *a*?

    The angle increases in size. The diffraction pattern produced by *c* is similar to that produced by *a* because pattern *c* is almost linear.

6. A close look at your sketches for diffraction from arrays *e* and *f* in Table 4 reveals that these diffraction patterns are mirror images of each other. Explain why this is not surprising.

    Because the arrays are also mirror images of one another.

7. What molecular shapes are simulated by arrays *g* and *h* in Table 3?

    Array *g* is T-shaped, while *h* is arranged to simulate a trigonal planar arrangement.

EXTENSIONS

For more information on this experiment there are a number of interesting web sites:

www.yorvic.york.ac.uk/~cowtan/sfapplet/sfintro.html

- This is an Interactive Structure Factor Tutorial.

There are many other websites linked to these.

The following figures are from A Material Science Companion, figures 4.6-4.9

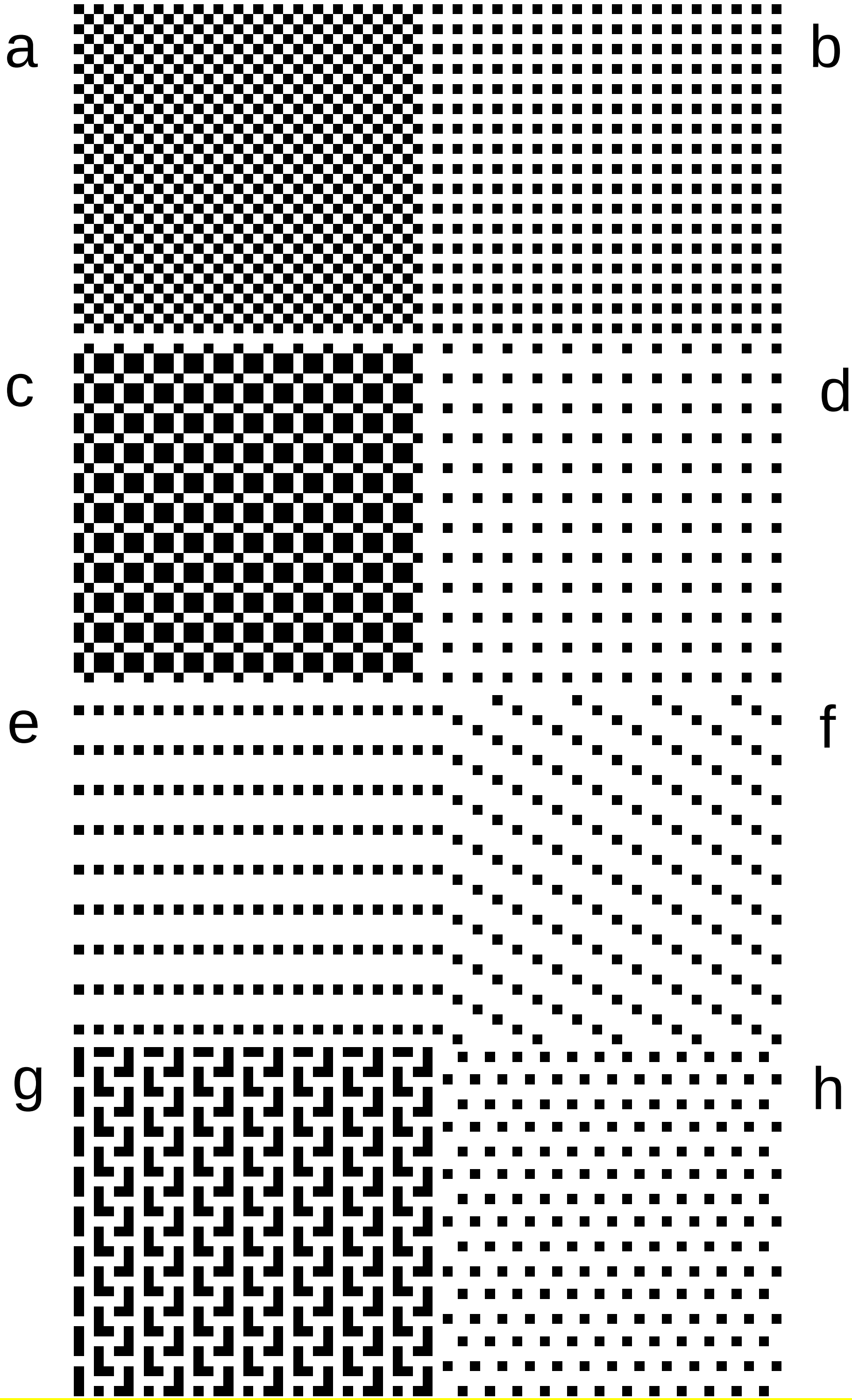

Figure 3. The arrays on the optical transform Unit Cell slide, available from ICE (oriented so that the ICE logo is on the right side as you look through the slide).

