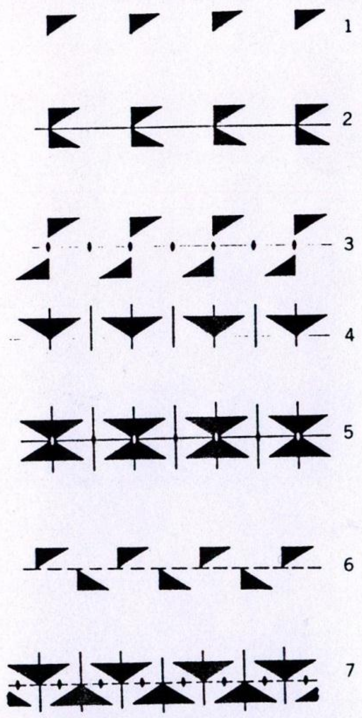


Figure 11.1 The seven classes of one-dimensional symmetry. [Adapted from I. Hargittai and G. Lengyel, *J. Chem. Educ.*, 1984, *61*, 1033.]

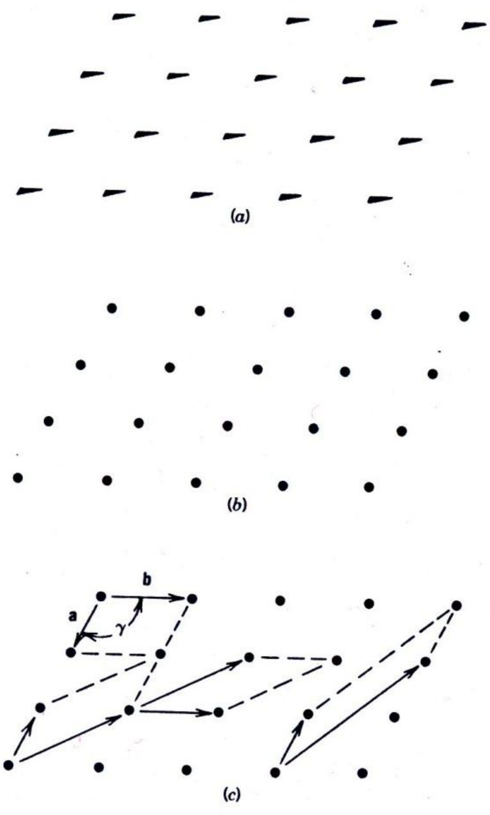


Figure 11.2. (*a*) A regular two-dimensional array of objects. (*b*) The lattice corresponding to this array. (*c*) Any pair of noncolinear translation vectors can be used to generate the lattice from one point.

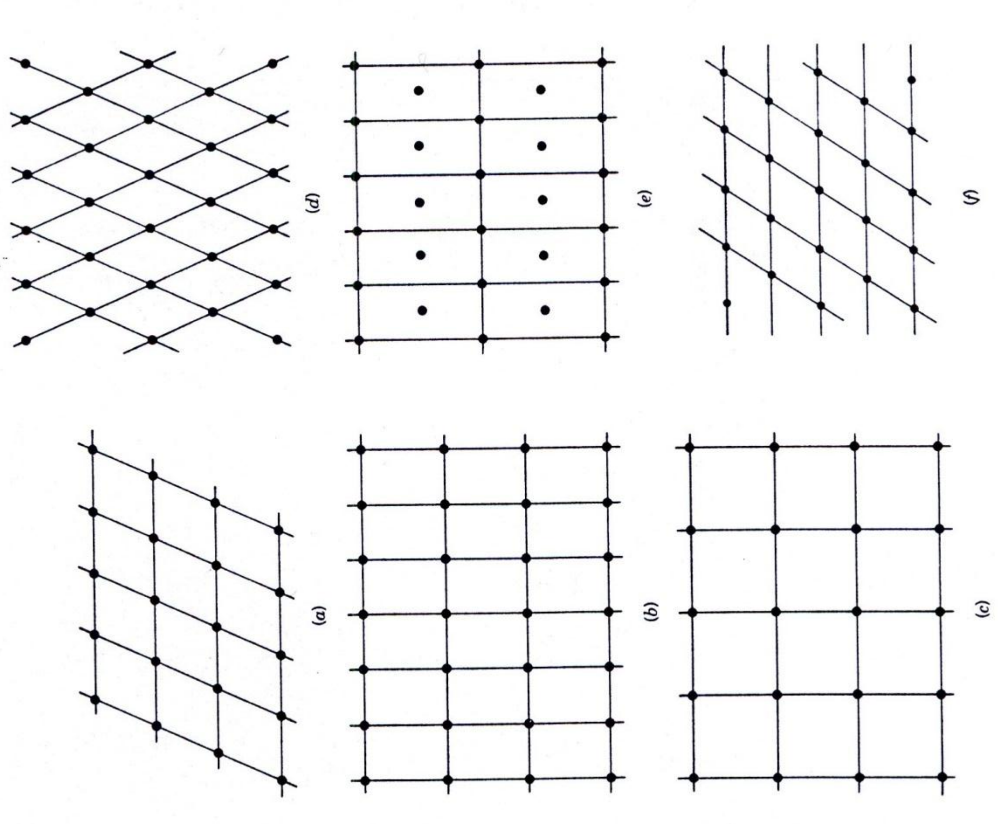


Figure 11.3. The five distinct plane (2D) lattices (*a*) oblique, (*b*) primitive rectangular, (*c*) square, (*d*) and (*e*) are both centered rectangular but show alternative choices of unit cell, (*f*) hexagonal.

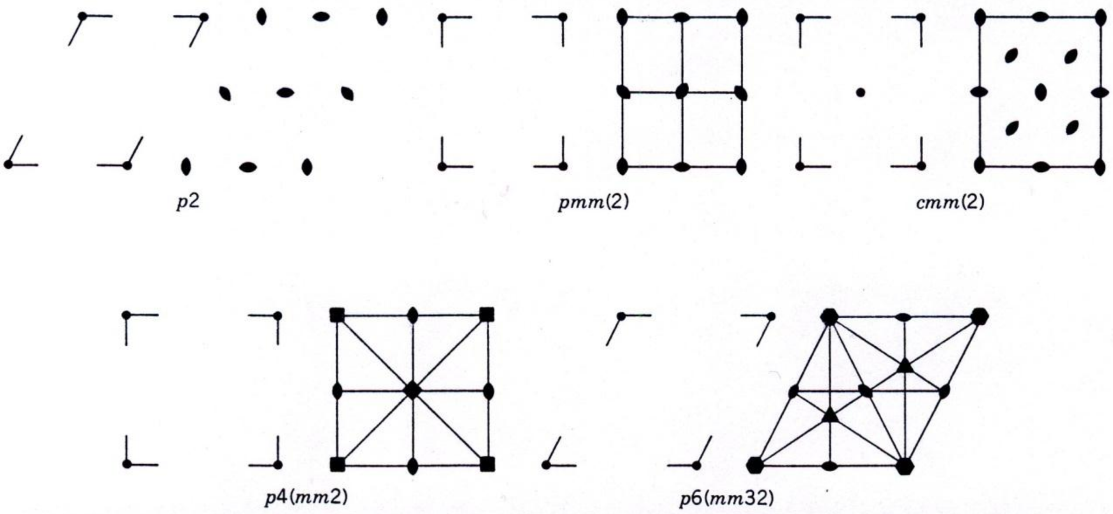


Figure 11.4. The symmetry elements of the five 2D lattices. For each pair the lattice is represented on the left by the points defining one unit cell and on the right are the symmetry elements. Different orientations of the symbols are used to differentiate nonequivalent axes of the same order. Symmetry symbols in parentheses are redundant, that is, indicate those that arise automatically from those preceding them.

