Space Groups

Internal Symmetry of Crystals
Dyar, Gunter, Tasa chapt 12

Space Groups

- *If translation operations are included with rotation and inversion,*
- *We have 230 three-dimensional space groups.*
- *Translation operations*
  - *Unit cell translations*
  - *Centering operations (Lattices) (A, B, C, I, F, R)*
  - *Glide planes (reflection + translation) (a, b, c, n, d*
  - *Screw axes (rotation + translation) (2_1, 3_1, 3_2)*

Space Groups: Learning Goals

- *Our knowledge of crystals is very well established and defined.*
- *Crystal structures are determined by X-ray diffraction methods (+neutron & electron)*
- *Recognize a space group symbol.*
  - *Pbnm, C2/c, Ia-3d, P-1, Imma, etc.*
  - *Every mineral structure has one.*

Space Groups

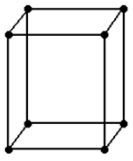
- *230 three-dimensional space groups*
- *Hermann-Mauguin symbols. (4 positions)*
- *First position is Lattice type (P, A, B, C, I, F or R)*
- *Second, third and fourth positions as with point groups*

Space Groups: Learning Goals

- Mineral structure is defined by:
  - Space Group (class, system)
  - Unit cell parameters (a, b, c, α, β, γ).
  - Coordinates (fractional) of unique atoms

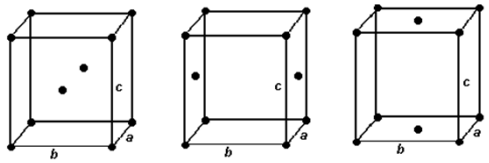
Lattices (centering operations)

- *P is for primitive*

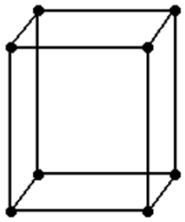


Lattices

- A, B, and C are end-centered



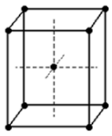
Lattices



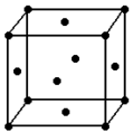
- A. P
- B. B
- C. I
- D. R
- E. F

Lattices

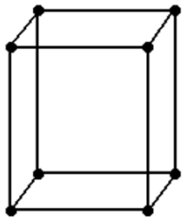
- I is body-centered
  - point @ (0.5, 0.5, 0.5)
  - multiplicity = 2



- F is face-centered
  - 0.5, 0.5, 0
  - 0.5, 0, 0.5
  - 0, 0.5, 0.5
  - multiplicity = 4



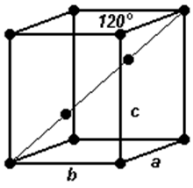
Lattices



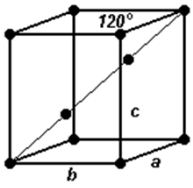
- A. P
- B. B
- C. I
- D. R
- E. F

Lattices

- R is rhombohedral
  - (2/3, 1/3, 1/3)
  - (1/3, 2/3, 2/3)
  - multiplicity = 3
  - Trigonal system

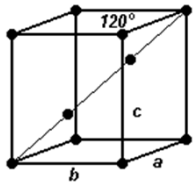


Lattices



- A. P
- B. B
- C. I
- D. R
- E. F

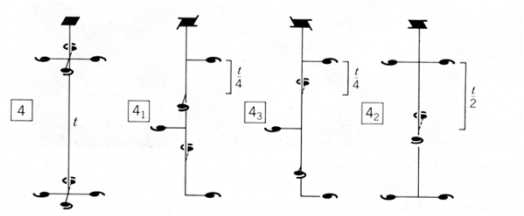
Lattices



- A. P
- B. B
- C. I
- D. R
- E. F

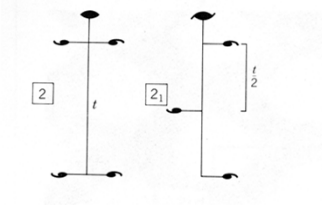
Screw Tetrads

- 4_1 is a 90º rotation plus a 1/4 cell translation (right-handed).
- 4_2 is a 90º rotation plus a 1/2 cell translation (no handedness).
- 4_3 is a 90º rotation plus a 3/4 cell translation (left-handed).