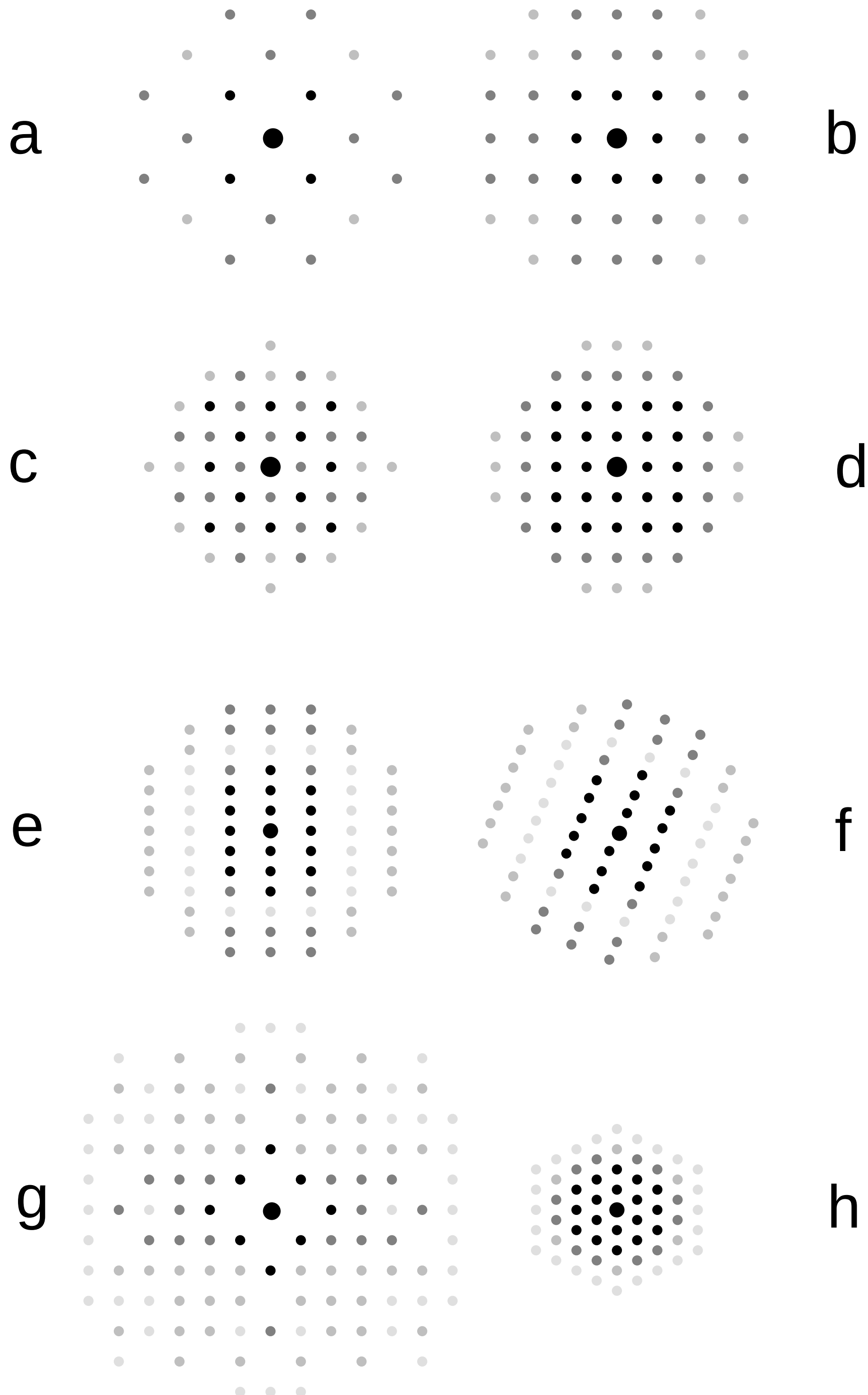

Figure 4. A simulation of the diffraction patterns from Figure 3. The letter by each pattern corresponds to the array from which the diffraction pattern is derived.

