

# GY302 Crystallography & Mineralogy Lab

## **Lab 3 Assignment: Determination of Point Groups from Orthorhombic and Tetragonal Block Models.**

There will be 10 wooden block models available in room 337 that you will need to determine the point group classification. Fill in the attached data sheet for each of the blocks to turn in as the weekly assignment. A flowchart is provided to aid in determining the point group. The data sheet form is also on the online site in "resources" when you need to print single sheets. You can assume that all of the block models in this lab are from the Tetragonal or Orthorhombic systems. The Orthorhombic models will in general have more symmetry elements than the ones in the previous lab.

## Crystal Model Data Sheet

Student Name: \_\_\_\_\_

J#: \_\_\_\_\_

Block Model No. : \_\_\_\_\_

1. Rotational axes: List below the number and types of rotational axes discovered in the block model. Use the notation  $nA_x$  where  $n$ = number of axes found, and  $x$ =the magnitude of the rotational axis (2,3,4,6).  
\_\_\_\_\_

2. Roto-inversion axes: List below the number and type of roto-inversion axes discovered in the block model. Use the notation  $nA_x$  where  $n$ = number of roto-inversion axes found, and  $x$ =the magnitude of the rotational axis (2,3,4,6).  
\_\_\_\_\_

3. Mirror planes: List below the number of mirror planes discovered in the model:  
\_\_\_\_\_

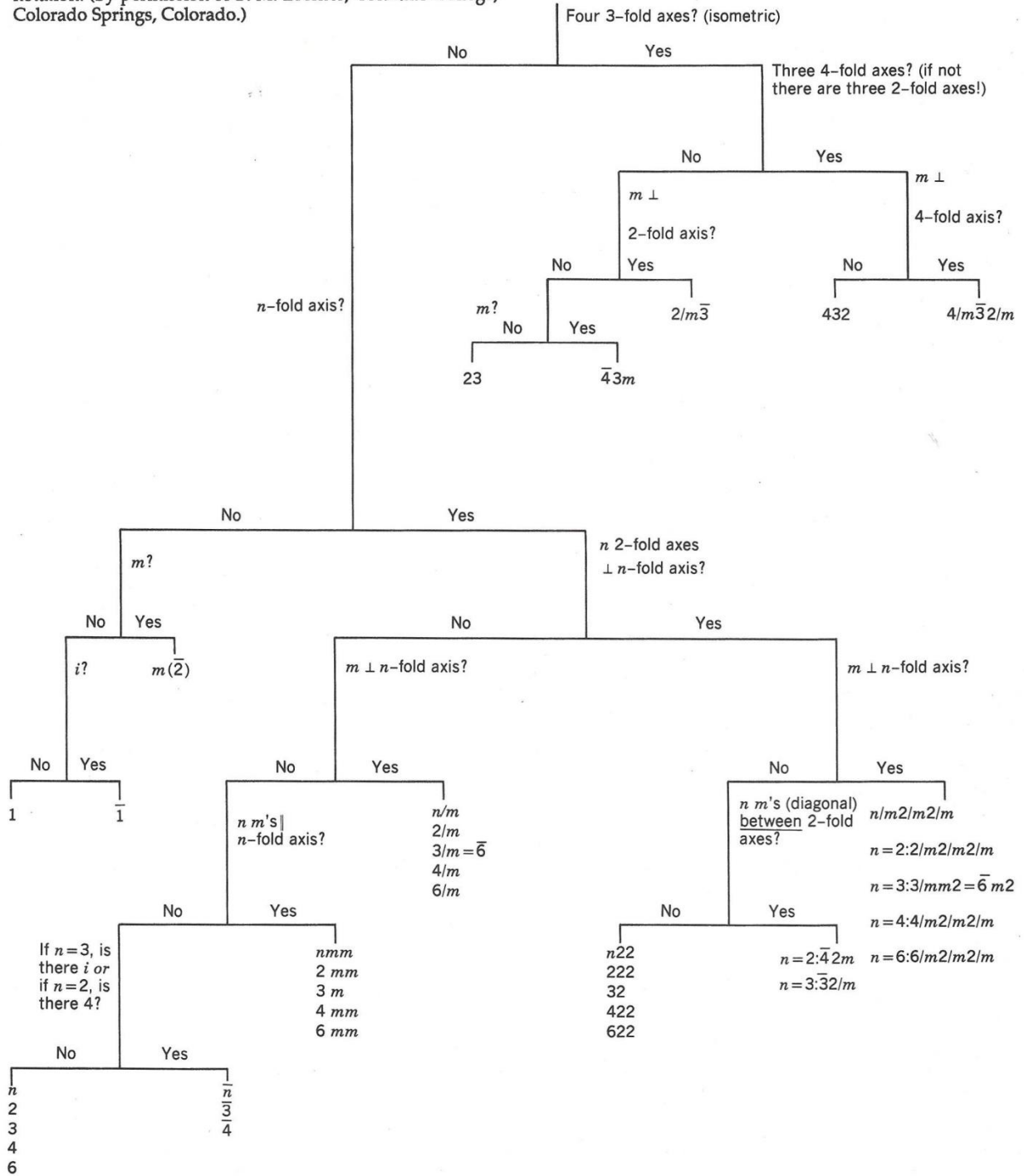
4. Center of symmetry (i): Does the model contain a center of symmetry (Yes/No): \_\_\_\_\_

5. Hermann-Mauguin Point Group Designation: \_\_\_\_\_

6. Crystal Class Name: \_\_\_\_\_

7. Crystal System (Triclinic, Monoclinic, Orthorhombic, Tetragonal, Trigonal/Hexagonal, Isometric) :  
\_\_\_\_\_

FIGURE 2.4 Scheme for the assignment of the symbolic point group notation on the basis of the symmetry content of a crystal. See Exercise 3 for further discussion of this symmetry notation. (By permission of B. M. Loeffler, Colorado College, Colorado Springs, Colorado.)