Rotation + Translation = Screw Axes Screw Diads

- 2 is a 180º rotation
- 2_1 is a 180º rotation plus 1/2 cell translation.

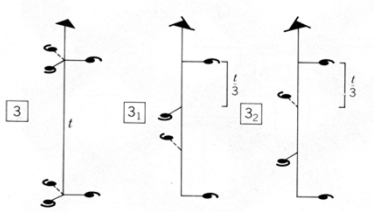


Screw Hexads

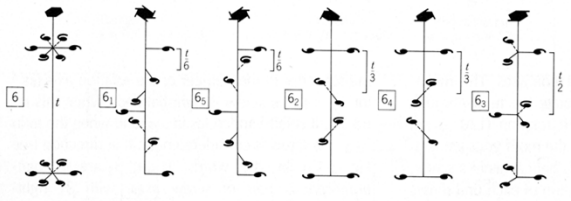
- 6_1 is a 60º rotation plus a 1/6 cell translation (right-handed).
- 6_2 is a 120º rotation plus a 1/3 cell translation (right-handed).
- 6_3 is a 180º rotation plus a 1/2 cell translation (no handedness).
- 6_4 is a 240º rotation plus a 2/3 cell translation (left-handed).
- 6_5 is a 300º rotation plus a 5/6 cell translation (left-handed).

Screw Triads

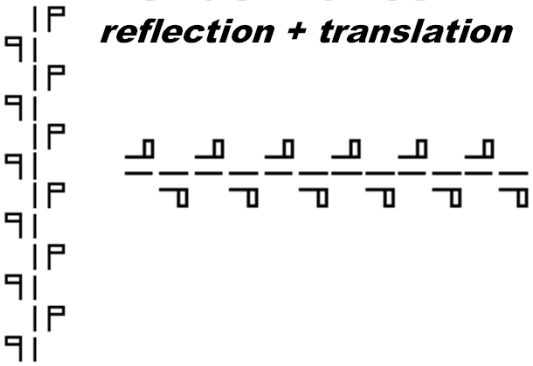
- 3_1 is a 120º rotation plus a 1/3 cell translation.
- 3_2 is a 120º rotation plus a 2/3 cell translation



Screw Hexads

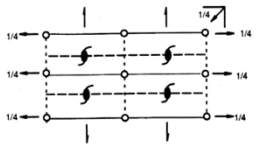


Glide Planes =
reflection + translation



Space Group Symmetry Diagrams

	Axis	Plane
– *a*	2_1	*b*
– *b*	2	*c*
– *c*	2_1	*n*



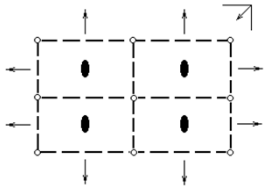
- $P\,2_1/b\,2/c\,2_1/n = Pbcn$

Glide Planes

- *Reflection plus 1/2 cell translation*
  - *a-glide: a/2 translation*
  - *b-glide: b/2 translation*
  - *c-glide: c/2 translation*
  - *n-glide(normal to a): b/2+c/2 translation*
  - *n-glide(normal to b): a/2+c/2 translation*
  - *n-glide(normal to c): a/2+b/2 translation*
  - *d-glide (tetragonal + cubic systems)*

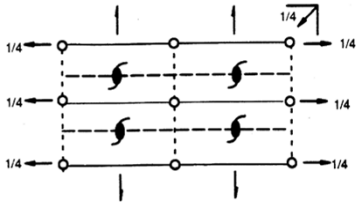
Space Group Symmetry Diagrams

	Axis	Plane
– *a*	2	*b*
– *b*	2	*a*
– *c*	2	*n*



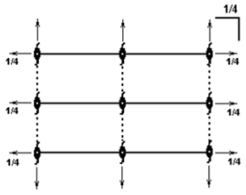
- $P\,2/b\,2/a\,2/n = Pban$

Space Group Symmetry Diagrams



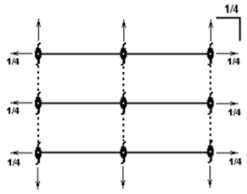
- *a-vertical*
- *b-horizontal*
- *c-normal to page*

