

Materials Science 142

Applications of Diffraction Techniques in Materials Science

Assigned: 1/11/12

Homework Assignment 1

Due: 1/18/12, 5pm

Point Group Identification

Goal: Identify the point group and crystal system of a high symmetry object. Seven objects are to be analyzed. [For your folding pleasure, instructions for making the objects are appended, but this is not part of the assignment.]

1. List and identify the symmetry elements in each. For example, when describing the cube, state “mirror plane in (110)”, or make drawings of the faces of the cube with the symmetry elements shown.
2. Identify the point group of each object.
3. Identify to which crystal system each of the models must belong.

Turn in a description of the symmetry elements in each object, the point group of the object, and the appropriate crystal system. Make sure your drawings are neat and legible. A formal lab write-up is not required.

Textbook Problems:

Chapter 2: #1, #5, #6 (reproduced below)

1. Consider two mirror planes that intersect at $\phi = 90^\circ$. Using a geometrical representation of two planes, establish which symmetry element(s) appear(s) as the result of this combination of mirror planes. What is(are) the location(s) of new symmetry element(s)? Name the point group symmetry formed by this combination of symmetry elements.
5. Determine both the crystal systems and point group symmetry of an ideal brick in which $a \neq b \neq c$ and $\alpha = \beta = \gamma = 90^\circ$.
6. Determine both the crystal system and point group symmetry of the benzene molecule, C_6H_6 . Treat atoms as spheres, not dimensionless points.

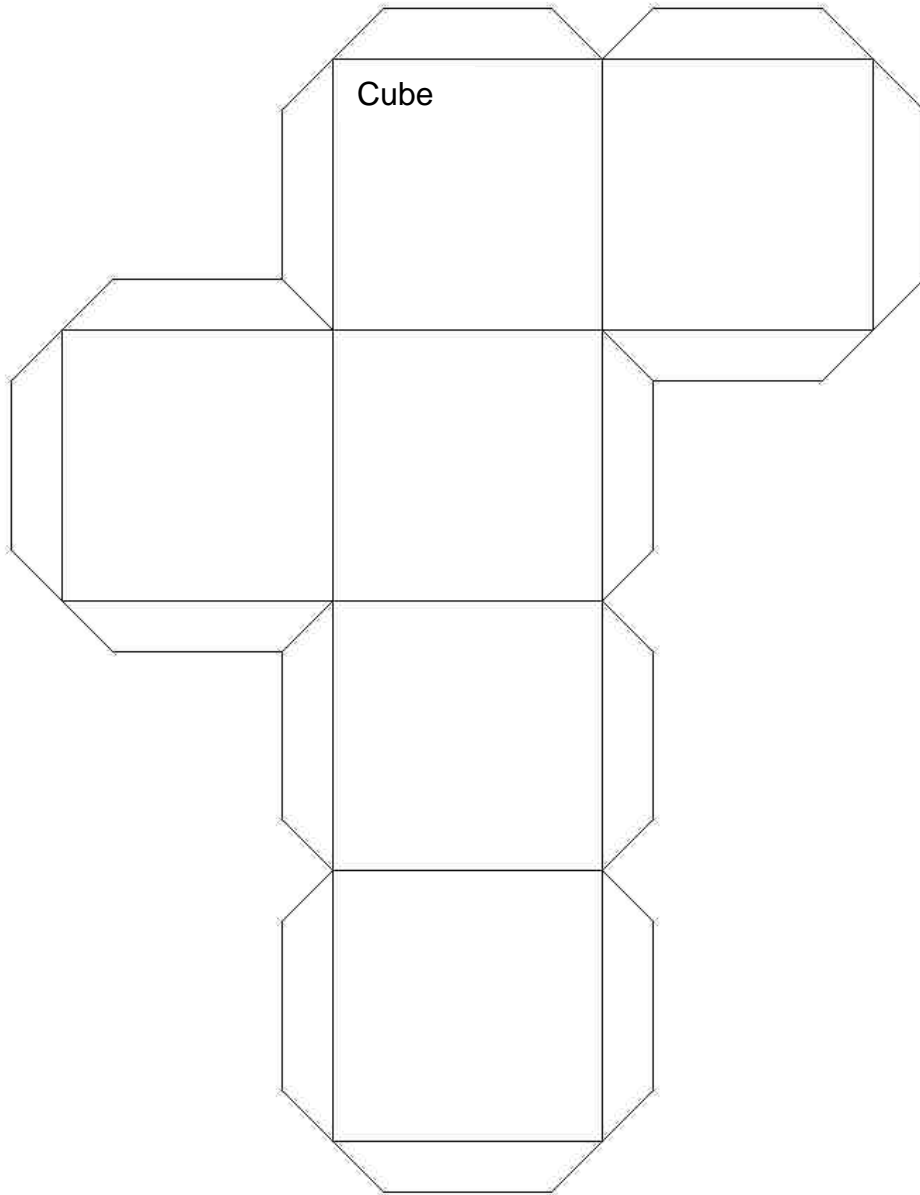
Preparation for X-ray Data Analysis:

