powder diffraction file

PDF

ICDD & PDF

ICDD - International Centre for Diffraction Data

- A non-profit scientific organization dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of crystalline materials
- Joint Committee for Chemical Analysis by Powder Diffraction Methods ; founded in 1941
- Joint Committee on Powder Diffraction Standards (JCPDS) ; established in 1969
- Renamed to ICDD in 1978

PDF - powder diffraction file

- a collection of single-phase XRPD patterns in the form of tables of characteristic **interplanar spacings (d's)** and corresponding **relative intensities (I's)** along with other pertinent physical and crystallographic properties
- dif file
- ###.dif

XRPD; X-ray Powder Diffraction

www.icdd.com

PDF card

Quality mark
* Highest quality
i reasonable quality
o low quality
blank quality lower than o
c calculated data
r d's from Rietveld refinement

Set number
Add 1950 → year

Chemical formula
Chemical name
Mineral name

Experimental info
Types of X-ray
Wavelength
Monochromator/filter
Method of d measurement
Max measurable d-spacing
Method of I measurement
I/I(corundum)
Literature source

Physical data
Xtal system
International tables space group symbol
Axial lengths
Axial ratios
Interaxial angles
Number of chemical formulas in unit cell
Melting point
Literature source
X-ray density
Measured density
Figure of Merit

5- 628

NaCl

Sodium Chloride

Halite, syn

Rad. CuKα$_1$ λ 1.5405 **Filter** Ni **d-sp**
Cutoff **Int.** Diffractometer **I/I$_{cor}$**: 4.40
Ref. Swanson, Fuyai, *Natl. Burl. Stand. (U.S.), Circ. 539, II 41 (1953)*

Sys. Cubic **S.G.** Fm3m(225)
A 5.6402 **b** **c** **AC**
α β γ **Z** 4 **mp** 804
Ref. Ibid.
D$_x$ 2.16 **D$_m$** 2.17 **SS/FOM F$_{17}$**=93(.011,17)
εα ηωβ 1.542 εγ **Sign** **2V**
Ref. *Dana's System of Mineralogy, 7th Ed.*, II 4

Color Colorless
Pattern taken at 26 C. CAS#: 7647-14-5. An ACS reagent grade sample recrystallized twice from hydrochloric acid. Halite group, halite subgroup. PSC: cF8.

d Å	Int	h k l	d Å	Int	h k l
3.26	13	111			
2.821	100	200			
1.994	55	220			
1.701	2	311			
1.628	15	222			
1.410	6	400			
1.294	1	331			
1.261	11	420			
1.1515	7	422			
1.0855	1	511			
0.9969	2	440			
0.9533	1	531			
0.9401	3	600			
0.8917	4	620			
0.8601	1	533			
0.8503	32	622			
0.8141	2	444			

General comments

D's, I's and Miller indices

Krawitz

PDF card

CAS; chemical abstracts service registry number

PDF # 050628,

05-0628 Quality: *
CAS Number: 7647-14-5
Molecular Weight: 58.44
Volume[CD]: 179.43
Dx: 2.163 Dm: 2.168
Sys: Cubic
Lattice: Face-centered
S.G.: Fm3m (225)
Cell Parameters:
a 5.640 b c
α β γ
SS/FOM: F17=93(.0108, 17)
I/Icor: 4.40
Rad: CuKa1
Lambda: 1.5405
Filter: Ni
d-sp:
Mineral Name:
Halite syn

PCPDFWIN

PDF

- PDF-2
- PDF-4+: most advanced database, designed for both phase ID and quantitative analysis.

Data Entry Source	PDF-2 2016	PDF-4+ 2016 WebPDF-4+ 2016	PDF-4/ Minerals 2016	PDF-4/ Organics 2017
00- ICDD	115,066	115,066	12,031	39,395
01- FIZ	165,264	67,498	12,294	12,185
02- CCDC	0	0	0	431,359
03- NIST	10,067	2,960	216	281
04- MPDS	0	198,367	19,748	0
05- ICDD Crystal Data	722	722	52	32,785
Total No. of Data Sets	**291,119**	**384,613**	**44,341**	**516,054**
Subfile Distribution:				
Inorganic	258,130	351,612	44,285	33,943
Organic	41,386	42,229	701	505,530
New Entries	12,616	18,736	1,489	14,090
Rietveld—No. with atomic coordinates	0	271,449	33,574	96,825
Reference Intensity Ratio (RIR)—I/I_c	193,567	286,885	33,362	484,021
Experimental Digital Patterns	0	11,287	127	6,062
Pattern Fitting—Calculated Digital Patterns	0	384,613	44,341	516,054

All ICDD databases combine the power of both powder diffraction and crystal structure reference data. We are the only crystallographic database in the world with quality marks and quality review processes that are ISO certified. Each PDF databas includes our integrated data mining software.