Perpendicular to a:



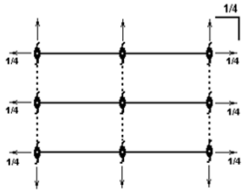
- *A. n-glide*
- *B. b-glide*
- *C. c-glide*
- *D. Mirror*
- *E. nothing*

Perpendicular to a:



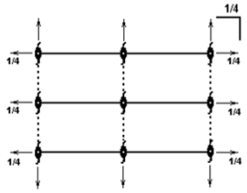
- *D. Mirror*

Perpendicular to c:



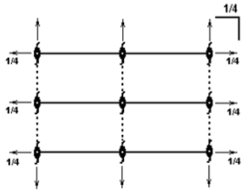
- *A. n-glide*
- *B. b-glide*
- *C. c-glide*
- *D. Mirror*
- *E. nothing*

Perpendicular to b:



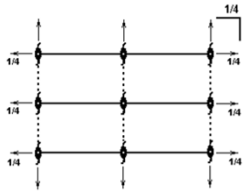
- *A. n-glide*
- *B. b-glide*
- *C. c-glide*
- *D. Mirror*
- *E. nothing*

Perpendicular to c:



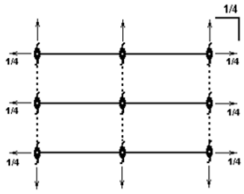
- *Mirror*

Perpendicular to b:



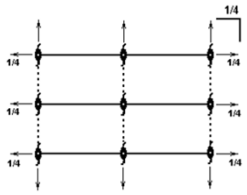
- *c-glide*

Axis Parallel to a:



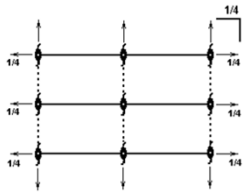
- *A. 2*
- *B. 2_1*
- *C. 4*
- *D. nothing*

Axis Parallel to a:



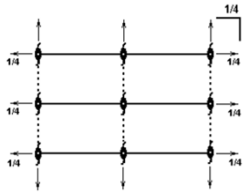
- A. 2
- B. 2_1
- C. 4
- D. nothing

Primitive space group



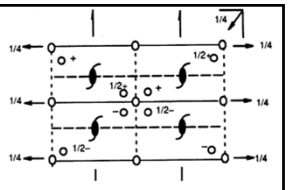
- P 2/m 2/c 2_1/m
- = Pmcm

Axis Parallel to c:



- A. 2
- B. 2_1
- C. 4
- D. nothing

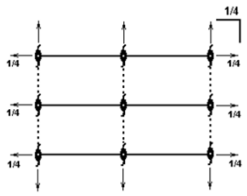
Pbcn



- (*x*, *y*, *z*)

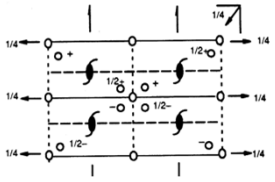
- We place an atom at fractional coordinates *x*, *y*, *z* in the unit cell.
- The symmetry operators repeat that atom 7 times to give 8 identical atoms in the cell.

Axis Parallel to c:



- A. 2
- B. 2_1
- C. 4
- D. nothing

Pbcn



- (*x*, *y*, *z*)
- (-*x*, -*y*, -*z*)
- (*x*, -*y* 1/2+*z*)
- (-*x*, *y* 1/2-*z*)
- (1/2 - *x*, 1/2 + *y*, *z*)
- (1/2 + *x*, 1/2 - *y*, -*z*)
- (1/2 - *x*, 1/2 - *y*, 1/2 + *z*)
- (1/2 + *x*, 1/2 + *y*, 1/2 - *z*)

Pbcn — *General*

- (*x*, *y*, *z*)
- (*-x*, *-y*, *-z*)
- (*x*, *-y* 1/2+*z*)
- (*-x*, *y* 1/2-*z*)
- (1/2 - *x*, 1/2 + *y*, *z*)
- (1/2 + *x*, 1/2 - *y*, *-z*)
- (1/2 - *x*, 1/2 - *y*, 1/2 + *z*)
- (1/2 + *x*, 1/2 + *y*, 1/2 - *z*)