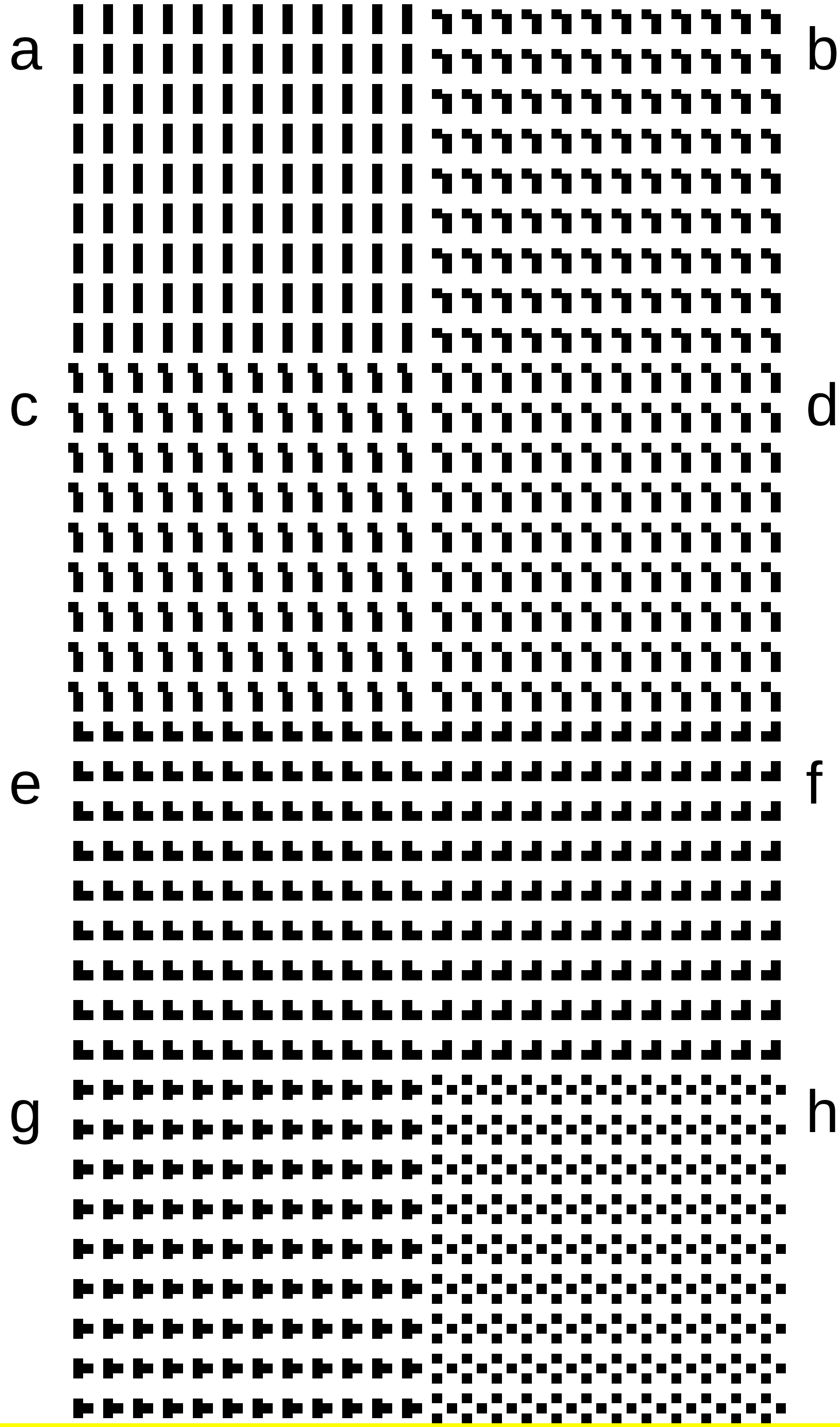

Figure 5. The arrays on the optical transform VSEPR slide, available from ICE (oriented so that the ICE logo is on the right side as you look through the slide).