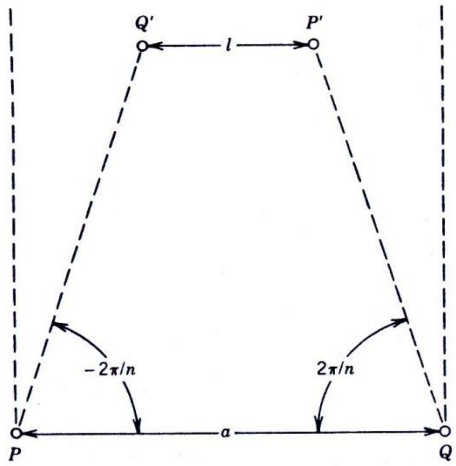


Figure 11.5. A geometrical construction used to show how rotation axes in a lattice are limited to those with orders 1, 2, 3, 4, and 6.

TABLE 11.1

Angle	Cosine	Order of Rotation Axis
60° = 2π/6	1/2	6
90° = 2π/4	0	4
120° = 2π/3	−1/2	3
180° = 2π/2	−1	2
0(≡360)° = 2π/1	1	1

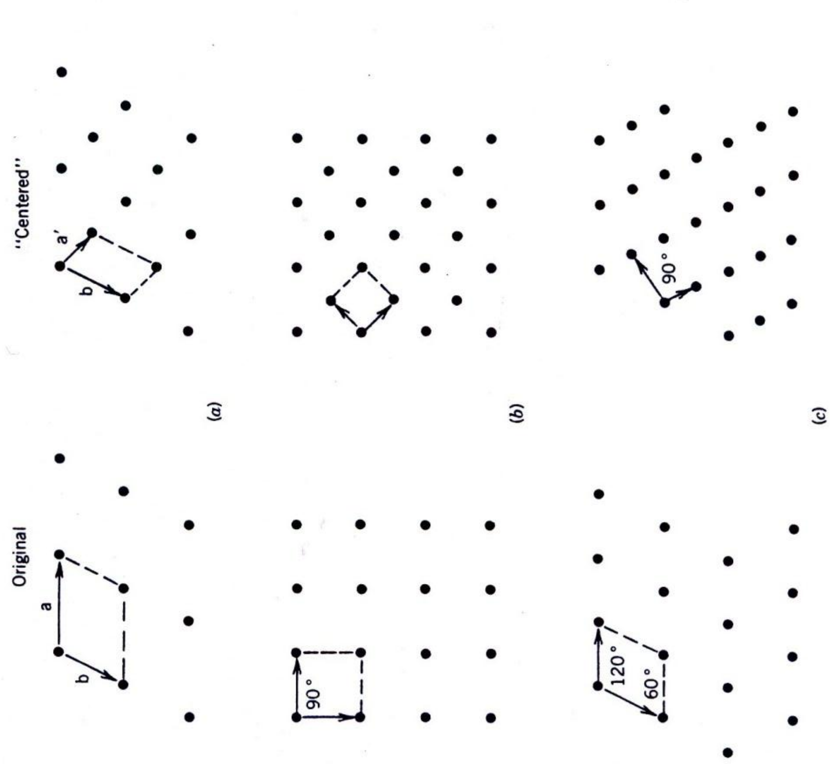


Figure 11.6. Drawings showing the consequences of attempting to produce centered lattices of oblique (*a*), square (*b*), and hexagonal (*c*) types.

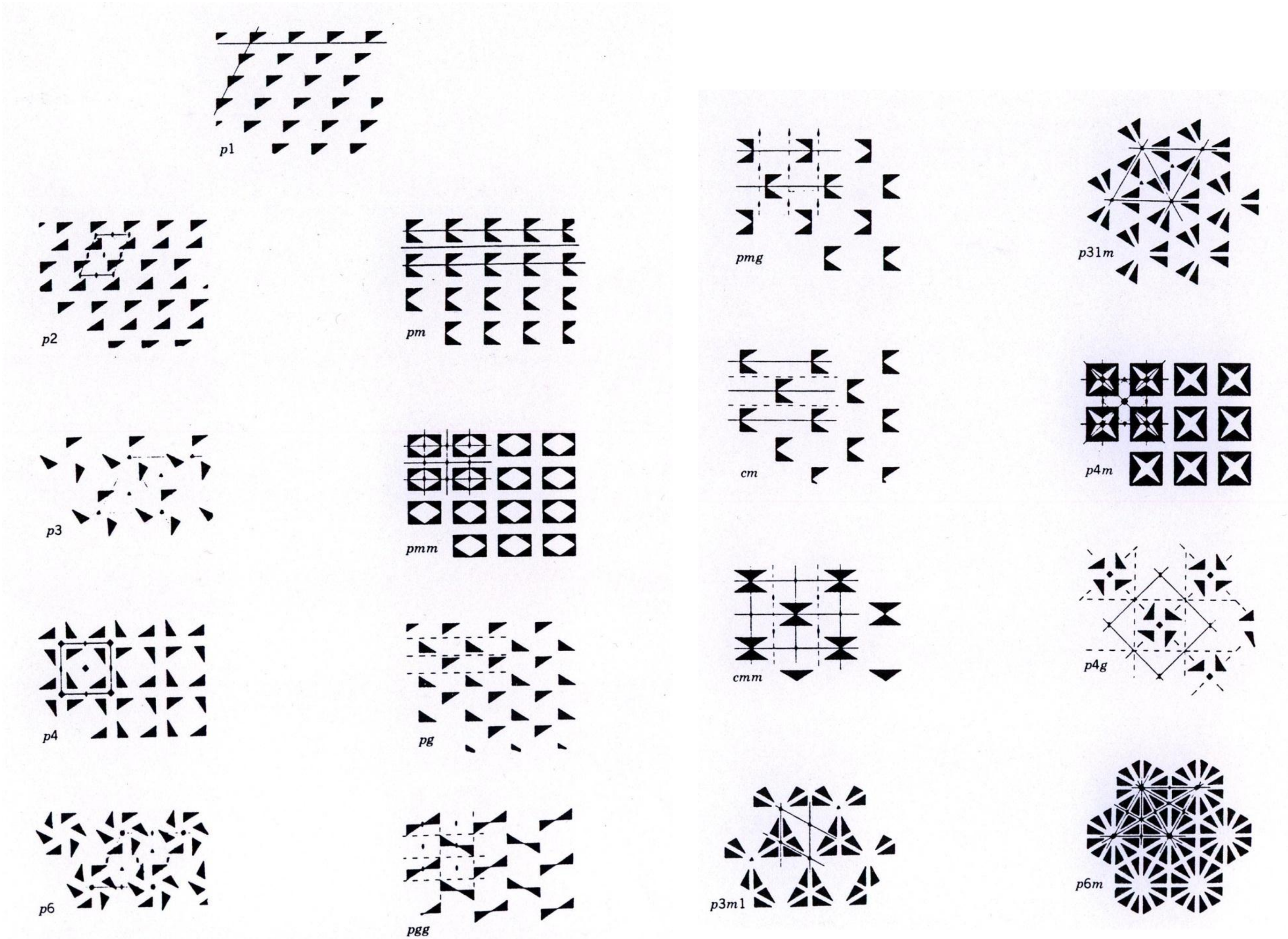


Figure 11.7 The 17 two-dimensional space groups; continuation on page 360.
[Adapted from I. Hargittai and G. Lengyel, *J. Chem. Educ.*, 1985, *62*, 35.]