- *(0.1, 0.2, 0.3)*
- *(0.9, 0.8, 0.7)*
- *(0.1, 0.8, 0.8)*
- *(0.9, 0.2, 0.2)*
- (0.4, 0.7, 0.3)
- (0.6, 0.3, 0.7)
- (0.4, 0.3, 0.8)
- (0.6, 0.7, 0.2)

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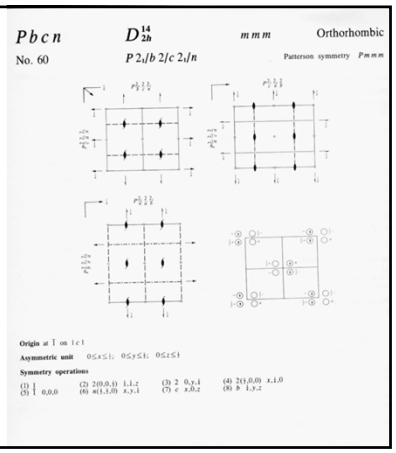


Pbcn — *Special*

- (*x*, *y*, *z*)
- (*-x*, *-y*, *-z*)
- (*x*, *-y* 1/2+*z*)
- (*-x*, *y* 1/2-*z*)
- (1/2 - *x*, 1/2 + *y*, *z*)
- (1/2 + *x*, 1/2 - *y*, *-z*)
- (1/2 - *x*, 1/2 - *y*, 1/2 + *z*)
- (1/2 + *x*, 1/2 + *y*, 1/2 - *z*)

- *(0, 0, 0)*
- *(0, 0, 0)*
- *(0, 0, 0.5)*
- *(0, 0, 0.5)*
- *(0.5, 0.5, 0)*
- *(0.5, 0.5, 0)*
- *(0.5, 0.5, 0.5)*
- *(0.5, 0.5, 0.5)*

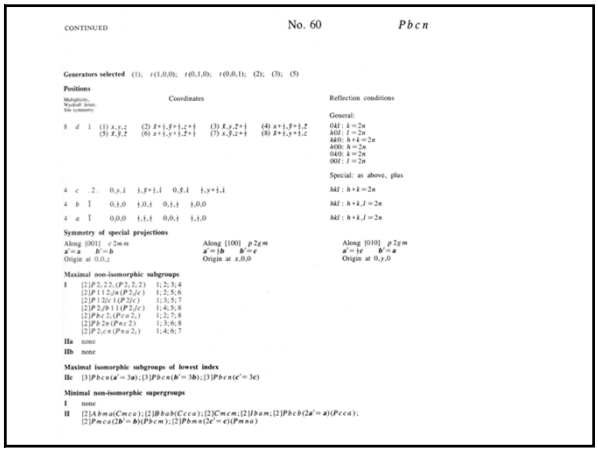
Half as many

Enstatite Pbcn

- *Cell a=9.306; b=8.892 c= 5.349 Å*

- *Mg1* *(0, 0.1006, 0.25)*
- *Mg2* *(0, 0.2625, 0.25)*
- *Si* *(0.2928, 0.0897,0.0739)*

- *O1* *(0.1200, 0.0942, 0.0770)*
- *O2* *(0.3773, 0.2463, 0.0677)*
- *O3* *(0.3481, 0.9836, 0.3079)*


CONTINUED No. 60 *Pbcn*

Generators selected (1); *t*(1,0,0); *t*(0,1,0); *t*(0,0,1); (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry | Coordinates | Reflection conditions

General:

8 *d* 1 (1) *x*,*y*,*z* (2) $\bar{x}$+½,$\bar{y}$+½,*z*+½ (3) $\bar{x}$,*y*,*z*+½ (4) *x*+½,$\bar{y}$+½,$\bar{z}$ (5) $\bar{x}$,$\bar{y}$,$\bar{z}$ (6) *x*+½,*y*+½,*z*+½ (7) *x*,$\bar{y}$,*z*+½ (8) $\bar{x}$+½,*y*+½,*z*

0kl : *k* = 2*n*
h0l : *l* = 2*n*
hk0 : *h*+*k* = 2*n*
h00 : *h* = 2*n*
0k0 : *k* = 2*n*
00l : *l* = 2*n*

