

Tables of the Characteristics of the Vector Representations of the 230 Space Groups

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All space groups can be distinguished in their vector representations, except that one cannot distinguish between the members of the eleven enantiomorphous pairs. This means that the space groups of all crystals can be distinguished in their Patterson syntheses, except that one cannot distinguish between the members of the eleven enantiomorphous pairs. All but eight of the distinguishable space groups can be recognized in Patterson synthesis merely by their symmetry plus the locations of heavy concentrations. Five of these eight can be distinguished by simple qualitative features of the patterns in the concentration loci, while the other three can be distinguished if the data for the Patterson synthesis is on an absolute basis. A table listing the symmetrical concentrations for the 230 space groups is given. These concentrations are also the only possible Harker sections.

At the 1946 meeting of the American Society for X-ray and Electron Diffraction at Lake George, New York, the writer pointed out (Buerger, 1946) that all space groups except a very limited number of pairs could be distinguished by their Patterson syntheses. The matter was touched upon again in discussing vector sets (Buerger, 1950*a*), and in some greater detail under the title *The Crystallographic Symmetries Determinable by X-ray Diffraction* (Buerger, 1950*b*). In preparing this last paper, the writer had available a manuscript table composed for inclusion in the *International Tables for X-ray Crystallography* listing the specific characteristics of the vector representations of the 230 space groups. In order to correct errors in these tables, and also because of the recent development of interest in symmetry determination by X-ray means (Wilson, 1949; Rogers, 1949), it appears desirable to publish these tables in advance of their appearance in the *International Tables*. The writer would be grateful to receive at the earliest possible date notice of errors which are discovered in them.

In the earlier contributions (Buerger, 1950*a, b*), it was pointed out that symmetry other than pure inversion symmetry leaves a record in vector sets in the form of characteristic concentrations of points. Reflection symmetries correspond to linear concentrations in the vector set, while rotational symmetries appear as planar concentrations. The translational component of the symmetry element can be identified from the specific locations of the concentrations. In the accompanying Table 1 the last two columns list the specific sets of concentrations for each of the 230 space groups.

It often occurs that a linear concentration is embedded in one or more planar concentrations. The relations between such coincidences are indicated by a subscript in the accompanying table. Thus, if the co-ordinates of

a linear concentration are followed by a subscript, the same subscript is appended to a planar concentration in which the linear concentration is embedded. A linear concentration can be embedded in no more than two symmetrically non-equivalent planar concentrations.

The table lists only linear and planar concentrations which are not symmetrically equivalent. In general, the co-ordinates of concentrations are given for a set of concentrations in the immediate vicinity of the origin lattice point.

Nineteen pairs of space groups are bracketed in the table. The individuals of these pairs cannot be separately distinguished by the symmetry of the vector set plus the mere co-ordinates of the concentrations. All but the eleven enantiomorphic pairs, however, can be distinguished by taking into account not only the co-ordinates, but also some simple qualitative aspects (for five pairs of space groups) or simple quantitative aspects (for three more pairs of space groups) of the *patterns* in the concentrations. The specific methods of distinguishing between pairs in these cases are discussed elsewhere (Buerger, 1950*b*).

Every concentration listed in the table is a Harker section (Harker, 1936). Where the table shows that a linear concentration is embedded in a planar concentration, the axial Harker synthesis has reflection satellites (Buerger, 1946). The table is thus a complete guide to the possible Harker syntheses of the space groups.

References

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 HARKER, D. (1936). *J. Chem. Phys.* **6**, 381.
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Table 1 (cont.)

