

3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

3.2.3. Tables of the crystallographic point-group types

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The crystallographic point-group types are listed in Tables 3.2.3.1 and 3.2.3.2 for two-dimensional and for three-dimensional space, respectively. No listings are presented for the noncrystallographic point-group types (*i.e.* having axes of orders other than 1, 2, 3, 4 and 6), but their symbols can be found in Tables 3.2.1.5, 3.2.1.6 and 3.2.3.3 (*cf.* Section 3.2.1.4 for a review of noncrystallographic point groups). The two icosahedral point groups 235 and $m\bar{3}5$ are treated in detail in Section 3.2.1.4.2, while their crystallographic data are shown in Table 3.2.3.3.

There is a physical difference between the point groups of crystals and those of molecules. For a molecule, the point group is the set of all symmetry operations that map its atoms onto one another. Macroscopic crystals, however, hardly ever exhibit their ideal symmetry because of the defects that occur during crystal

growth. For a crystal, its point group is the set of all symmetry operations that map the set of the vectors normal to the crystal faces onto one another; it does not operate in point space, but in vector space.

In Tables 3.2.3.1 and 3.2.3.2 the point-group types are presented for crystals as well as for molecules. However, parts of the tables concern either crystals only or molecules only. The names of crystal forms in the fifth column (in roman type) and the *hkl* face indices in the last column are only relevant for crystals. The names of the point forms in the second line of each pair of entries in the fifth column (given in italics) and the other data (multiplicities, Wyckoff letters, site symmetries and sets of symmetry-equivalent coordinates) concern both crystals and molecules. However, for point groups with an origin fixed by symmetry, the Wyckoff position with the Wyckoff letter *o* is only of interest for molecules.

Because the meanings of the entries are not identical for crystals and for molecules, they are not explained here, but in Sections 3.2.1 (for crystals) and 3.2.4 (for molecules).

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Table 3.2.3.1

The ten two-dimensional crystallographic point groups

The point groups are listed in blocks according to crystal system and are specified by their Hermann–Mauguin symbols. For each point group, the stereographic projections show (on the left) the general position and (on the right) the symmetry elements.

The list of Wyckoff positions includes:

Columns 1 to 4: multiplicity, Wyckoff letter, oriented site-symmetry symbol, coordinate doublets;

Under the stereographic projections: edge forms (in roman type) and point forms (in italics); if there are two entries, the second entry refers to a limiting (noncharacteristic) form;

Last column: Miller indices of equivalent edges [for hexagonal groups, Bravais–Miller indices (*hki*) are used].

OBLIQUE SYSTEM							
1							
1	<i>a</i>	1	<i>x, y</i>		Single edge <i>Single point</i>	(<i>hk</i>)	
2							
2	<i>a</i>	1	<i>x, y</i> \bar{x}, \bar{y}		Pair of parallel edges <i>Line segment through origin</i>	(<i>hk</i>) ($\bar{h}\bar{k}$)	
1	<i>o</i>	2	0, 0		<i>Point in origin</i>		

3.2. POINT GROUPS AND CRYSTAL CLASSES

Table 3.2.3.1 (continued)

RECTANGULAR SYSTEM					
<i>m</i>					
2	<i>b</i>	1	$x, y \quad \bar{x}, y$	Pair of edges Line segment	$(hk) \quad (\bar{h}k)$
				Pair of parallel edges Line segment through origin	$(10) \quad (\bar{1}0)$
1	<i>a</i>	<i>.m.</i>	$0, y$	Single edge Single point	$(01) \text{ or } (0\bar{1})$
<i>2mm</i>					
4	<i>c</i>	1	$x, y \quad \bar{x}, \bar{y} \quad \bar{x}, y \quad x, \bar{y}$	Rhomb Rectangle	$(hk) \quad (\bar{h}\bar{k}) \quad (\bar{h}k) \quad (h\bar{k})$
2	<i>b</i>	<i>.m.</i>	$0, y \quad 0, \bar{y}$	Pair of parallel edges Line segment through origin	$(01) \quad (0\bar{1})$
2	<i>a</i>	<i>.m.</i>	$x, 0 \quad \bar{x}, 0$	Pair of parallel edges Line segment through origin	$(10) \quad (\bar{1}0)$
1	<i>o</i>	<i>2mm</i>	$0, 0$	Point in origin	
SQUARE SYSTEM					
4					
4	<i>a</i>	1	$x, y \quad \bar{x}, \bar{y} \quad \bar{y}, x \quad y, \bar{x}$	Square Square	$(hk) \quad (\bar{h}\bar{k}) \quad (\bar{k}h) \quad (k\bar{h})$
1	<i>o</i>	<i>4..</i>	$0, 0$	Point in origin	
<i>4mm</i>					
8	<i>c</i>	1	$x, y \quad \bar{x}, \bar{y} \quad \bar{y}, x \quad y, \bar{x}$ $\bar{x}, y \quad x, \bar{y} \quad y, x \quad \bar{y}, \bar{x}$	Ditetragon Truncated square	$(hk) \quad (\bar{h}\bar{k}) \quad (\bar{k}h) \quad (k\bar{h})$ $(\bar{h}k) \quad (h\bar{k}) \quad (kh) \quad (k\bar{h})$
4	<i>b</i>	<i>.m.</i>	$x, x \quad \bar{x}, \bar{x} \quad \bar{x}, x \quad x, \bar{x}$	Square Square	$(11) \quad (\bar{1}\bar{1}) \quad (\bar{1}1) \quad (1\bar{1})$
4	<i>a</i>	<i>.m.</i>	$x, 0 \quad \bar{x}, 0 \quad 0, x \quad 0, \bar{x}$	Square Square	$(10) \quad (\bar{1}0) \quad (01) \quad (0\bar{1})$
1	<i>o</i>	<i>4mm</i>	$0, 0$	Point in origin	