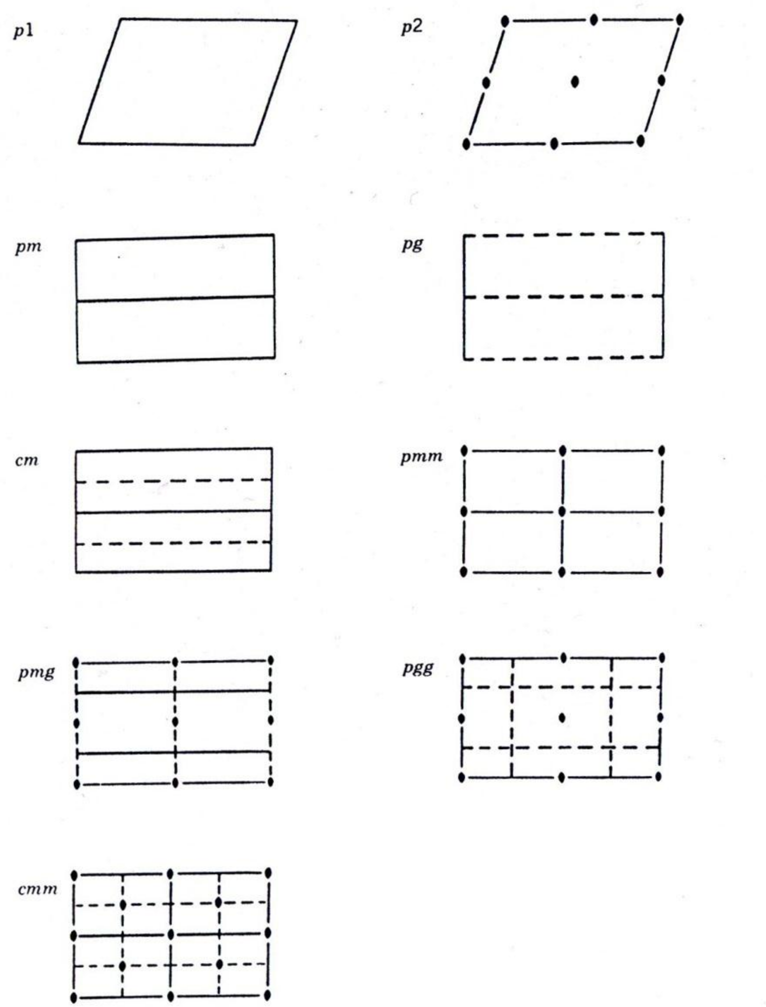


Figure 11.8. Diagrams showing all symmetry elements for the 17 two-dimensional symmetry classes; continuation on page 364. (Adapted from the International Tables for X-ray Crystallography, 1965.)

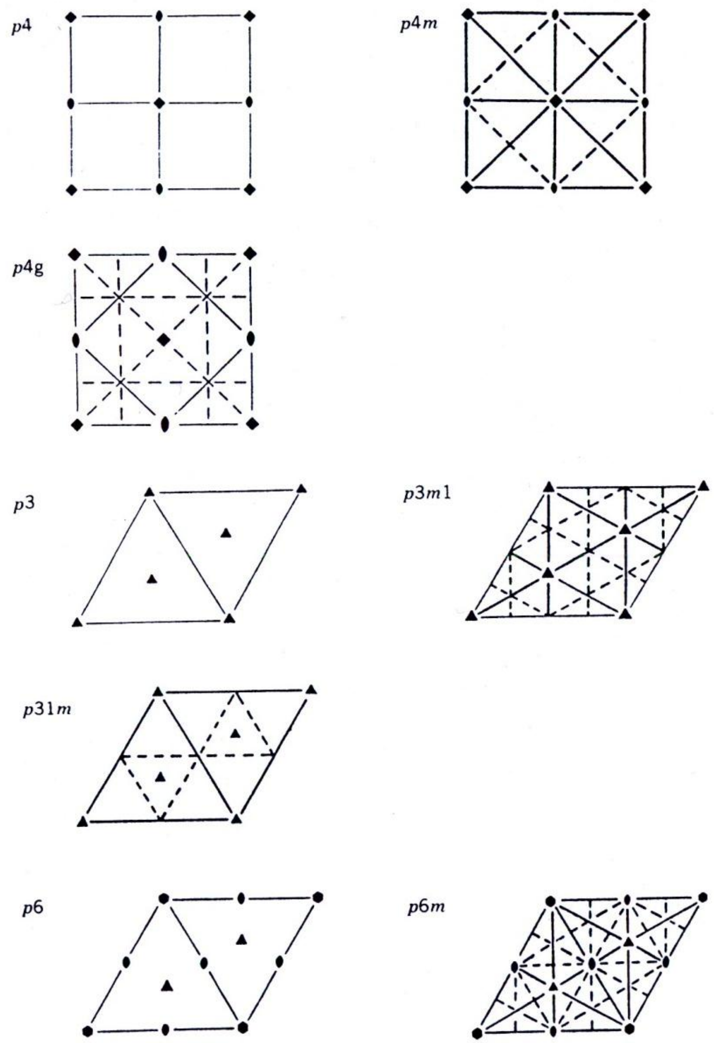


Figure 11.8. (*Continued*)

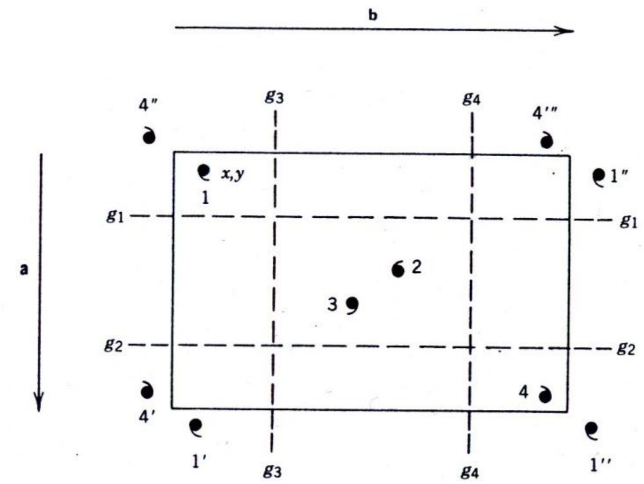


Figure 11.9. A diagram showing how an entire set of objects is generated from an initial one (No. 1) at a general position (x, y) by the combined action of glide lines and the lattice translations.

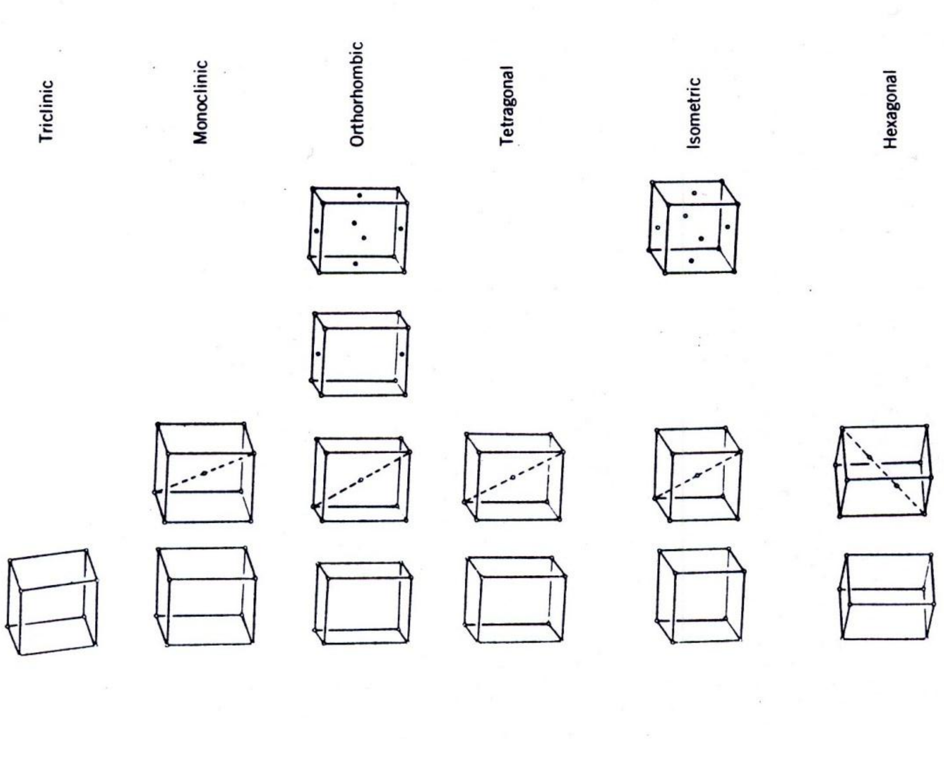


Figure 11.11. The 14 Bravais lattices arranged into the 6 crystal systems.