**TABLE 3.2** Crystal Systems and Their Coordinate Axes

<i>Crystal System</i>	<i>Coordinate Axes</i>
Triclinic	No symmetry constraints on choice of axes ( $a \neq b \neq c$ ; $\alpha \neq \beta \neq \gamma$ ) <sup>a</sup>
Monoclinic	If 2-fold axis is present, set this as $b$ ; if only mirror present, choose $b$ perpendicular to it ( $a \neq b \neq c$ ; $\alpha = \gamma = 90^\circ$ ; $\beta > 90^\circ$ )
Orthorhombic	The three mutually perpendicular directions about which there is binary symmetry (2 or $m$ ) are chosen as the axial directions, $a$ , $b$ , and $c$ ( $a \neq b \neq c$ ; $\alpha = \beta = \gamma = 90^\circ$ )
Tetragonal	The unique 4-fold axis is chosen as $c$ ; the two $a$ axes are in a plane perpendicular to $c$ ( $a \neq b$ , which results in $a_1 = a_2$ ; $\alpha = \beta = \gamma = 90^\circ$ )
Hexagonal	The unique 6-fold (or 3-fold) axis is chosen as $c$ ; the three $a$ axes are in a plane perpendicular to $c$ ( $a = b$ , which results in $a_1 = a_2 = a_3$ ; $\alpha = \beta = 90^\circ$ ; $\gamma = 120^\circ$ )
Isometric	The three 4-fold rotation axes (when present) are chosen parallel to the three coordinate axes ( $a_1, a_2, a_3$ ); if 4-fold rotation axes are absent, locate the four 3-fold axes at $54^\circ 44'$ to the $a$ axes (the 3-fold directions are parallel to diagonal directions from corner to corner in a cube) ( $a_1 = a_2 = a_3$ ; $\alpha = \beta = \gamma = 90^\circ$ )

<sup>a</sup>The notation  $a = b$  means that the  $a$  axis is nonequivalent to the  $b$  axis. Similarly,  $\alpha = \beta$  means that the angle  $\alpha$  is not equivalent to the angle  $\beta$ . When a specific axis turns out to be equivalent to another axis,  $a = b$  results, which crystallographers rename as  $a_1 = a_2$ .

**TABLE 3.3** Relationship of Hermann–Mauguin Symbols to Coordinate Axes in Crystals

<i>Point Group (crystal class)</i>	<i>Crystal System</i>	<i>Symmetry Constraints on Hermann-Mauguin Notations</i>
1, $\bar{1}$	Triclinic	No symmetry constraints on location of coordinate axes
2, $m$ , $2/m$	Monoclinic	2-fold = $b$ ("second setting"); mirror is the $a$ - $c$ plane
222, $mm2$ , $2/m2/m2/m$	Orthorhombic	2-fold axes coincide with coordinate axes in the order $a$ , $b$ , $c$ .
4, 4, $4/m$ , 422, $4mm$ , $42m$ , $4/m2/m2/m$	Tetragonal	4-fold axis (unique) is $c$ axis; second symbol (if present) refers to both $a_1$ and $a_2$ axial directions; third symbol (if present) refers to directions at $45^\circ$ to the $a_1$ and $a_2$ axes. <i>Example:</i> 422: 4 = $c$ ; first 2 means 2-fold axes along $a_1$ and $a_2$ ; second 2 means two more 2-fold axes along diagonal directions.
6, $\bar{6}$ , $6/m$ , 622, $6mm$ , $6m2$ , $6/m2/m2/m$ , 3, $\bar{3}$ , $32$ , $3m$ , $32m$	Hexagonal	6-fold axis (or 3-fold axis) is $c$ axis; second symbol (if present) refers to three axial directions ( $a_1, a_2,$ and $a_3$ ); and third symbol (if present) refers to directions at $30^\circ$ to the $a_1, a_2, a_3$ axes. <i>Example:</i> $6m2$ ; 6 is coincident with $c$ axis; $m$ 's present along the three axial directions ( $a_1, a_2, a_3$ ) and 2-fold rotations occur along the directions half-way to the crystallographic axes ( $a_1, a_2, a_3$ )
23, $2/m\bar{3}$ , 432, $43m$ , $4/m\bar{3}2/m$	Isometric	The first entry refers to the three crystallographic axes ( $a_1, a_2, a_3$ ); the second symbol refers to four directions at $54^\circ 44'$ to the crystallographic axes (these directions run from corner to corner in a cube); the third symbol (if present) refers to six directions that run from edge to edge in the cube. <i>Example:</i> $4/m\bar{3}2/m$ ; all three $a$ axes are axes of 4-fold rotation, with mirrors perpendicular to them; the "corner to corner" directions (in a cube) are 3 (there are four such directions); the "edge to edge" directions (in a cube) are 2-fold rotations (there are six such directions) with mirrors perpendicular to them.