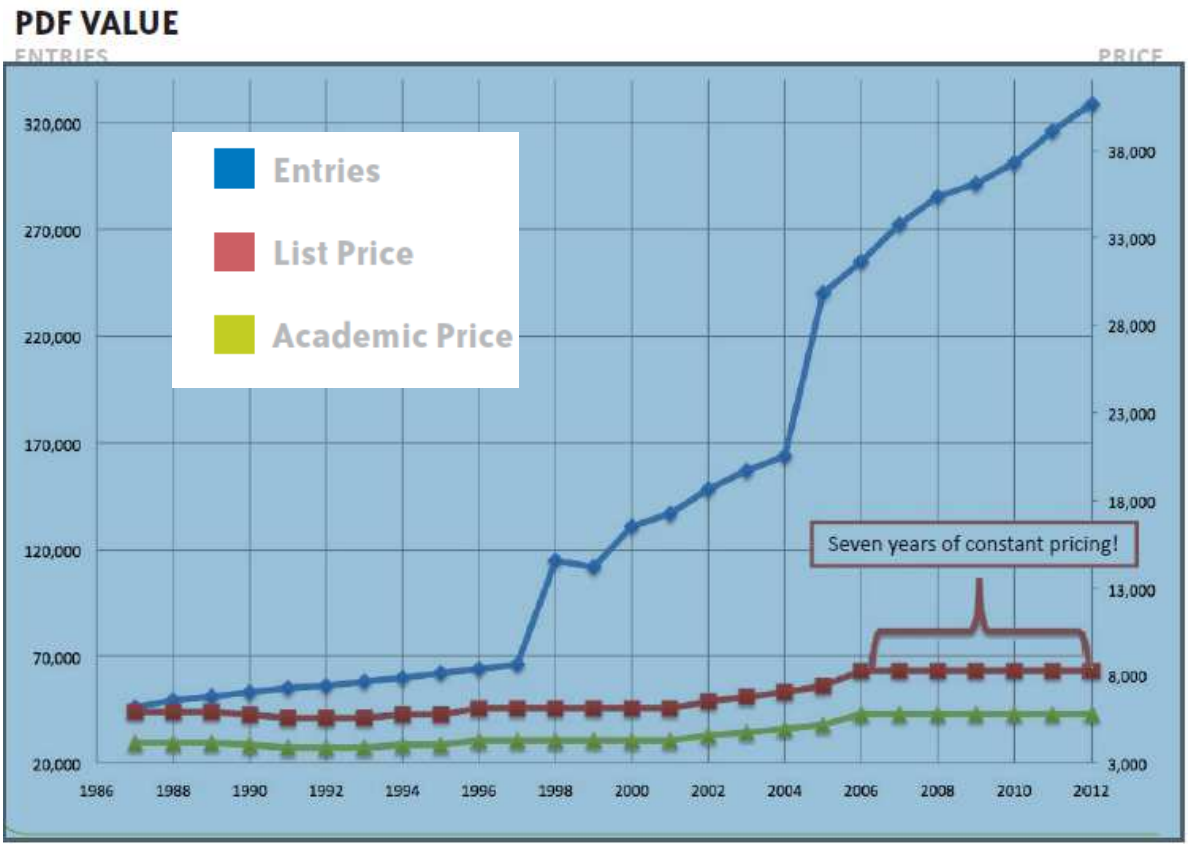
www.icdd.com/products/flyers/Product_Summary.pdf

PDF

- The initial term of the license for PDF-2 and SIeve is five (5) years from the license registration key date.
- All PDF-4 products are licensed for 12 months.

PDF-4+ 2016	List	Academic
New - Single License	$8,660	$5,775
Renewal from 2015 to 2016	$1,760	$1,150
PDF-4+ 2016 Multi-year License*		
Renewal - 3 year license	$4,750	$3,105
Renewal - 5 year license	$7,480	$4,890
PDF-4+Scholar Multi-year License		
Renewal - 5 year license	NA	$5,925
PDF-4+ 2016 Site License*		
New Master License	$8,660	$5,775
New - additional licenses, each	$1,760	$1,150
Renewal - Yearly Master License	$1,760	$1,150
Renewal - additional licenses, each	$550	$395
PDF-4+ 2016 Site/Multi-year Licens		
Renewal - 3 year Master Site License	$5,495	$3,810
Renewal - 3 year additional licenses, eac	$1,820	$1,310
Renewal - 5 year Master Site License	$9,340	$6,680
Renewal - 5 year additional licenses, eac	$3,190	$2,290
PDF-2 to PDF-4+ 2016 Conversion		
PDF-2 2015 to PDF-4+ 2016	$1,760	$1,150
PDF-2 2014 to PDF-4+ 2016	$3,520	$2,300
PDF-2 2013 to PDF-4+ 2016	$5,280	$3,450
PDF-2 2012 to PDF-4+ 2016	$7,040	$4,600