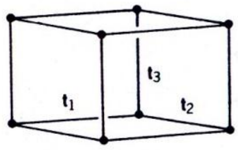


Figure 11.14. The formation of a primitive hexagonal lattice by stacking 2D lattices of $p6$ symmetry.

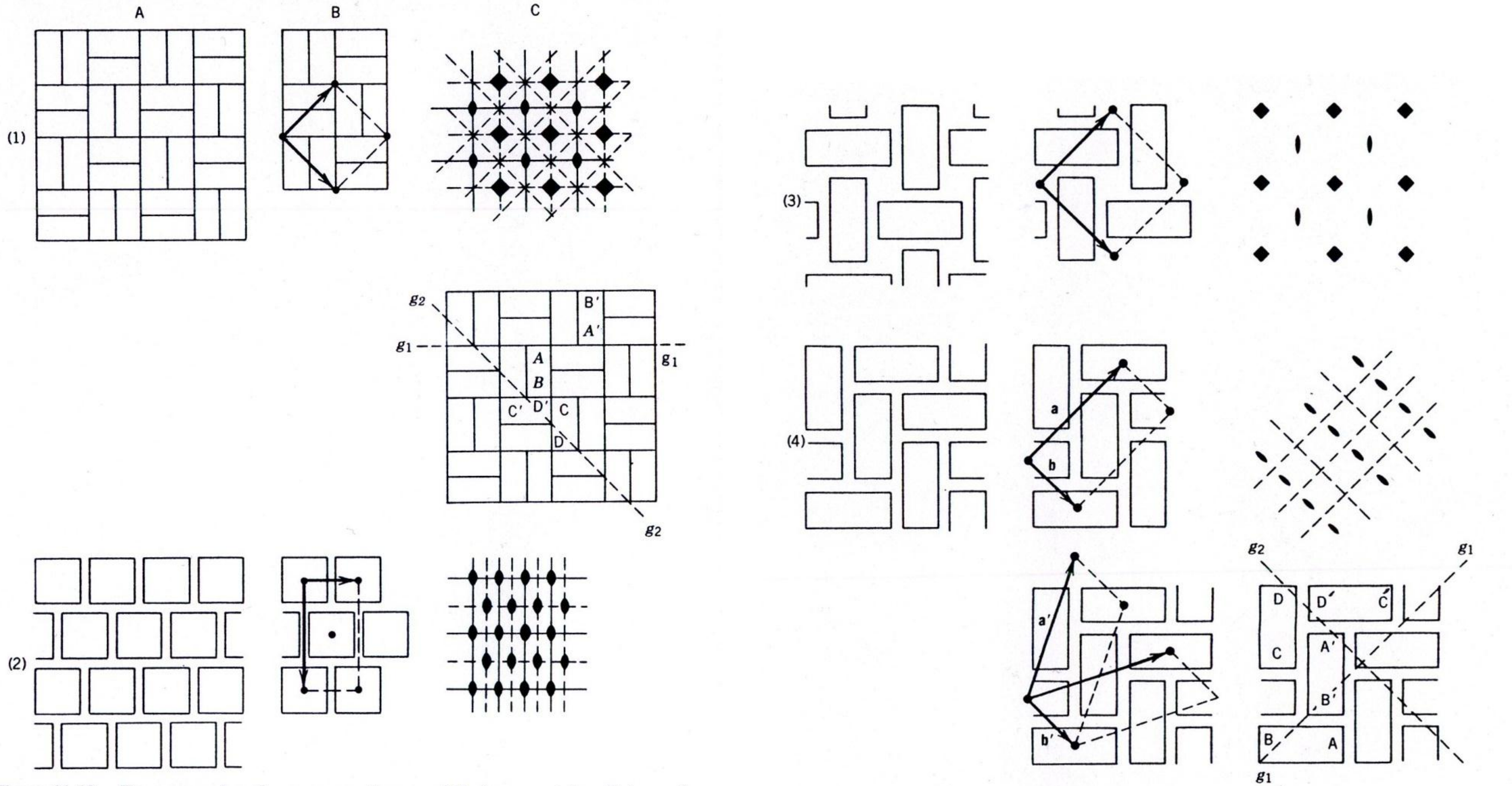


Figure 11.10. Four examples of masonry patterns and their symmetries. Column A shows the patterns; B shows the correct or incorrect choices of lattice vectors and unit cells; C shows the symmetry elements.

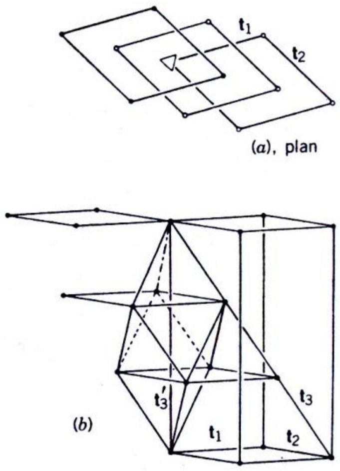


Figure 11.15. The formation of a primitive rhombohedral or triply primitive hexagonal lattice by stacking of 2D lattices of $p6$ symmetry.

TABLE 11.2 Properties of 3D Lattices

Crystal System	Lattice Symmetry		Axial Relations	Cell Types
	Schönflies	Crystallographic[a]		
Triclinic	C_i	$\bar{1}$	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	P
Monoclinic	C_{2h}	$2/m$	$a \neq b \neq c$ $\gamma \neq \alpha \equiv \beta = 90°$	P, I (or A or B)
Orthorhombic	D_{2h}	mmm	$a \neq b \neq c$ $\alpha \equiv \beta \equiv \gamma = 90°$	P, I, A, F
Tetragonal	D_{4h}	$4/mmm$	$a \equiv b \neq c$ $\alpha \equiv \beta \equiv \gamma = 90°$	P, I
Isometric (cubic)	O_h	$m3m$	$a \equiv b \equiv c$ $\alpha \equiv \beta \equiv \gamma = 90°$	P, I, F
Trigonal-hexagonal	D_{3d} D_{6h}	$\bar{3}m$ $6/mmm$	$a \equiv b \neq c$ $\alpha \equiv \beta = 90°$ $\gamma = 120°$	P or rhombohedral

[a]The use of these symbols is explained in Section 11.5.