Space group		Space group vector set	Linear concentrations in vector set	Planar concentrations in vector set	
Short symbol	Full symbol				
Orthorhombic (cont.)	C ₂ 2 ₂ C ₂ 2 ₂	C ₂ mm	—	yz x0z xy0	
			—	—	
	C ₂ mm2 C ₂ m2 ₁ C ₂ cc2	(A ₂ mm2) tr. → C ₂ 2mm (A ₂ bm2) tr. → C ₂ m { b a} (A ₂ ma2) tr. → C ₂ cm (A ₂ ba2) tr. → C ₂ c { b a}	C ₂ mm	xy0 ₂ xy0 ₁ xy0 _{1,2} xy0 ₁	xy0 _{1,2} xy0 ₁ xy0 _{1,2} xy0 ₁
				—	—
				—	—
				—	—
				—	—
	C ₂ mm C ₂ cm C ₂ ca	C ₂ /m2/c2 ₁ /m C ₂ /m2/c2 ₁ /a C ₂ /m2/m2/m C ₂ /c2/c2/m C ₂ /m2/m2/a C ₂ /c2/c2/a	C ₂ mm	xy0 _{1,2,3} xy0 _{2,3} xy0 _{3,5} xy0 _{2,3,4} xy0 _{2,3} xy0 _{2,3,5} xy0 _{2,3,5}	x0z _{1,5} x0z _{1,5} x0z _{1,6} x0z _{1,6} x0z _{1,4} x0z _{1,4} x0z _{1,3}
				—	—
				—	—
				—	—
				—	—
	Tetragonal	I ₂ 22 I ₂ 1 ₁ 2 ₁	I ₂ mm	—	yz x0z xy0
				—	—
		I ₂ mm2 I ₂ ba2 I ₂ ma2	I ₂ mm	xy0 ₂ xy0 ₂ xy0 ₂	xy0 _{1,2} xy0 _{1,2} xy0 _{1,2}
—				—	
—				—	
I ₂ mm I ₂ bm I ₂ ba I ₂ ma		I ₂ /m2/m2/m I ₂ /b2/a2/m I ₂ /b2/c2 ₁ /a I ₂ /m2 ₁ /m2 ₁ /a	I ₂ mm	xy0 _{3,4} xy0 _{3,4} xy0 _{3,4} xy0 _{3,4}	xy0 _{2,4} xy0 _{2,4} xy0 _{2,4} xy0 _{2,4}
				—	—
				—	—
F ₂ 22 F ₂ mm2 F ₂ dd2		F ₂ mm	—	yz x0z xy0	
			—	—	
F ₂ mm F ₂ dd	F ₂ /m2/m2/m F ₂ /d2/d2/d	F ₂ mm	xy0 _{1,2} xy0 _{1,2}	x0z _{1,5} x0z _{1,5}	
			—	—	
P ₄	P ₄ P ₄ P ₄ P ₄	P ₄ /m	—	yz x0z xy0	
			—	—	
			—	—	
			—	—	
			—	—	
P ₄ /m P ₄ /m P ₄ /m P ₄ /m	P ₄ /m P ₄ /m P ₄ /m P ₄ /m	P ₄ /m	xy0 _{3,4} xy0 _{3,4} xy0 _{3,4} xy0 _{3,4}	xy0 _{1,2} xy0 _{1,2} xy0 _{1,2} xy0 _{1,2}	
			—	—	
			—	—	

Table 1 (cont.)