www.icdd.com/products/flyers/Product_Summary.pdf



PDF - Quality Mark & Figure of Merit

Quality Mark

- * highest quality - average $\Delta 2\theta$ < 0.03 degree, all lines were indexed, I measured quantitatively
- i reasonable quality - average $\Delta 2\theta$ < 0.06 degree, indexed with no more than two lines being unaccounted for, I measured quantitatively
- o low quality - low precision, poorly characterized, no unit cell data
- blank quality lower than o
- c calculated data
- r d's from Rietveld refinement
- h (hypothetical)

www.icdd.com/resources/webpdf/explain.htm
"Evaluating Data Quality" from ICDD

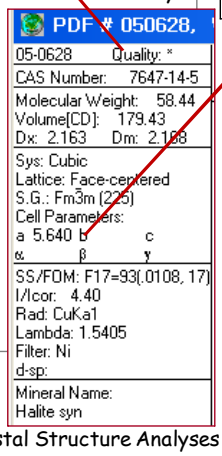


Figure of Merit

- To quantify better the quality of a given set of d-spacings
- To judge the credibility and worth of the results
- To evaluate the quality of d measurements
- The higher, the better < 20 → poor quality

SS/FOM (Smith & Snyder FOM)

$$F_N = \frac{1}{|\Delta 2\theta|} \frac{N_{obs}}{N_{poss}}$$

F_N	=	Figure of merit
$\Delta 2\theta$	=	The average error in 2θ
N_{obs}	=	The number of lines observed
N_{poss}	=	Number of lines possible

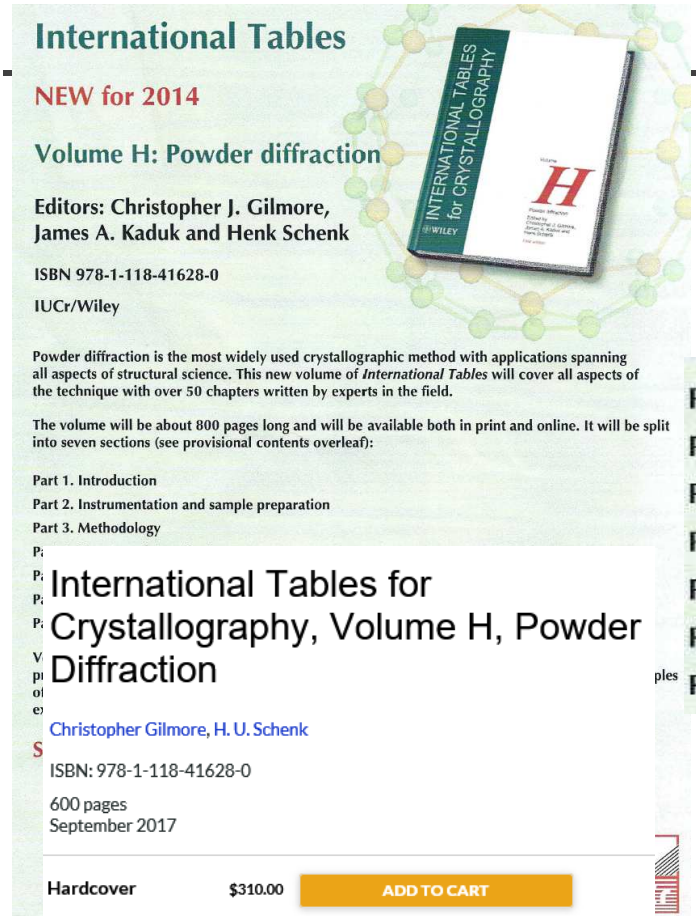
Jenkins & Snyder page 315

Space Group, International Table

International Tables for Crystallography, Brief teaching edition of Volume A: Space-group symmetry
Edited by Theo Hahn

International Tables for Crystallography, Volume A: Space-group symmetry
Edited by Theo Hahn

International Tables for Crystallography, Volume H: Powder Diffraction
Edited by C.J. Gilmore, J.A. Kaduk and H. Schenk



2019

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Part 2. Instrumentation and sample preparation
Part 3. Methodology
Part 4. Structure determination
Part 5. Defects, texture, microstructure and fibres
Part 6. Software
Part 7. Applications

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Electrons (J. M. Zuo, J. L. Lábár, J. Zhang, T. E. Gorelik and U. Kolb)
Two-dimensional powder diffraction (B. B. He)
Temperature (C. Reiss)
Sample environment – high-pressure devices (A. Katrusiak)
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Cells for *in situ* powder diffraction investigation of chemical reactions (W. van Beek and P. Pattison)
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Data reduction to $|F_{obs}|$ (A. Le Bail)
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Fibres (P. Langan)