TABLE 11.4 Symmetry Groups for the Six Crystal Systems

System	Essential Symmetry	Lattice Symmetry	Point Groups	Diffraction (Laue) Symmetry
Triclinic	None	$\bar{1}$	$1(C_1)$, $\bar{1}(C_i)$	$\bar{1}$
Monoclinic	2 or $m(\equiv \bar{2})$	$2/m$	$2(C_2)$, $m(C_s)$, $2/m(C_{2h})$	$2/m$
Orthorhombic	222 or $2mm$	mmm	$222(D_2)$, $2mm(C_{2v})$, $mmm(D_{2h})$	mmm
Tetragonal	4 or $\bar{4}$	$4/mmm$	$4(C_4)$, $\bar{4}(S_4)$, $4/m(C_{4h})$	$4/m$
			$422(D_4)$, $4mm(C_{4v})$, $\bar{4}2m(D_{2d})$, $4/mmm(D_{4h})$	$4/mmm$
Trigonal-hexagonal	3 or $\bar{3}$	$\bar{3}m$	$3(C_3)$, $\bar{3}(S_6)$	$\bar{3}$
			$32(D_3)$, $3m(C_{3v})$, $\bar{3}m(D_{3d})$	$\bar{3}m$
	6 or $\bar{6}$	$6/mmm$	$6(C_6)$, $\bar{6}(C_{3h})$, $6/m(C_{6h})$	$6/m$
			$622(D_6)$, $6mm(C_{6v})$, $\bar{6}m2(D_{3h})$, $6/mmm(D_{6h})$	$6/mmm$
Isometric	23	$m3m$	$23(T)$, $m3(T_h)$	$m3$
			$432(O)$, $\bar{4}3m(T_d)$, $m3m(O_h)$	$m3m$

TABLE 11.3 The 32 Crystallographic Point Groups

Number	Schönflies Symbol	Crystallographic Symbol	Crystal System
1	C_1	1	Triclinic
2	C_i	$\bar{1}$	
3	C_s	m	Monoclinic
4	C_2	2	
5	C_{2h}	$2/m$	
6	C_{2v}	mm	Orthorhombic
7	D_2	222	
8	D_{2h}	mmm	
9	C_4	4	Tetragonal
10	S_4	$\bar{4}$	
11	C_{4h}	$4/m$	
12	C_{4v}	$4mm$	
13	D_{2d}	$\bar{4}2m$	
14	D_4	422	
15	D_{4h}	$4/mmm$	
16	C_3	3	Trigonal—Hexagonal
17	S_6	$\bar{3}$	
18	C_{3v}	$3m$	
19	D_3	32	
20	D_{3d}	$\bar{3}m$	
21	C_{3h}	$\bar{6}$	
22	C_6	6	
23	C_{6h}	$6/m$	
24	D_{3h}	$\bar{6}m2$	
25	C_{6v}	$6mm$	
26	D_6	622	
27	D_{6h}	$6/mmm$	
28	T	23	Cubic
29	T_h	$m3$	
30	T_d	$\bar{4}3m$	
31	O	432	
32	O_h	$m3m$	

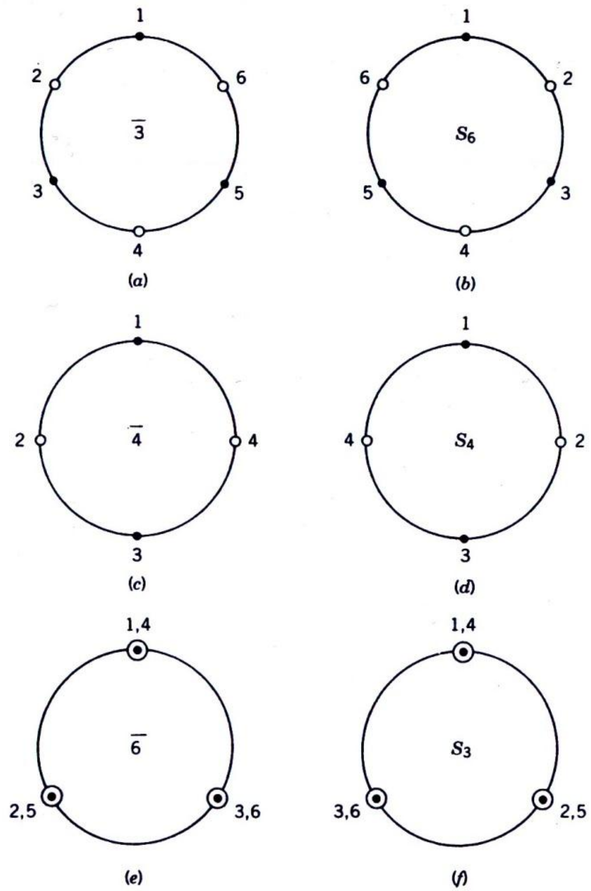


Figure 11.16. Diagrams comparing rotoinversion and rotoreflections operations.

TABLE 11.5 The Types of Glide Planes and Operations

Glide Type	Translation	Symbol
Axial	**a**/2	*a*
	b/2	*b*
	c/2	*c*
Diagonal	(**a** + **b**)/2	*n*
	(**a** + **c**)/2	
	(**b** + **c**)/2	
	(**a** + **b** + **c**)/2	
Diamond	(**a** ± **b**)/4	*d*
	(**a** ± **c**)/4	
	(**b** ± **c**)/4	
	(**a** ± **b** ± **c**)/4	

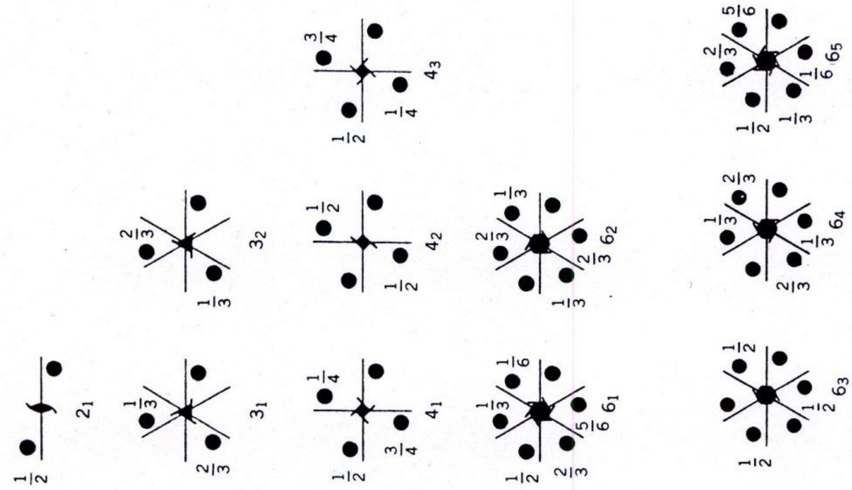


Figure 11.17. Diagrams showing the effects of screw rotations in projection down the screw axis. Fractions represent the fractional distances of each new point above the level of the initial point (which carries no fraction).

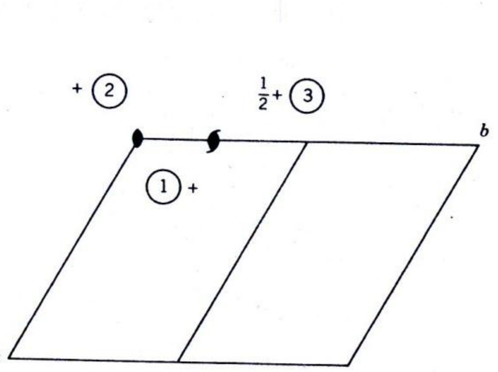


Figure 11.20. A diagram showing how the operations 2, 2_1, and *A* centering move an initial point 1 to other positions, 2 and 3 (see text).