Space group		Space group, vector set	Linear concentrations in vector set	Planar concentrations in vector set	
Short symbol	Full symbol				
$I\bar{4}$		$I4/m$	—	—	
$I4$		—	—	$xy0$	
$I4_1$		—	—	$xy\frac{1}{2}$	
$I4/m$		—	$00z$	$xy0$	
$I4_1/a$		—	$\frac{1}{2}0z$	$xy\frac{1}{2}$	
$P4_22$		$P4/mmm$	—	—	
$P4_212$			—	—	—
$P4_122$			—	—	—
$P4_222$			—	—	—
$P4_1212$			—	—	—
$P4_2212$			—	—	—
$P4_222$			—	—	—
$P4_2212$			—	—	—
$P4/mmm$			$xx0_1$	$xx0_2$	xxz
$P4bm$			$xx0_1$	$xx0_2$	xxz
$P4_2cm$			$xx\frac{1}{2}1$	$xx0_2$	xxz
$P4_2mm$			$xx\frac{1}{2}1$	$xx0_2$	xxz
$P4cc$			$xx\frac{1}{2}$	$xx\frac{1}{2}$	xxz
$P4nc$		$xx\frac{1}{2}$	$xx\frac{1}{2}$	xxz	
$P4_2mc$		$xx\frac{1}{2}$	$xx\frac{1}{2}$	xxz	
$P4_2bc$		$xx\frac{1}{2}$	$xx\frac{1}{2}$	xxz	
$P4_2m$		—	—	—	
$P4_2c$		—	—	—	
$P4_2/m$		—	—	—	
$P4_2-c$		—	—	—	
$P4_1m2$		—	—	—	
$P4_22$		—	—	—	
$P4_12$		—	—	—	
$P4_1m2$		—	—	—	
$P4_1m2/m2/m$		—	—	—	
$P4_1m2/c2/c$		—	—	—	
$P4_1m2/c2/c$		—	—	—	
$P4_2/m2/m2/m$		—	—	—	
$P4_2/m2/c2/c$		—	—	—	
$P4_2/m2/c2/m$		—	—	—	
$P4_2/m2/b2/c$		—	—	—	
$P4_2/m2/b2/c$		—	—	—	
$P4_2/m2_1/b2/c$		—	—	—	
$P4_2/m2_1/b2/c$		—	—	—	
$P4_2/m2_1/m2/c$		—	—	—	
$P4_2/m2_1/m2/c$		—	—	—	
$P4_2/m2_1/c2/c$		—	—	—	
$P4_2/m2_1/m2/c$		—	—	—	
$P4_2/m2_1/c2/m$		—	—	—	
$P4_2/m2_1/b2/c$		—	—	—	
$P4_2/m2_1/b2/c$		—	—	—	
$P4_2/m2_1/m2/c$		—	—	—	
$P4_2/m2_1/m2/c$		—	—	—	
$P4_2/m2_1/c2/m$		—	—	—	
$P4_2/m2_1/c2/m$		—	—	—	
$P4_1mcc$		—	—	—	
$P4_1nbn$		—	—	—	
$P4_1nbc$		—	—	—	
$P4_1mbn$		—	—	—	
$P4_1mnc$		—	—	—	
$P4_1mmn$		—	—	—	
$P4_1ncc$		—	—	—	
$P4_2/mnc$		—	—	—	
$P4_2/mcm$		—	—	—	
$P4_2/nbc$		—	—	—	
$P4_2/mnm$		—	—	—	
$P4_2/mbc$		—	—	—	
$P4_2/mnm$		—	—	—	
$P4_2/mnc$		—	—	—	
$P4_2/ncm$		—	—	—	

Tetragonal (cont.)

Table I (cont.)

Space group		Space group, vector set	Linear concentrations in vector set	Planar concentrations in vector set		
Short symbol	Full symbol					
Tetragonal (cont.)		$I4/mmm$	—	xxz	$xy0$	
			—	xxz	$xy0$	
			$x00_1$	—	—	$xy0_{1,2}$
			$x0\frac{1}{2}_1$	$xx0_2$	—	$xy0_{1,2}$
			$x00_1$	$x(x+\frac{1}{2})\frac{1}{2}_2$	—	$xy\frac{1}{2}_2$
			$x0\frac{1}{2}_1$	$x(x+\frac{1}{2})\frac{1}{2}_2$	—	$xy\frac{1}{2}_2$
		$I4/m2/m2/m$ $I4/m2/c2/m$ $I4_1/amd$ $I4_1/acd$	—	—	—	—
			—	—	—	—
			$x00_1$	—	—	—
			$x0\frac{1}{2}_1$	$xx0_1$	—	—
			—	$x(x+\frac{1}{2})\frac{1}{2}$	—	—
			—	—	—	—
Hexagonal		$P\bar{3}$	$x00_{1,2}$	$xxz_{3,6}$	$xy0_{2,4}$	
			$x0\frac{1}{2}_{1,2}$	$xxz_{3,6}$	$xy0_{2,4}$	
			$x00_{1,2}$	xxz	$xy0_2$	
			$x0\frac{1}{2}_{1,2}$	xxz	$xy0_2$	
			—	—	—	
			—	—	—	
		$P\bar{3}1m$	—	—	—	—
			—	—	—	—
			—	$xx0_1$	—	—
			—	$xx\frac{1}{2}$	$xy0_1$	—
			—	$xx0_1$	$xy0_1$	—
			—	$xx\frac{1}{2}$	$xy0_1$	—
$P\bar{3}1m$	—	—	—	—		
	—	—	—	—		
	$x2x0_1$	—	—	—		
	$x2x\frac{1}{2}$	—	—	—		
	$x2x0_1$	—	—	—		
	$x2x\frac{1}{2}$	—	—	—		
$R\bar{3}m$	—	—	—	—		
	—	—	—	—		
	—	$xx0_1$	—	—		
	—	$xx\frac{1}{2}$	$xy0_1$	—		
	—	$xx0_1$	$xy0_1$	—		
	—	$xx\frac{1}{2}$	$xy0_1$	—		

Table 1 (cont.)