Special: as above, plus

4 *c* .2. 0,*y*,¼ ½,$\bar{y}$+½,¼ 0,$\bar{y}$,¼ ½,*y*+½,¼ *hkl* : *h*+*k* = 2*n*

4 *b* $\bar{1}$ 0,½,0 ½,0,½ 0,½,½ ½,0,0 *hkl* : *h*+*k*,*l* = 2*n*

4 *a* $\bar{1}$ 0,0,0 ½,½,½ 0,0,½ ½,½,0 *hkl* : *h*+*k*,*l* = 2*n*

Symmetry of special projections

Along [001] *c*2*mm* — *a*′ = *a* *b*′ = *b* — Origin at 0,0,*z*

Along [100] *p*2*gm* — *a*′ = ½*b* *b*′ = *c* — Origin at *x*,0,0

Along [010] *p*2*gm* — *a*′ = ½*c* *b*′ = *a* — Origin at 0,*y*,0

Maximal non-isomorphic subgroups

I [2]*P*2,2,2 (*P*2,2,2) 1; 2; 3; 4
[2]*P*1 1 2$_1$/*a* (*P*2$_1$/*c*) 1; 2; 5; 6
[2]*P* 1 2/*c* 1 (*P*2/*c*) 1; 3; 5; 7
[2]*P*2$_1$/*b* 1 1 (*P*2$_1$/*c*) 1; 4; 5; 8
[2]*P*2*c* 2$_1$ (*Pc*2$_1$) 1; 2; 7; 8
[2]*P*2*b* 2*n* (*Pnc*2) 1; 3; 6; 8
[2]*P*2$_1$*c* 2*n* (*Pnc*2$_1$) 1; 4; 6; 7

IIa none

IIb none

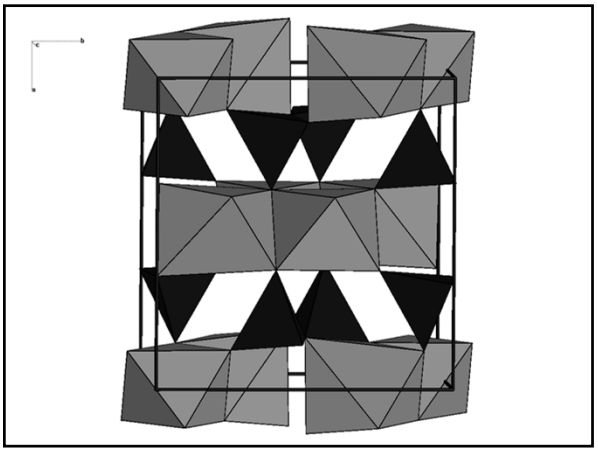
Maximal isomorphic subgroups of lowest index

IIc [3]*Pbcn* (*a*′ = 3*a*); [3]*Pbcn* (*b*′ = 3*b*); [3]*Pbcn* (*c*′ = 3*c*)

Minimal non-isomorphic supergroups

I none

II [2]*Abma* (*Cmca*); [2]*Bbab* (*Ccca*); [2]*Cmcm*; [2]*Ibam*; [2]*Pbcb* (2*a*′ = *a*) (*Pcca*); [2]*Pmca* (2*b*′ = *b*) (*Pbcm*); [2]*Pbnn* (2*c*′ = *c*) (*Pnna*)



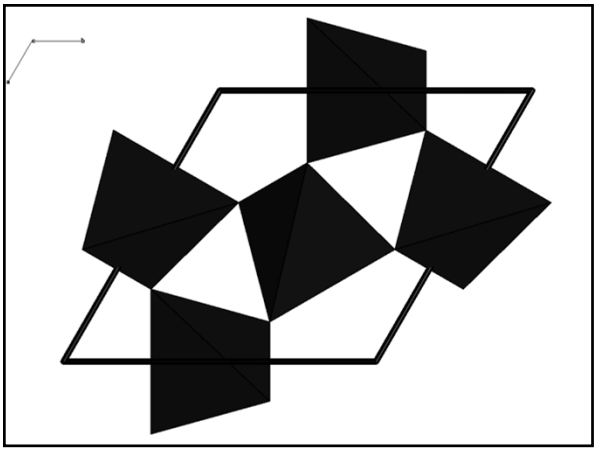
Quartz $P3_121$

- Cell a=4.9137; b=4.9137 c= 5.4047Å
- Space Group: $P3_121$
- Si (0.4697, 0.0, 0.0)
- O (0.4133, 0.2672, 0.1188)