Install Origin Software. It can be downloaded from the company website www.originlab.com. A one-year student license can be purchased for \$50. A sample ascii data file of diffraction data will be provided. Plot this using properly label axes and provide a meaningful figure caption: “Figure 1. X-ray powder diffraction pattern collected from xxxx using CuK_α radiation (Panalytical X’Pert Pro) over the two-theta range xxx to xxx.”

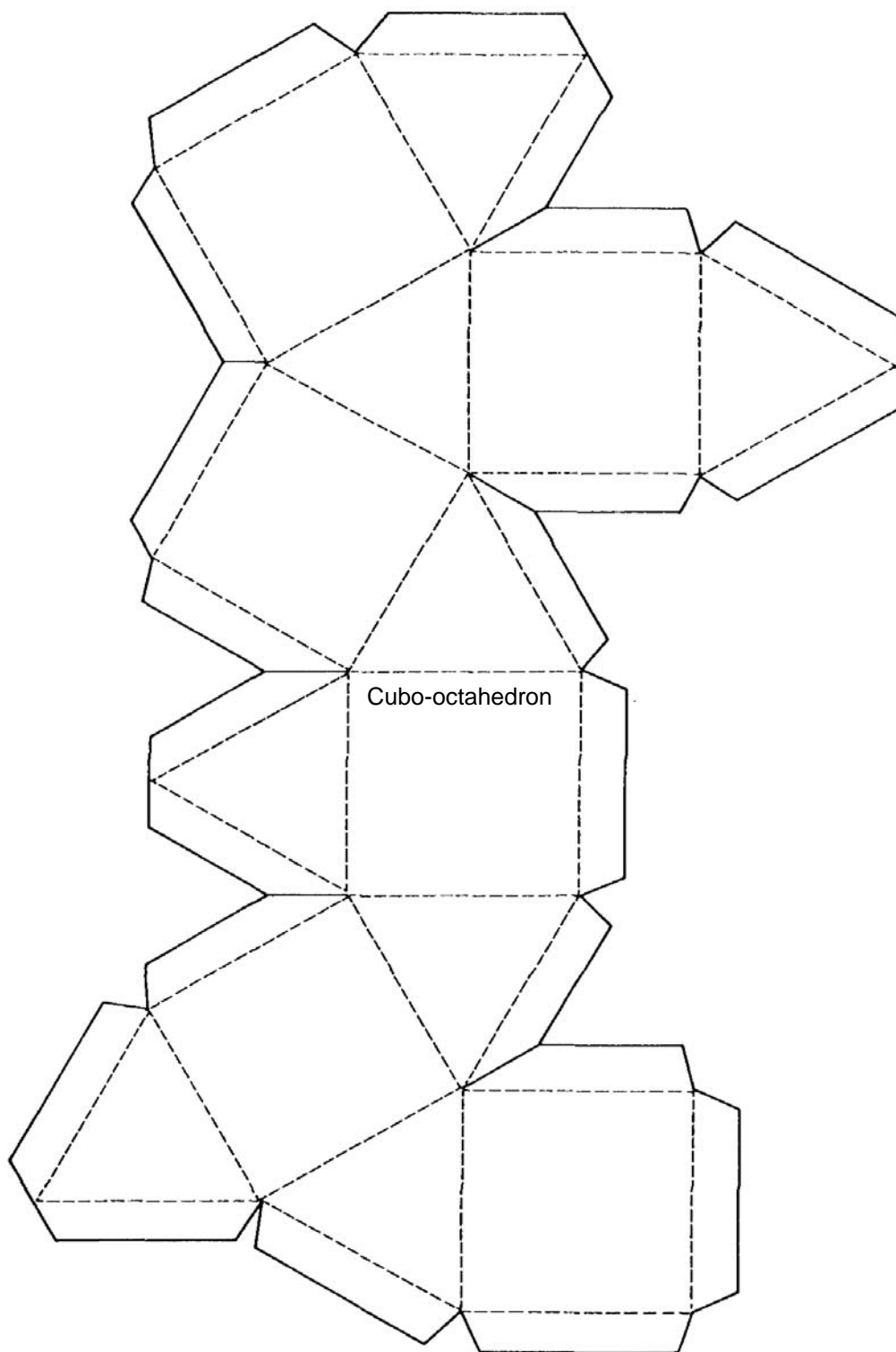
Reading:

