

TABLE 3.2 Crystal Systems and Their Coordinate Axes

Crystal System	Coordinate Axes
Triclinic	No symmetry constraints on choice of axes ($a \neq b \neq c$; $\alpha \neq \beta \neq \gamma$) ^a
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) ($a_1 = a_2 = a_3$; $\alpha = \beta = \gamma = 90^\circ$)

^aThe notation $a \neq b$ means that the a axis is nonequivalent to the b axis. Similarly, $\alpha \neq \beta$ means that the angle α is not equivalent to the angle β . 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

Point Group (crystal class)	Crystal System	Symmetry Constraints on Hermann–Mauguin Notations
$1, \bar{1}$	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° to the a_1 and a_2 axes. Example: $422: 4 = c$; first 2 means 2-fold axes along a_1 and a_2 ; second 2 means two more 2-fold axes along diagonal directions.
$6, \bar{6}, 6/m, 622, 6mm, \bar{6}m2, 6/m2/m2/m, 3, 3, 32, 3m, 32m$	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° to the a_1, a_2, a_3 axes. Example: $6m2$; 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)
$23, 2/m\bar{3}, 432, 43m, 4/m32/m$	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. Example: $4/m32/m$; 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.