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Part 7. Applications

Symmetry operation

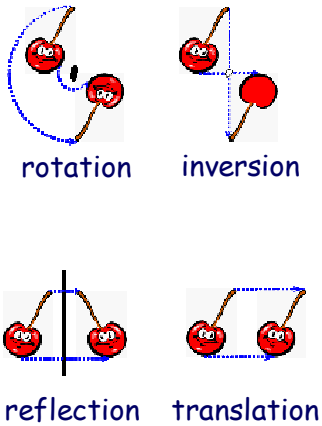
(1) Rotation; **1 2 3 4 6** (2) Reflection; **m** (= $\bar{2}$)

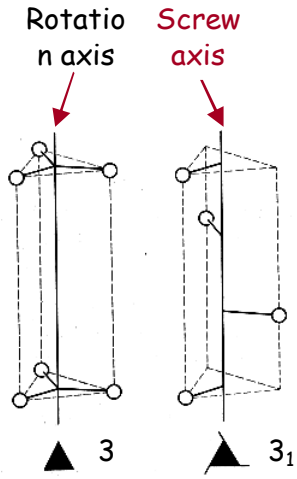
(3) Inversion (center of symmetry) (= $\bar{1}$)

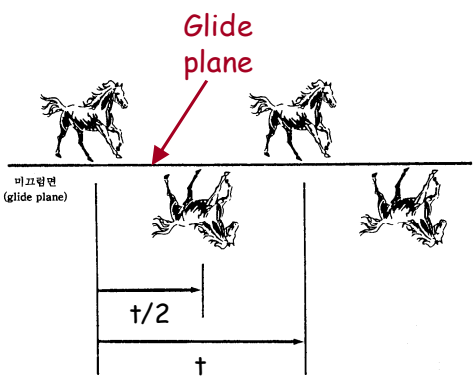
(4) Rotation-inversion; $\bar{1}$ (=center of symmetry), $\bar{2}$ (= mirror), $\bar{3}$, $\bar{4}$, $\bar{6}$

(5) Screw axis; rotation + translation **2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1,---, 6_5**

(6) Glide plane; reflection + translation, **a, b, c, n, d**







Crystal symmetry, 14 Bravais lattice

Crystal System	Bravais Lattices	Symmetry	Symmetry	Axis System
Cubic	P, I, F	m3m	m**3**m	a=b=c, α=β=γ=90
Tetragonal	P, I	4/mmm	**4**/mmm	a=b≠c, α=β=γ=90
Orthorhombic	P, C, I, F	mmm	**mmm**	a≠b≠c, α=β=γ=90
Hexagonal	P	6/mmm	**6**/mmm	a=b≠c, α=β=90, γ=120
Rhombohedral	R	3m	**3**m	a=b=c, α=β=γ≠90
Monoclinic	P, C	2/m	**2**/m	a≠b≠c, α=γ=90, β≠90
Triclinic	P	1	1	a≠b≠c, α≠β≠γ≠90

Quartz
Crystal System: trigonal
Bravais Lattice: primitive
Space Group: $P3_221$
Lattice Parameters: 4.9134 x 4.9134 x 5.4052 A
Atom Positions:

	x	y	z
Si	0.47 0	0	0.667
O	0.414	0.268	0.786

$P3_221$
P 3_2 2 1

6/mmm
6/m m m

Symmetry directions, Space group

Xtal systems	Symmetry directions		
Triclinic			
Monoclinic	b		
Orthorhombic	a	b	c
Tetragonal	c	<a>	<110>
Trigonal	c	<a>	
Hexagonal	c	<a>	<210>
Cubic	<a>	<111>	<110>

Fmmm
Face centered lattice
m ⊥ to a axis
m ⊥ to b axis
m ⊥ to c axis

$P3_221$
Primitive lattice
3_2 along the c axis
2 fold rot axis along the a axis
1 fold rot axis along the <210>

Fd3m
Face centered lattice
d ⊥ to a axis
3 fold axis along the <111>
m ⊥ to c axis