Fundamentals of Powder Diffraction and Structural Characterization of Materials, 2nd Ed: Chapters 1 and 2.

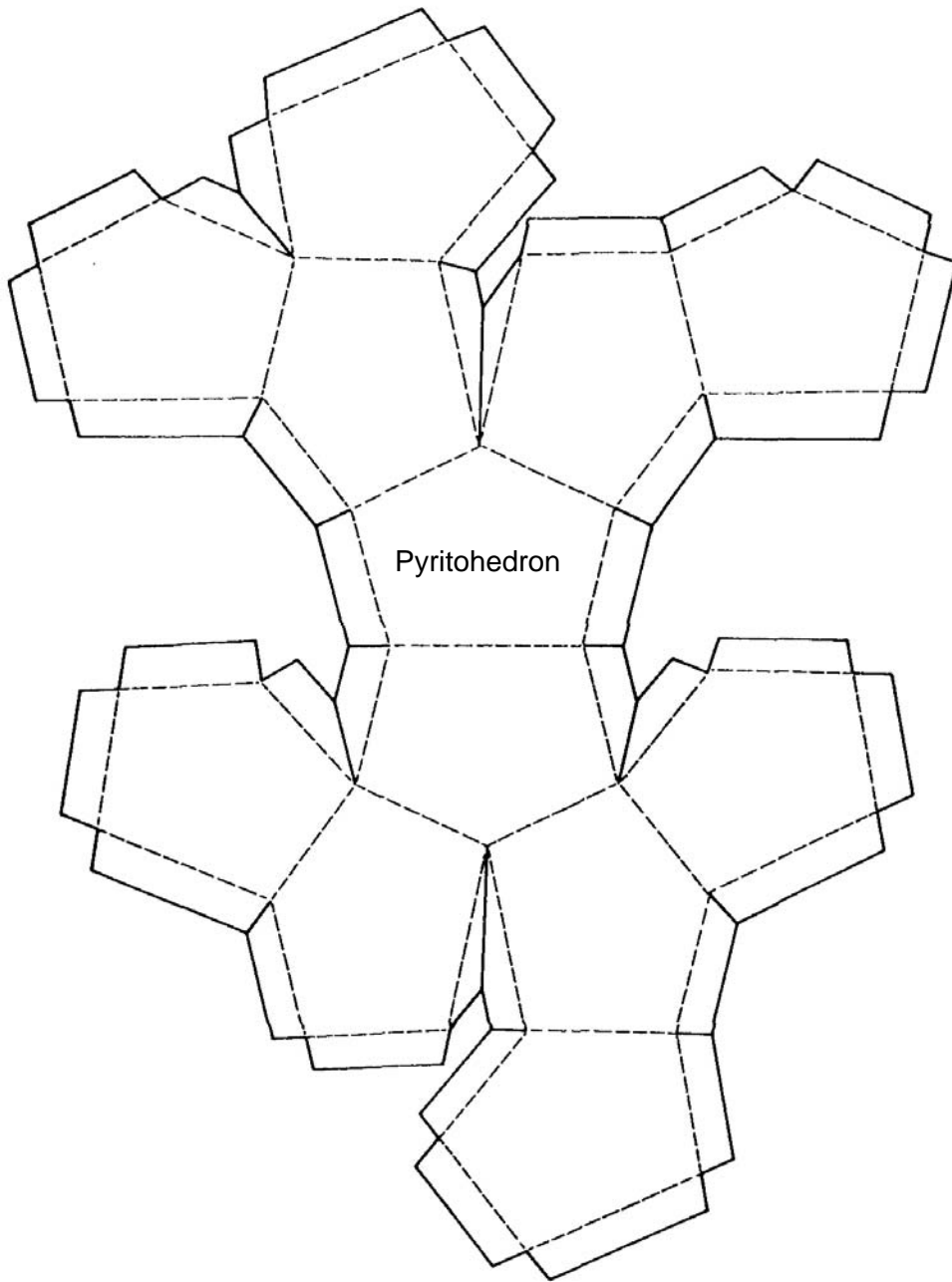
Cube



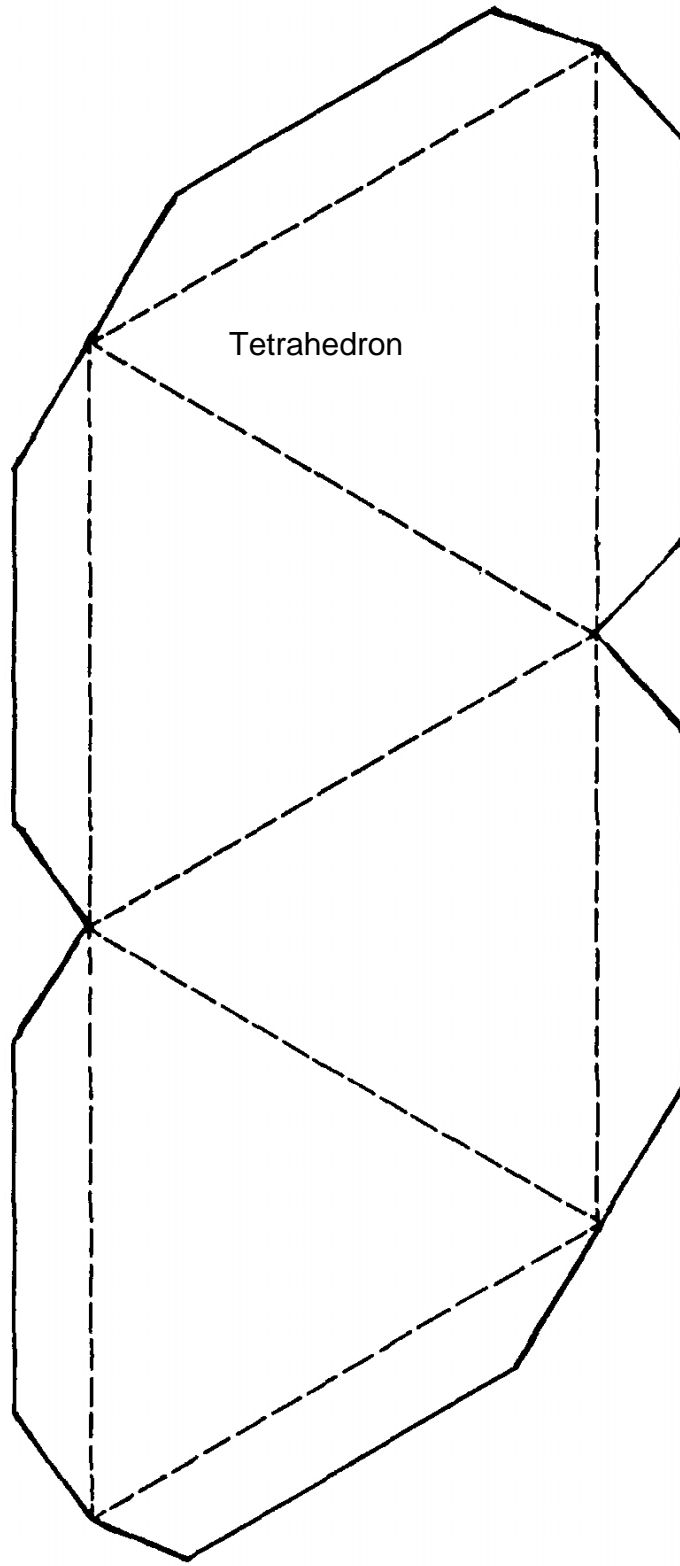