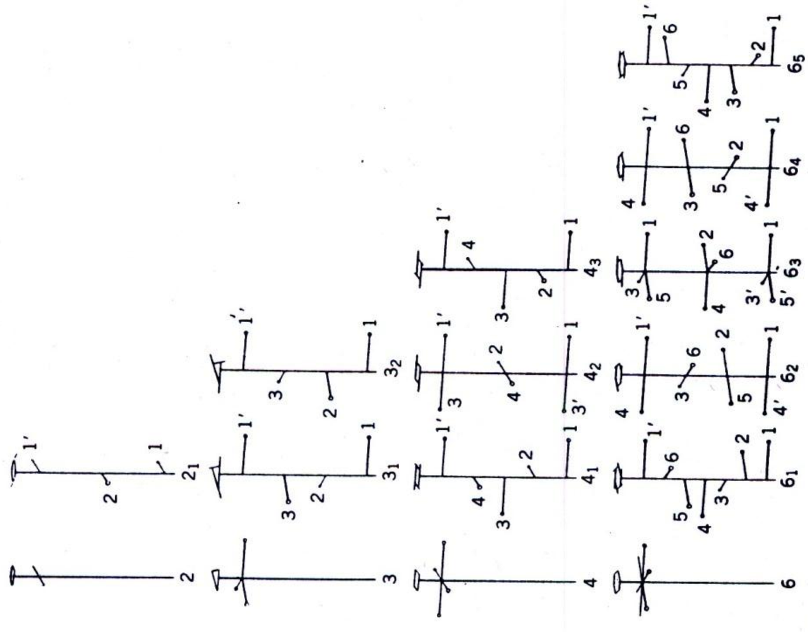


Figure 11.18. A second type of diagram showing the way screw operations replicate an initial point 1, until finally it reaches its original position but translated up by one vector distance (point 1′).

TABLE 11.6 Standard Symbols for Space Group Symmetry Elements

Element	Symbol	⊥ to Projection Plane	In or ∥ to Projection Plane
Simple mirror	m	———	⌐ or ⌐\
Axial glide	$a,b,c,$	- - - - - - - - - (glide in projection plane) · · · · · · · · · (glide ⊥ to projection plane)	←⌐ or ⌐↓ or ←⌐↓
Diagonal glide	n	- · - · - · - ·	⌐↙
Diamond glide	d	·—·⇆·—·	⌐↙ ⌐↘
Center of inversion	$\bar{1}$	○	
Rotation axis	2, 3, 4, 6	⬮ ▲ ◆ ⬢	⟶
Rotation–inversion axis	$\bar{3}, \bar{4}, \bar{6}$	△ ◈ ⬡	
Screw axis	2_1 $3_1, 3_2$ $4_1, 4_2, 4_3$ $6_1, 6_2, 6_3, 6_4, 6_5$	(screw axis symbols)	⟶

TABLE 11.7 The 13 Space Groups in the Monoclinic System

Lattice Type	Added Symmetry Elements	Space Group Symbol: Standard	Space Group Symbol: Alternate
P	2	*P*2	
	2_1	$P2_1$	
	m	*Pm*	
	a	*Pa*	*Pc*
	2 and *m*	*P*2/*m*	
	2_1 and *m*	$P2_1/m$	
	2 and *a*	*P*2/*a*	*P*2/*c*
	2_1 and *a*	$P2_1/a$	$P2_1/c$
A	2	*A*2	*C*2
	m	*Am*	*Cm*
	a	*Aa*	*Cc*
	2 and *m*	*A*2/*m*	*C*2/*m*
	2 and *a*	*A*2/*a*	*C*2/*c*

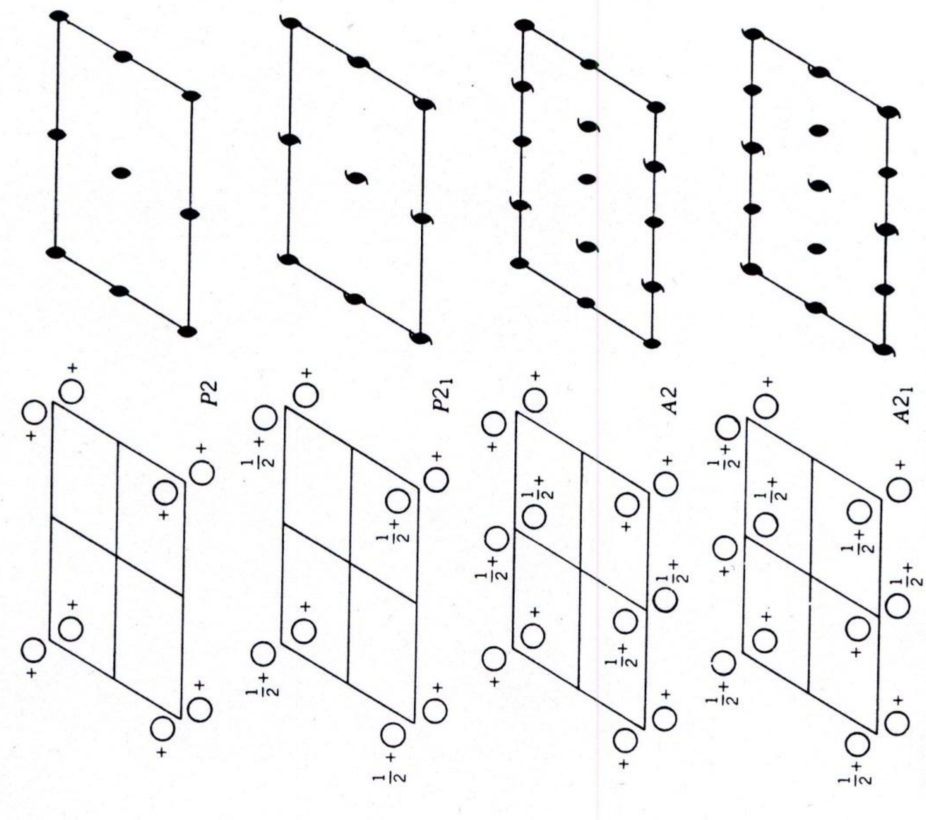
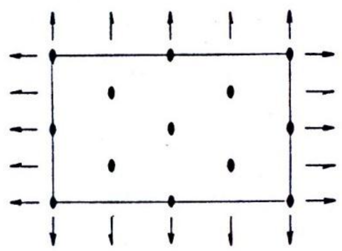
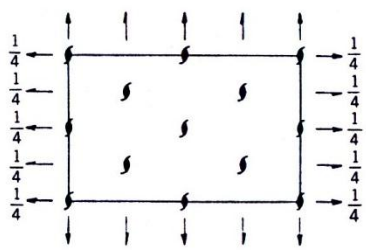


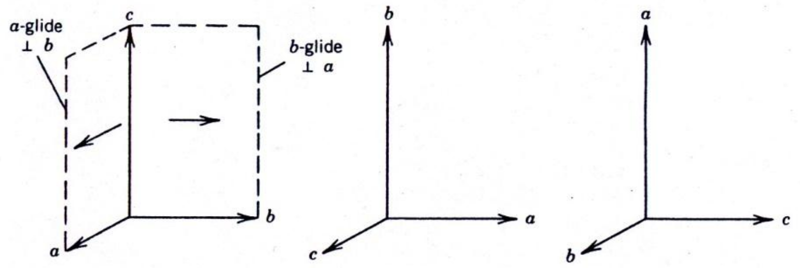
Figure 11.19. Diagrams showing symmetry elements and general point positions for space groups *P*2, $P2_1$, *A*2, and $A2_1$ (which is not different from *A*2 except for placement of the origin).