Short Hermann-Mauguin symbol

Point group

Schoenflies symbol

Crystal system symbol

Space group number

Full Hermann-Mauguin symbol

Patterson symmetry

Projection of symmetry elements

from International Tables for X-ray Crystallography

Projection of a general position

Choice of origin

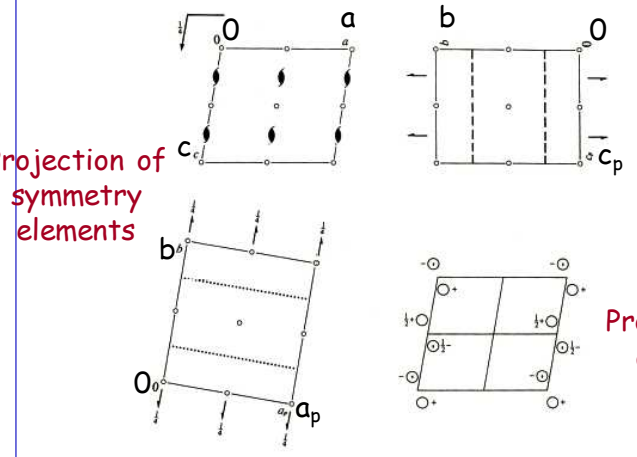
Asymmetric unit

Symmetry operations

$P2_1/c$ C_{2h}^5 $2/m$ Monoclinic

No. 14 $P12_1/c1$ Patterson symmetry $P12/m1$

UNIQUE AXIS b, CELL CHOICE 1



Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1;\ 0 \le y \le \frac{1}{2};\ 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{4},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ 0,0,0 (4) c $x,\frac{1}{4},z$

International Tables for X-ray Crystallography

General & special positions

CONTINUED No. 14 $P2_1/c$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry		Coordinates				Reflection conditions
						General:
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
				General position			Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl : $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
				Special position			

Symmetry of special projections

Along [001] $p2gm$ $\mathbf{a}' = \mathbf{a}_p$ $\mathbf{b}' = \mathbf{b}$ Origin at $0,0,z$

Along [100] $p2gg$ $\mathbf{a}' = \mathbf{b}$ $\mathbf{b}' = \mathbf{c}_p$ Origin at $x,0,0$

Along [010] $p2$ $\mathbf{a}' = \frac{1}{2}\mathbf{c}$ $\mathbf{b}' = \mathbf{a}$ Origin at $0,y,0$

Maximal non-isomorphic subgroups

I [2] $P1c1$ (Pc, 7) 1; 4
[2] $P12_11$ ($P2_1$, 4) 1; 2
[2] $P\bar{1}$ (2) 1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P12_1/c1$ ($\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{a}' = 2\mathbf{a}, \mathbf{c}' = 2\mathbf{a} + \mathbf{c}$) ($P2_1/c$, 14); [3] $P12_1/c1$ ($\mathbf{b}' = 3\mathbf{b}$) ($P2_1/c$, 14)

Minimal non-isomorphic supergroups

I [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pbcn$ (60); [2] $Pbca$ (61); [2] $Pnma$ (62); [2] $Cmce$ (64)

II [2] $A12/m1$ ($C2/m$, 12); [2] $C12/c1$ ($C2/c$, 15); [2] $I12/c1$ ($C2/c$, 15); [2] $P12_1/m1$ ($\mathbf{c}' = \frac{1}{2}\mathbf{c}$) ($P2_1/m$, 11); [2] $P12/c1$ ($\mathbf{b}' = \frac{1}{2}\mathbf{b}$) ($P2/c$, 13)

- Asymmetric unit
  - ✓ a region of space which fills all space when all the symmetry operations of the space group are applied
  - ✓ smaller than a unit cell
- Unit cell
  - ✓ a region of space which fills all space when the translation operations are applied

Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{4},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ 0,0,0 (4) c $x,\frac{1}{4},z$

International Tables for X-ray Crystallography

- Symmetry operations
  - ✓ (n) of the general equivalent position can be obtained from (1) x,y,z by symmetry operation number (n)
  - ✓ (3) -x,-y,-z ← 1bar with 0,0,0 as inversion point

4 e 1 (1) x,y,z (2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (3) $\bar{x},\bar{y},\bar{z}$ (4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$

Origin at $\bar{1}$

Asymmetric unit $0 \le x \le 1;\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{4},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ 0,0,0 (4) c $x,\frac{1}{4},z$

c glide, glide plane $x,\frac{1}{4},z$

Screw part Screw axis Location of inversion point

International Tables for X-ray Crystallography

- Generators
  - ✓ Symmetry operations and their sequence, selected to generate all symmetrically equivalent points of the general position from a point x,y,z
  - ✓ Set of symmetry operators which when successfully multiplied yield ALL of the operators of the group
  - ✓ List of symmetry operations selected that can generate all of the symmetry operations of the space group

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

translations

Symmetry operations

(1) 1 (2) $2(0,\frac{1}{4},0)$ $0,y,\frac{1}{4}$ (3) $\bar{1}$ 0,0,0 (4) c $x,\frac{1}{4},z$

International Tables for X-ray Crystallography

- Positions
  - ✓ Multiplicity (rank); # equivalent points per unit cell
  - ✓ Wyckoff letter
  - ✓ Site symmetry (point symmetry of the position)
  - ✓ Coordinates of the equivalent positions

Positions

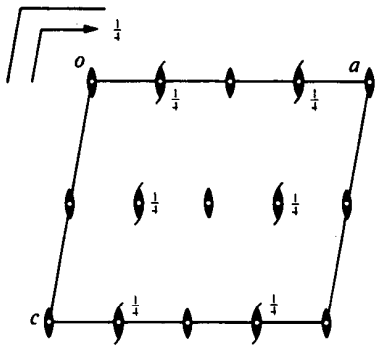
Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$		
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$		
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$		