Space group		Space group, vector set	Linear concentrations in vector set	Planar concentrations in vector set	•				
Short symbol	Full symbol								
Hexagonal (cont.)									
P6		P6/m	—	—	—				
P6 ₁									
P6 ₂									
P6 ₃									
P6 ₄									
P6 ₅									
P6 = P3/m			00z	xy0	xy $\frac{1}{2}$				
P6/m		P6/mmm	—	—	—				
P6 ₃ /m									
P622									
P6 ₃ 22									
P6 ₂ 22									
P6 ₃ 22									
P6mm		P6/mmm	—	—	—				
P6cc									
P6 ₃ cm									
P6 ₃ mc									
P6m2 = P3/m2									
P6c2 = P3/mc2									
P62m = P3/m2m		Pm3	—	—	—				
P62c = P3/m2c									
P6/mmm	P6/m2/m2/m								
P6/mcc	P6/m2/c2/c								
P6 ₃ /mcm	P6 ₃ /m2/c2/m								
P6 ₃ /mmc	P6 ₃ /m2/m2/c								
P23		Pm3	—	—	—				
P2 ₁ 3									
Pm3	P2/m3								
Pn3	P2/m3								
Pa3	P2 ₁ /a3								
I23						Im3	—	—	—
I2 ₁ 3									
Im3	I2/m3								
Ic3	I2 ₁ /a3								
F23		Fm3	—	—	—				
F2/m3									
Fm3	F2/d3								
Fd3	F2/d3								
Isometric						Fm3	—	—	—
I23									
Im3	I2/m3								
Ic3	I2 ₁ /a3								
F23									
Fm3	F2/m3								
Fd3	F2/d3								

Table 1 (cont.)