Cubo-octahdron



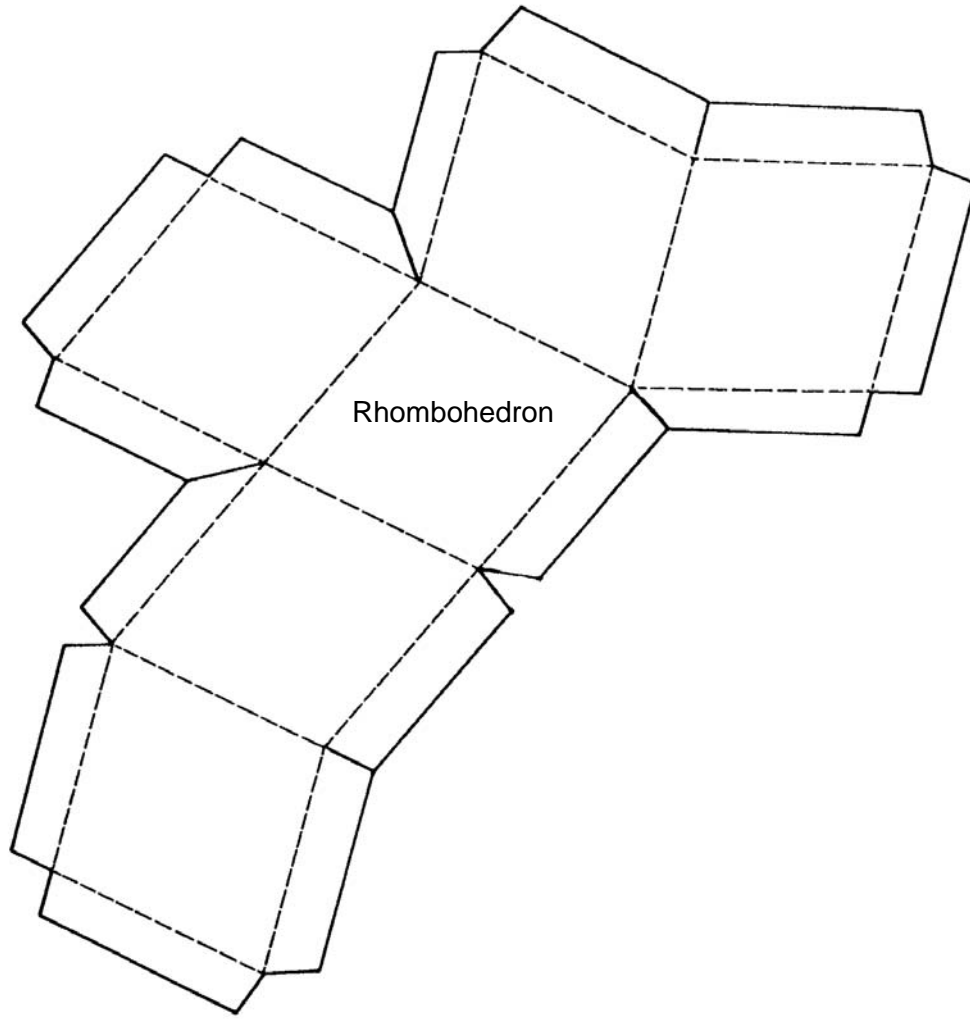
Pyritohedron