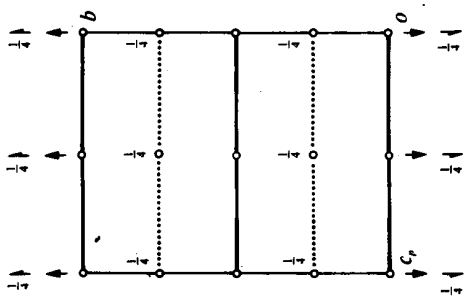
General position

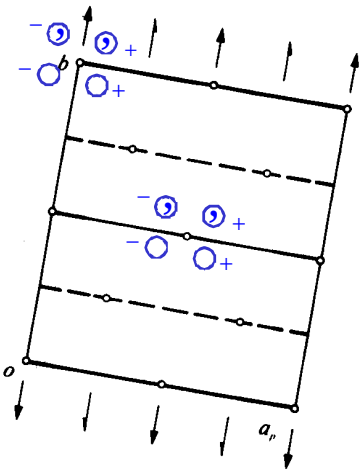
Special position

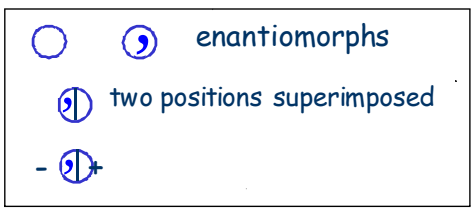
- The number of equivalent points in the unit cell = multiplicity
- A general position is a set of equivalent points with point symmetry (site symmetry) 1
- A special position is a set of equivalent points with point symmetry (site symmetry) higher than 1
- The asymmetric unit of a space group is the smallest part of the unit cell from which the whole cell may be filled by the operation of all the symmetry operations

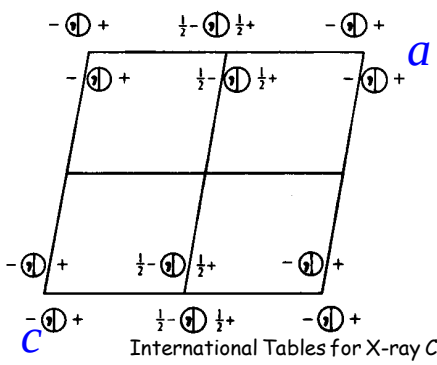
$C\frac{2}{m}$







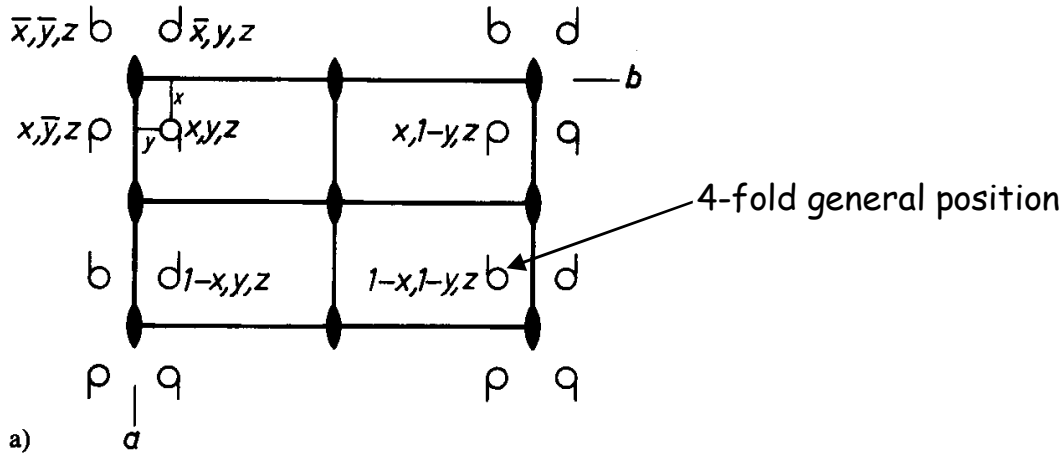




Space Group - Pmm2

- for a point x, y, z (general point),
  symmetry element generates $\bar{x}, y, z;\ x, \bar{y}, z;\ \bar{x}, \bar{y}, z$

$x, y, z;\ \bar{x}, y, z;\ x, \bar{y}, z;\ \bar{x}, \bar{y}, z$ are equivalent (multiplicity of 4)