Space group		Space group, vector set	Linear concentrations in vector set	Planar concentrations in vector set
Short symbol	Full symbol			
<i>Pm</i> 3 <i>m</i>	<i>P</i> 432	<i>Pm</i> 3 <i>m</i>	—	<i>xxz</i>
	<i>P</i> 4 ₃ 32		—	<i>xxz</i>
	<i>P</i> 4 ₃ 32		—	<i>xxz</i>
	<i>P</i> 4 ₁ 32		—	<i>xy</i> 0
<i>P</i> 43 <i>m</i>	<i>P</i> 43 <i>m</i>	<i>P</i> 43 <i>m</i>	<i>xx</i> 0 ₁	<i>xy</i> 0 ₁
	<i>P</i> 43 <i>m</i>		<i>xx</i> ½	<i>xy</i> 0
	<i>P</i> 4 ₁ / <i>m</i> 32/ <i>m</i>		<i>xx</i> 0 _{3,4}	<i>xy</i> 0 _{3,4}
	<i>P</i> 4 ₂ / <i>m</i> 32/ <i>n</i>		<i>xx</i> ½ ₂	<i>xy</i> 0
<i>Pm</i> 3 <i>m</i>	<i>P</i> 4 ₂ / <i>m</i> 32/ <i>n</i>	<i>Pm</i> 3 <i>m</i>	<i>xx</i> 0 _{1,2}	<i>xy</i> 0 _{1,2}
	<i>P</i> 4 ₂ / <i>m</i> 32/ <i>n</i>		<i>xx</i> ½ ₁	<i>xy</i> 0 _{3,4}
	<i>P</i> 4 ₂ / <i>m</i> 32/ <i>m</i>		<i>xx</i> 0 _{1,2}	<i>xy</i> 0 _{3,4}
<i>Pm</i> 3 <i>m</i>	<i>P</i> 4 ₂ / <i>m</i> 32/ <i>m</i>	<i>Pm</i> 3 <i>m</i>	<i>xx</i> ½ _{1,2}	<i>xy</i> 0 _{3,4}
	<i>P</i> 4 ₂ / <i>m</i> 32/ <i>m</i>		<i>xx</i> 0 _{3,4}	<i>xy</i> 0 _{3,4}
<i>Im</i> 3 <i>m</i>	<i>I</i> 432	<i>Im</i> 3 <i>m</i>	—	<i>xxz</i>
	<i>I</i> 4 ₁ 32		—	<i>xxz</i>
	<i>I</i> 43 <i>m</i>		<i>xx</i> 0 ₁	<i>xy</i> 0 ₁
<i>Im</i> 3 <i>m</i>	<i>I</i> 43 <i>m</i>	<i>Im</i> 3 <i>m</i>	<i>xx</i> 0 ₁	<i>xy</i> 0 ₁
	<i>I</i> 43 <i>m</i>		<i>x(x+½)</i> ½	<i>xy</i> 0
<i>Im</i> 3 <i>m</i>	<i>I</i> 4/ <i>m</i> 32/ <i>m</i>	<i>Im</i> 3 <i>m</i>	<i>xx</i> 0 _{1,2}	<i>xy</i> 0 _{2,4}
	<i>I</i> 4 ₁ / <i>a</i> 32/ <i>d</i>		<i>x(x+½)</i> ½	<i>xy</i> 0 ₁
<i>Fm</i> 3 <i>m</i>	<i>F</i> 432	<i>Fm</i> 3 <i>m</i>	—	<i>xxz</i>
	<i>F</i> 4 ₁ 32		—	<i>xxz</i>
	<i>F</i> 43 <i>m</i>		<i>xx</i> 0 _{1,2}	<i>xy</i> 0
<i>Fd</i> 3 <i>m</i>	<i>F</i> 43 <i>m</i>	<i>Fd</i> 3 <i>m</i>	<i>xx</i> ½ _{1,2}	<i>xy</i> 0 ₂
	<i>F</i> 43 <i>m</i>		<i>xx</i> 0 _{3,4}	<i>xy</i> 0 ₂
	<i>F</i> 4 ₁ / <i>d</i> 32/ <i>m</i>		<i>xx</i> ½ ₂	<i>xy</i> 0 ₂
<i>Fd</i> 3 <i>m</i>	<i>F</i> 4 ₁ / <i>d</i> 32/ <i>m</i>	<i>Fd</i> 3 <i>m</i>	<i>xx</i> 0 _{1,2}	<i>xy</i> 0 _{2,4}
	<i>F</i> 4 ₁ / <i>d</i> 32/ <i>m</i>		<i>xx</i> 0 _{1,2}	<i>xy</i> 0 _{2,4}
	<i>F</i> 4 ₁ / <i>d</i> 32/ <i>c</i>		<i>xx</i> ½ _{1,2}	<i>xy</i> 0 _{2,4}

Isometric (cont.)

The symbols used in Table 1 are those which will be used in the new *International Tables*. The short symbols for certain space groups have been discarded to give a better picture of the symmetry of the group and, in general, the full symbols have been abbreviated only where they would constitute an unduly complicated list of axes with their normal planes. In such instances the shortened symbol omits certain axes.

For the monoclinic system, the symbols in parentheses apply to the orientation (now current) in which the *b* axis is chosen parallel to the twofold axis, or normal to the symmetry plane. The symbols not in parentheses apply to the orientation where the *c* axis is so chosen. When the lattice is centered on one face of the cell parallel to the axis, this has been chosen as the *A* face in Table 1, which brings the

convention into conformity with the established one used for the orthorhombic hemimorphic class.

It is customary to fix the direction of the symmetry axis of the orthorhombic hemimorphic class as the *c* axis, and then permit the lattice, if centered on only one face of the cell, to be either *C* centered or *A* centered. On the other hand, the orthorhombic holohedral class is always referred to a *C* centered cell. In vector space, the symmetries of all these point distributions are the same, and should all be referred to a cell with the same centering. This has been chosen as *C* centering. In order to provide *C* centering for orthorhombic hemimorphic class, the standard *A*-centered orientation has been transformed as indicated by such symbols as (*Amm*2) tr. → *C2mm*, for example.