Enstatite Pbcn

- Cell a=9.306; b=8.892 c= 5.349 Å
- What's in the cell??
- Mg1 special 4
- Mg2 special 4
- Si general 8
- O1 general 8
- O2 general 8
- O3 general 8

8 Mg, 8 Si, 24 O



Enstatite Pbcn

- Cell a=9.306; b=8.892 c= 5.349 Å
- What's in the cell??

8 Mg, 8 Si, 24 O

- 8 x ($MgSiO_3$)
- Z = 8 (formula units per cell)

Quartz $P3_121$

- Cell a=4.9137; b=4.9137 c= 5.4047Å
- Space Group: $P3_121$ or $P3_221$
- Si (3)
- O (6)
- Formula 3 x (SiO2)

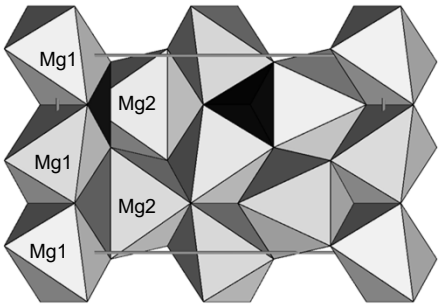
Olivine Pbnm Mg_2SiO_4

- Cell a=4.756; b=10.207 c= 5.980 Å

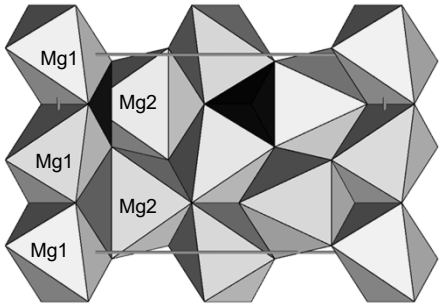
- Mg1 4 (0.0, 0.0, 0.0)
- Mg2 4 (0.991, 0.277, 0.25)
- Si 4 (0.426, 0.094,0.25)

- O1 4 (0.766, 0.091, 0.25)
- O2 4 (0.222, 0.447, 0.25)
- O3 8 (0.278, 0.163, 0.033)

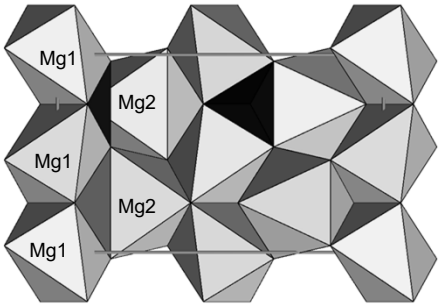
Cation Substitution Olivine



Olivine Pbnm Mg_2SiO_4



Fe^{2+} substitutes for Mg^{2+} in octahedral sites



Olivine Pbnm Mg_2SiO_4

- Cell a=4.756; b=10.207 c= 5.980 Å

- Mg1 4, Mg2 4, Si 4
- O1 4, O2 4, O3 8

- = 4 x (Mg_2SiO_4)

- This is why minerals have formulas with integer atom ratios.

Cation Substitution

- Mg_2SiO_4 - Fe_2SiO_4 Olivine

- Mg_2SiO_4 Forsterite
- Fe_2SiO_4 Fayalite
-
- $(Mg,Fe)_2SiO_4$ Any intermediate composition

- 2 divalent, 1 tetravalent, 4 oxygens

Cation Substitution

- Mg_2SiO_4 - Fe_2SiO_4 Olivine

- Mg_2SiO_4 Forsterite Fo
- Fe_2SiO_4 Fayalite Fa
-
- $Fo_{90}Fa_{10}$

Lab Next Week: XTALDRAW

- Bring: Your mineral
  - Unit Cell information
    - a, b, c, α, β, γ
  - Formula
  - Atom positions