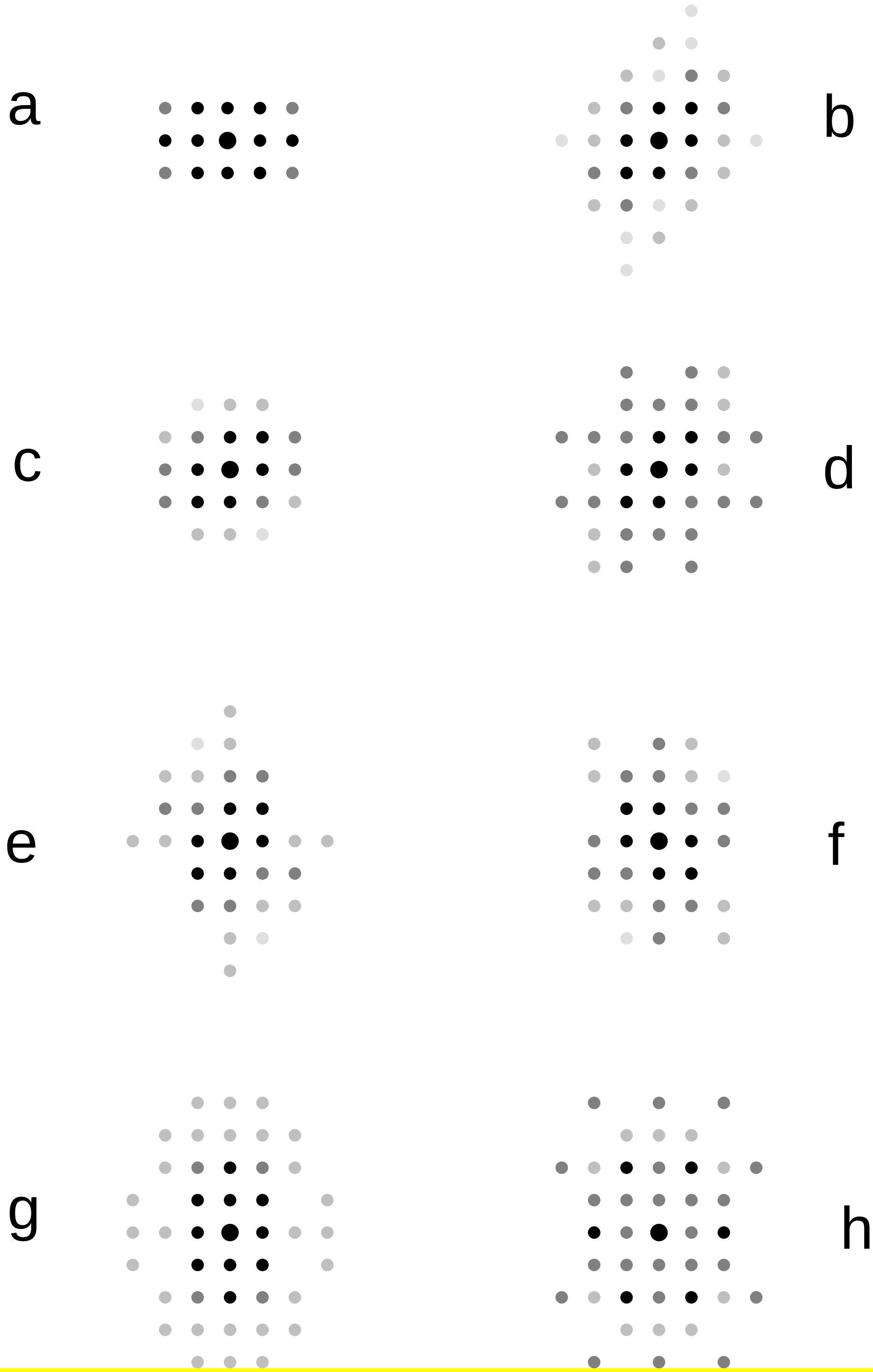

Figure 6. A simulation of the diffraction patterns from Figure 5. The indicated letter corresponds to the array from which the diffraction pattern is produced.