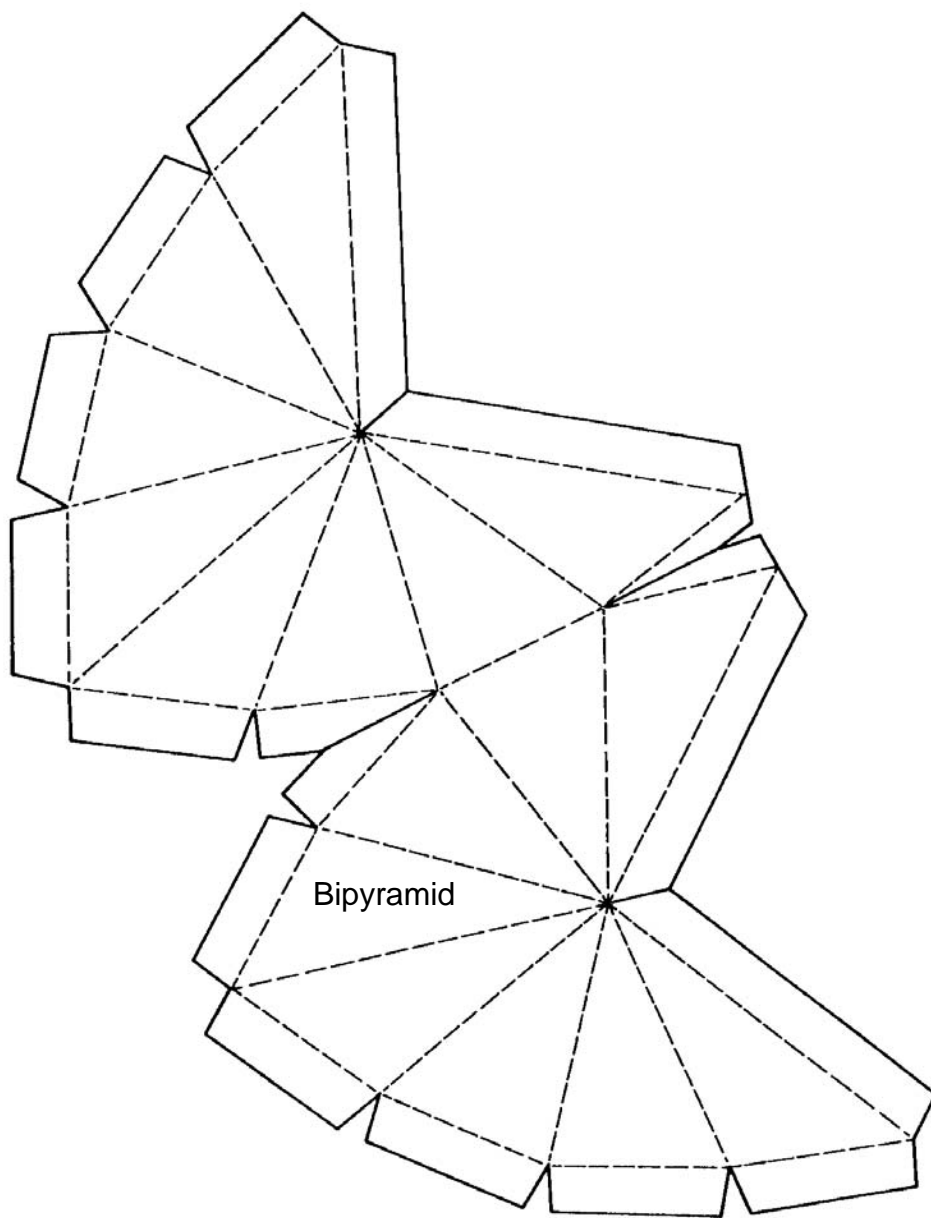
Tetrahedron



Rhombohedron



Bipyramidal crystal



Dodecahedron