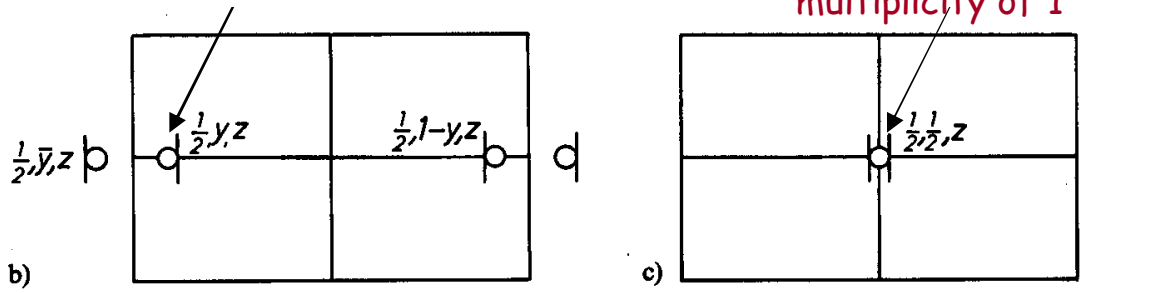


Space Group - Pmm2

- move a point x, y, z on to mirror plane at $\frac{1}{2}, y, z$
  x, y, z and $1\text{-}x, y, z$ coalesce to $\frac{1}{2}, y, z$
  $x, 1-y, z$ and $1\text{-}x, 1-y, z$ coalesce to $\frac{1}{2}, 1-y, z$
- multiplicity of 2
  - ✓ as long as the point remains on the mirror plane, its multiplicity is unchanged - degree of freedom 2

2-fold special position

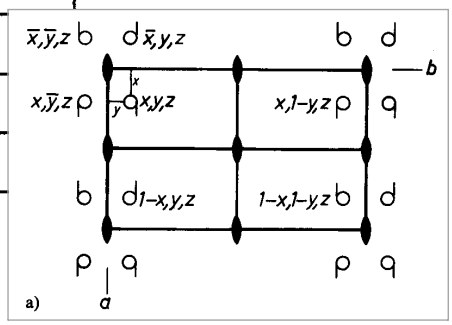
point symmetry mm2
multiplicity of 1



A special point arises from the merging of equivalent positions

Space Group Pmm2

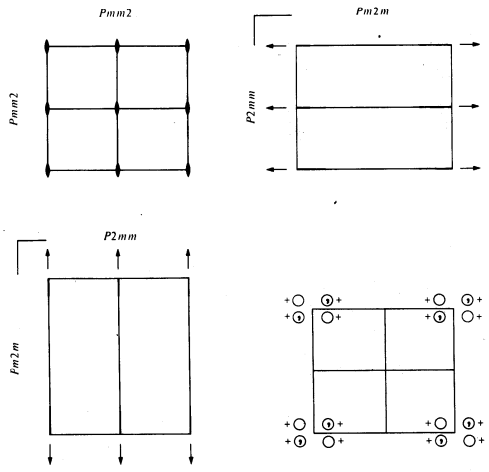
Position	Degrees of freedom	Multi-plicity	Site symmetry	Coordinates of equivalent points
general	3	4	1	x,y,z; $\bar{x},\bar{y},z$; x,$\bar{y}$,z; $\bar{x}$,y,z
special	2	2	m	$\frac{1}{2}$,y,z; $\frac{1}{2}$,$\bar{y}$,z
		2	m	0,y,z; 0,$\bar{y}$,z
		2	m	x,$\frac{1}{2}$,z; $\bar{x}$,$\frac{1}{2}$,z
		2	m	x,0,z; $\bar{x}$,0,z
	1	1	mm2	$\frac{1}{2}$,$\frac{1}{2}$,z
		1	mm2	$\frac{1}{2}$,0,z
		1	mm2	0,$\frac{1}{2}$,z
		1	mm2	0, 0, z



Space Group - Pmm2

P m m 2 C_{2v}^{1} *m m* 2 Orthorhombic

No. 25 *P m m* 2 Patterson symmetry *P m m m*



Origin on *m m* 2

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le \frac{1}{4}$; $0 \le z \le 1$

Symmetry operations

(1) 1 (2) 2 0,0,*z* (3) *m* *x*,0,*z* (4) *m* 0,*y*,*z*

- short space group symbol
- Schoenflies symbol
- point group
- crystal system
- number of space group
- full space group symbol
- projection of symmetry elements
- projection of general position

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
4	*i*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	General: no conditions
2	*h*	*m* . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			Special: no extra conditions
2	*g*	*m* . .	$0,y,z$	$0,\bar{y},z$			
2	*f*	. *m* .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2	*e*	. *m* .	$x,0,z$	$\bar{x},0,z$			
1	*d*	*mm*2	$\frac{1}{2},\frac{1}{2},z$				
1	*c*	*mm*2	$\frac{1}{2},0,z$				
1	*b*	*mm*2	$0,\frac{1}{2},z$				
1	*a*	*mm*2	$0,0,z$				