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Table 3.2.3.1 (continued)

HEXAGONAL SYSTEM					
3					
3	<i>a</i>	1	$x, y \quad \bar{y}, x - y \quad \bar{x} + y, \bar{x}$	Trigon Trigon	(<i>hki</i>) (<i>ihk</i>) (<i>kih</i>)
1	<i>o</i>	3..	0, 0	Point in origin	
3m1					
6	<i>b</i>	1	$x, y \quad \bar{y}, x - y \quad \bar{x} + y, \bar{x}$ $\bar{y}, \bar{x} \quad \bar{x} + y, y \quad x, x - y$	Ditrigon Truncated trigon	(<i>hki</i>) (<i>ihk</i>) (<i>kih</i>) (<i>khī</i>) (<i>īkh</i>) (<i>hīk</i>)
				Hexagon Hexagon	(<i>112̄</i>) (<i>2̄11</i>) (<i>12̄1</i>) (<i>112</i>) (<i>211</i>) (<i>121</i>)
3	<i>a</i>	. <i>m</i> .	$x, \bar{x} \quad x, 2x \quad 2\bar{x}, \bar{x}$	Trigon Trigon	(<i>101̄</i>) (<i>1̄10</i>) (<i>011</i>) or (<i>101</i>) (<i>110</i>) (<i>011</i>)
1	<i>o</i>	3 <i>m</i> .	0, 0	Point in origin	
31m					
6	<i>b</i>	1	$x, y \quad \bar{y}, x - y \quad \bar{x} + y, \bar{x}$ $y, x \quad x - y, \bar{y} \quad \bar{x}, \bar{x} + y$	Ditrigon Truncated trigon	(<i>hki</i>) (<i>ihk</i>) (<i>kih</i>) (<i>khī</i>) (<i>īkh</i>) (<i>hīk</i>)
				Hexagon Hexagon	(<i>101̄</i>) (<i>1̄10</i>) (<i>011</i>) (<i>011̄</i>) (<i>1̄01</i>) (<i>110</i>)
3	<i>a</i>	.. <i>m</i>	$x, 0 \quad 0, x \quad \bar{x}, \bar{x}$	Trigon Trigon	(<i>112̄</i>) (<i>2̄11</i>) (<i>12̄1</i>) or (<i>112</i>) (<i>211</i>) (<i>121</i>)
1	<i>o</i>	3. <i>m</i>	0, 0	Point in origin	
6					
6	<i>a</i>	1	$x, y \quad \bar{y}, x - y \quad \bar{x} + y, \bar{x}$ $\bar{x}, \bar{y} \quad y, \bar{x} + y \quad x - y, x$	Hexagon Hexagon	(<i>hki</i>) (<i>ihk</i>) (<i>kih</i>) (<i>hki</i>) (<i>ihk</i>) (<i>kih</i>)
1	<i>o</i>	6..	0, 0	Point in origin	
6mm					
12	<i>c</i>	1	$x, y \quad \bar{y}, x - y \quad \bar{x} + y, \bar{x}$ $\bar{x}, \bar{y} \quad y, \bar{x} + y \quad x - y, x$ $\bar{y}, \bar{x} \quad \bar{x} + y, y \quad x, x - y$ $y, x \quad x - y, \bar{y} \quad \bar{x}, \bar{x} + y$	Dihexagon Truncated hexagon	(<i>hki</i>) (<i>ihk</i>) (<i>kih</i>) (<i>hki</i>) (<i>ihk</i>) (<i>kih</i>) (<i>khī</i>) (<i>īkh</i>) (<i>hīk</i>) (<i>khī</i>) (<i>īkh</i>) (<i>hīk</i>)
6	<i>b</i>	. <i>m</i> .	$x, \bar{x} \quad x, 2x \quad 2\bar{x}, \bar{x}$ $\bar{x}, x \quad \bar{x}, 2\bar{x} \quad 2x, x$	Hexagon Hexagon	(<i>101̄</i>) (<i>1̄10</i>) (<i>011</i>) (<i>101</i>) (<i>110</i>) (<i>011</i>)
6	<i>a</i>	.. <i>m</i>	$x, 0 \quad 0, x \quad \bar{x}, \bar{x}$ $\bar{x}, 0 \quad 0, \bar{x} \quad x, x$	Hexagon Hexagon	(<i>112̄</i>) (<i>2̄11</i>) (<i>12̄1</i>) (<i>112</i>) (<i>211</i>) (<i>121</i>)
1	<i>o</i>	6 <i>mm</i>	0, 0	Point in origin	