*C*222

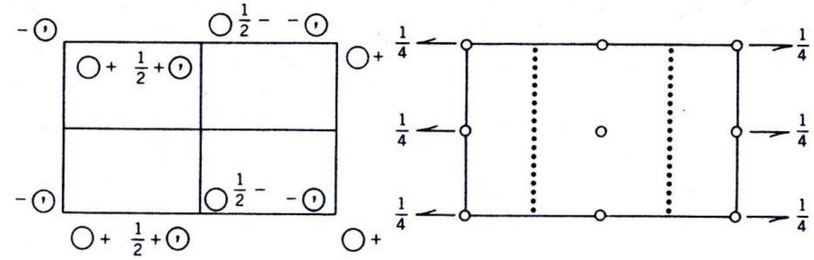


$C222_1$



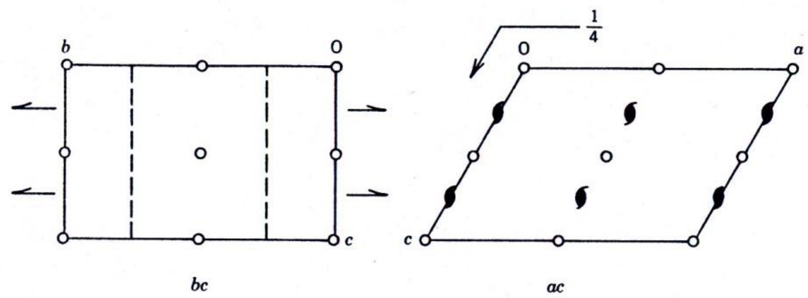
Pba2 *Pc2a* *P2cb*

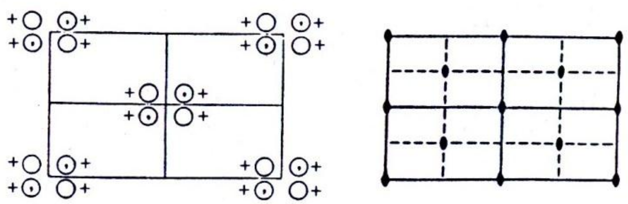
Figure 11.22. Diagrams showing how three different choices for labeling the axes lead to different symbols for the same space group. At left, where the positions of the glide planes are shown is the standard setting, that is, the conventional, tabulated, choice.



Number of positions, Wyckoff notation, and point symmetry			
4	*e*	1	x,y,z; $\bar{x},\bar{y},\bar{z}$; $\bar{x},\frac{1}{2}+y,\frac{1}{2}-z$; $x,\frac{1}{2}-y,\frac{1}{2}+z$.
2	*d*	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$; $\frac{1}{2},\frac{1}{2},0$.
2	*c*	$\bar{1}$	$0,0,\frac{1}{2}$; $0,\frac{1}{2},0$.
2	*b*	$\bar{1}$	$\frac{1}{2},0,0$; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.
2	*a*	$\bar{1}$	$0,0,0$; $0,\frac{1}{2},\frac{1}{2}$.

Figure 11.21. The diagrams and list of positions for space group $P2_1/c$, as given in the International Tables for X-ray Crystallography (1965). The diagrams are projections on the *ab* plane.





Number of positions, Wyckoff notation, and point symmetry

8	f	1	$x,y,z;\ \bar{x},\bar{y},z;\ \bar{x},y,z;\ x,\bar{y},z.$
4	e	m	$0,y,z;\ 0,\bar{y},z.$
4	d	m	$x,0,z;\ \bar{x},0,z.$
4	c	2	$\frac{1}{4},\frac{1}{4},z;\ \frac{1}{4},\frac{3}{4},z.$
2	b	mm	$0,\frac{1}{2},z.$
2	a	mm	$0,0,z.$

Figure 11.23. The standard diagrams and list of positions for the space group *Cmm*2.

TABLE 11.8 Conditions for Systematic Absences

Condition			Absent Reflections
1. *Lattice Centering*			
A-centered lattice (*A*)		hkl	$k + l = 2n + 1$
B-centered lattice (*B*)			$h + l = 2n + 1$
C-centered lattice (*C*)			$h + k = 2n + 1$
Face-centered lattice (*F*)			$h + k = 2n + 1$, $h + l = 2n + 1$, $k + l = 2n + 1$ } that is, h, k, l not all even or all odd
Body-centered lattice (*I*)			$h + k + l = 2n + 1$
2. *Glides Planes*			
perpendicular to	a		
translation $b/2$ (b glide)		$0kl$	$k = 2n + 1$
$c/2$ (c glide)			$l = 2n + 1$
$b/2 + c/2$ (n glide)			$k + l = 2n + 1$
$b/4 + c/4$ (d glide)			$k + l = 4n + 1, 2,$ or 3
perpendicular to	b		
translation $a/2$ (a glide)		$h0l$	$h = 2n + 1$
$c/2$ (c glide)			$l = 2n + 1$
$a/2 + c/2$ (n glide)			$h + l = 2n + 1$
$a/4 + c/4$ (d glide)			$h + l = 4n + 1, 2,$ or 3
perpendicular to	c		
translation $a/2$ (a glide)		$hk0$	$h = 2n + 1$
$b/2$ (b glide)			$k = 2n + 1$
$a/2 + b/2$ (n glide)			$h + k = 2n + 1$
$a/4 + b/4$ (d glide)			$h + k = 4n + 1, 2,$ or 3
3. *Screw Axes*			
Twofold screw (2_1) } along	a	$h00$	$h = 2n + 1 =$ odd
Fourfold screw (4_2) } along	b	$0k0$	$k = 2n + 1$
Sixfold screw (6_3) } along	c	$00l$	$l = 2n + 1$
Threefold screw (3_1, 3_2), Sixfold screw (6_2, 6_4) } along	c	$00l$	$l = 3n + 1, 3n + 2,$ that is, not evenly divisible by 3
Fourfold screw (4_1, 4_3) along	a	$h00$	$h = 4n + 1, 2,$ or 3
	b	$0k0$	$k = 4n + 1, 2,$ or 3
	c	$00l$	$l = 4n + 1, 2,$ or 3
Sixfold screw (6_1, 6_5) along	c	$00l$	$l = 6n + 1, 2, 3, 4,$ or 5

TABLE 11.9 Classification of Space Groups Based on Systematic Absences for the Triclinic, Monoclinic, and Orthorhombic Systems

System	Uniquely Determined	Sets with Identical Absences
Triclinic		$P1$, $P\bar{1}$
Monoclinic	$P2_1/a$	$P2$, Pm, $P2/m$
		$P2_1$, $P2_1/m$
		Pa, $P2/a$
		$A2$, Am, $A2/m$
		Aa, $A2/a$
Orthorhombic	$P222_1$	$P222$, $Pmm2$, $Pmmm$
	$P2_12_12$	$C222$, $Cmm2$, $Amm2$, $Cmmm$
	$P2_12_12_1$	$F222$, $Fmm2$, $Fmmm$
	$C222_1$	$I222$, $I2_12_12_1$, $Imm2$, $Immm$
	$Pnnn$	$Pmc2_1$, $Pma2$, $Pmma$
	$Pban$	$Pcc2$, $Pccm$
	$Pnna$	$Pca2_1$, $Pbcm$
	$Pcca$	$Pnc2$, $Pmna$
	$Pccn$	$Pmn2_1$, $Pmmn$
	$Pbcn$	$Pba2$, $Pbam$
	$Pbca$	$Pna2_1$, $Pnma$
	$Ccca$	$Pnn2$, $Pnnm$
	$Fdd2$	$Cmc2_1$, $Ama2$, $Cmcm$
	$Fddd$	$Ccc2$, $Cccm$
	$Ibca$	$Abm2$, $Cmma$
		$Aba2$, $Cmca$
		$Iba2$, $Ibam$
		$Ima2$, $Imma$