Zinc Blende, ZnS — $F\bar{4}3m$ (No.216)

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates (0,0,0)+	(0,½,½)+	(½,0,½)+	(½,½,0)+	Reflection conditions
96	*i*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	*h,k,l* permutable
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$	General:
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$	*hkl* : $h+k,h+l,k+l=2n$
			(13) y,x,z	(14) $\bar{y},\bar{x},z$	(15) $y,\bar{x},\bar{z}$	(16) $\bar{y},x,\bar{z}$	0*kl* : $k,l=2n$
			(17) x,z,y	(18) $\bar{x},z,\bar{y}$	(19) $\bar{x},\bar{z},y$	(20) $x,\bar{z},\bar{y}$	*hhl* : $h+l=2n$
			(21) z,y,x	(22) $z,\bar{y},\bar{x}$	(23) $\bar{z},y,\bar{x}$	(24) $\bar{z},\bar{y},x$	*h*00: $h=2n$
48	*h*	. . *m*	x,x,z $\bar{z},\bar{x},x$	$\bar{x},\bar{x},z$ $\bar{z},x,\bar{x}$	$\bar{x},x,\bar{z}$ x,z,x	$x,\bar{x},\bar{z}$ $\bar{x},z,\bar{x}$	z,x,x $x,\bar{z},\bar{x}$	$z,\bar{x},\bar{x}$ $\bar{x},\bar{z},x$	Special: no extra conditions
24	*g*	2 . *mm*	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$	
24	*f*	2 . *mm*	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$	
16	*e*	. 3*m*	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$			
4	*d*	$\bar{4}$3*m*	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$						
4	*c*	$\bar{4}$3*m*	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$						
4	*b*	$\bar{4}$3*m*	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$						
4	*a*	$\bar{4}$3*m*	$0,0,0$						

General position

Special position

Zinc Blende, ZnS

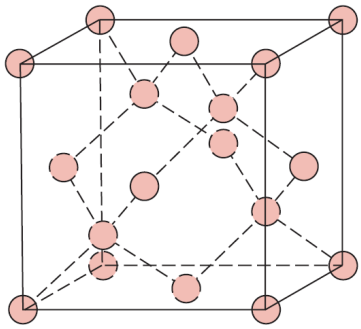
- diamond derivative structure
- Zn and S replace the C atoms in diamond
- Zn cubic close packing; S ½ tetrahedral site
- Zn and S cubic close packing displaced by $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

$F\bar{4}3m$ (No.216)

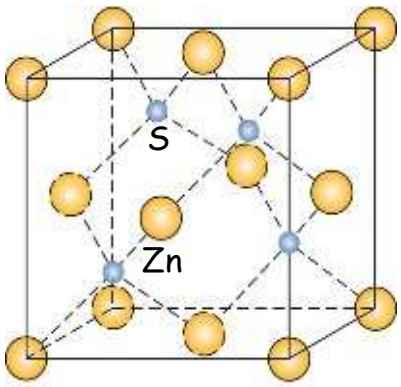
Zn: 4a, $\bar{4}3m$, $0,0,0$

Zn: 4c, $\bar{4}3m$, $\frac{1}{4},\frac{1}{4},\frac{1}{4}$

Diamond, Si, Ge



Zinc blende structure ZnS, SiC



Point group vs. space group

Point groups: A group of point symmetry operations, whose operation leaves at least one point unaltered. Any operation involving lattice translations is thus excluded	Space groups: A group of symmetry operations which include lattice translations
1 $\bar{1}$ 2 m 3 $\bar{3}$ 4 $\bar{4}$ 6 $\bar{6}$	1 $\bar{1}$ 2 m 2_1; a, b, c, n, e, d 3 $\bar{3}$ $3_1, 3_2$ 4 $\bar{4}$ $4_1, 4_2, 4_3$ 6 $\bar{6}$ $6_1, 6_2, 6_3, 6_4, 6_5$ lattice translations
a, b, c α, β, γ	a_0, b_0, c_0 α, β, γ
Order of the symmetry operations e.g. 4/m 2/m 2/m | | | c < a > < 110 >	Order of the symmetry operations e.g. $P4_2/m$ 2/m 2/m | | | c < a > < 110 >
General form: Set of equivalent faces each with face symmetry 1	General position: Set of equivalent points each with site symmetry 1
$f_{\text{asymmetric face unit}} = \frac{f_{\text{sphere}}}{\text{multiplicity of general form}}$	$V_{\text{asymmetric unit}} = \frac{V_{\text{unit cell}}}{\text{multiplicity of general point}}$
Multiplicity of general form of the point group	Multiplicity of the general position in all space groups with a P-lattice that are isomorphous with that point group
Special form: Set of equivalent faces each with face symmetry >1	Special position: Set of equivalent points each with site symmetry >1