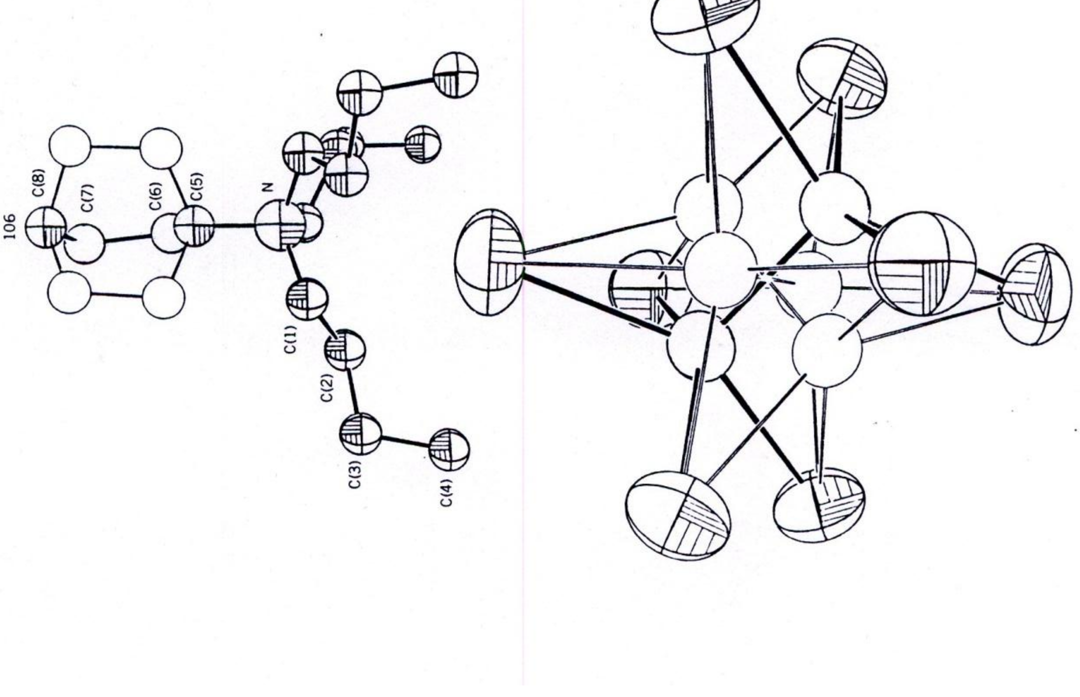


Figure 11.25. The disordered cation and anion in $[N(C_4H_9)_4]_2[Re_2I_8]$. Each one lies on a threefold axis of the unit cell. The hatched atoms are ordered, while the open circles show the sets of atoms (C above, Re below) that are disordered over three positions about the axis.

APPENDIX VIII

THE 230 SPACE GROUPS

Crystal System	Crystal Class	Space Groups					
Triclinic	1	$P1$					
	$\bar{1}$	$P\bar{1}$					
Monoclinic	2	$P2$	$P2_1$	$A2(C2)$			
	m	Pm	$Pa(Pc)$	$Am(Cm)$	$Aa(Cc)$		
	$2/m$	$P2/m$	$P2_1/m$	$A2/m(C2/m)$	$P2/a(P2/c)$	$P2_1/a(P2_1/c)$	$A2/a(C2/c)$
	222	$P222$	$P222_1$	$P2_12_12$	$P2_12_12_1$	$C222_1$	$C222$
		$F222$	$I222$	$I2_12_12_1$			
	$mm2$	$Pmm2$	$Pmc2_1$	$Pcc2$	$Pma2$	$Pca2_1$	$Pnc2$
		$Pmn2_1$	$Pba2$	$Pna2_1$	$Pnn2$	$Cmm2$	$Cmc2_1$
		$Ccc2$	$Amm2$	$Abm2$	$Ama2$	$Aba2$	$Fmm2$
Orthorhombic		$Fdd2$	$Imm2$	$Iba2$	$Ima2$		
	mmm	$Pmmm$	$Pnnn$	$Pccm$	$Pban$	$Pmma$	$Pnna$
		$Pmna$	$Pcca$	$Pbam$	$Pccn$	$Pbcm$	$Pnnm$
		$Pmmn$	$Pbcn$	$Pbca$	$Pnma$	$Cmcm$	$Cmca$
		$Cmmm$	$Cccm$	$Cmma$	$Ccca$	$Fmmm$	$Fddd$
		$Immm$	$Ibam$	$Ibca$	$Imma$		
	4	$P4$	$P4_1$	$P4_2$	$P4_3$	$I4$	$I4_1$
	$\bar{4}$	$P\bar{4}$	$I\bar{4}$				
	$4/m$	$P4/m$	$P4_2/m$	$P4/n$	$P4_2/n$	$I4/m$	$I4_1/a$
Tetragonal	422	$P422$	$P42_12$	$P4_122$	$P4_12_12$	$P4_222$	$P4_22_12$
		$P4_322$	$P4_32_12$	$I422$	$I4_122$		
	$4mm$	$P4mm$	$P4bm$	$P4_2cm$	$P4_2nm$	$P4cc$	$P4nc$
		$P4_2mc$	$P4_2bc$	$I4mm$	$I4cm$	$I4_1md$	$I4_1cd$
	$\bar{4}2m$	$P\bar{4}2m$	$P\bar{4}2c$	$P\bar{4}2_1m$	$P\bar{4}2_1c$	$P\bar{4}m2$	$P\bar{4}c2$
		$P\bar{4}b2$	$P\bar{4}n2$	$I\bar{4}m2$	$I\bar{4}c2$	$I\bar{4}2m$	$I\bar{4}2d$
	$4/mmm$	$P4/mmm$	$P4/mcc$	$P4/nbm$	$P4/nnc$	$P4/mbm$	$P4/mnc$
		$P4/nmm$	$P4/ncc$	$P4_2/mmc$	$P4_2mcm$	$P4_2/nbc$	$P4_2/nnm$
		$P4_2/mbc$	$P4_2/mnm$	$P4_2/nmc$	$P4_2/ncm$	$I4/mmm$	$I4/mcm$
		$I4_1/amd$	$I4_1/acd$				
	3	$P3$	$P3_1$	$P3_2$	$R3$		
	$\bar{3}$	$P\bar{3}$	$R\bar{3}$				
	32	$P312$	$P321$	$P3_112$	$P3_121$	$P3_212$	$P3_221$
		$R32$					
	$3m$	$P3m1$	$P31m$	$P3c1$	$P31c$	$R3m$	$R3c$
	$\bar{3}m$	$P\bar{3}1m$	$P\bar{3}1c$	$P\bar{3}m1$	$P\bar{3}c1$	$R\bar{3}m$	$R\bar{3}c$
Trigonal-hexagonal	6	$P6$	$P6_1$	$P6_5$	$P6_2$	$P6_4$	$P6_3$
	$\bar{6}$	$P\bar{6}$					
	$6/m$	$P6/m$	$P6_3/m$				
	622	$P622$	$P6_122$	$P6_522$	$P6_222$	$P6_422$	$P6_322$
	$6mm$	$P6mm$	$P6cc$	$P6_3cm$	$P6_3mc$		
	$\bar{6}m2$	$P\bar{6}m2$	$P\bar{6}c2$	$P\bar{6}2m$	$P\bar{6}2c$		
	$6/mmm$	$P6/mmm$	$P6/mcc$	$P6_3/mcm$	$P6_3/mmc$		
	23	$P23$	$F23$	$I23$	$P2_13$	$I2_13$	
	$m3$	$Pm3$	$Pn3$	$Fm3$	$Fd3$	$Im3$	$Pa3$
		$Ia3$					
Cubic	432	$P432$	$P4_232$	$F432$	$F4_132$	$I432$	$P4_332$
		$P4_132$	$I4_132$				
	$\bar{4}3m$	$P\bar{4}3m$	$F\bar{4}3m$	$I\bar{4}3m$	$P\bar{4}3n$	$F\bar{4}3c$	$I\bar{4}3d$
	$m3m$	$Pm3m$	$Pn3n$	$Pm3n$	$Pn3m$	$Fm3m$	$Fm3c$
		$Fd3m$	$Fd3c$	$Im3m$	$Ia3d$		