Computational Materials Physics

Center for Molecular Modeling

Department of Materials Science and Engineering

crystallographic vocabulary

part 2

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http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

Terminology and definitions

Terminology list:

- crystal
- (primitive) unit cell
- lattice points
- lattice vectors
- Wigner-Seitz cell
- Bravais lattice
- lattice system
- centering
- conventional cell
- point group → of a Bravais lattice / of a crystal / of a Wyckoff position
- origin choice
- space group
- Wyckoff positions
- asymmetric unit
- cif file

One of the goals of this lecture is to have a good understanding of these concepts.

Terminology and definitions

Now consider the atoms again (and not only the lattice points).

- Keep the origin fixed.
- Search all symmetry operations that leave the crystal (≠ Bravais lattice) unchanged, keeping the origin fixed.

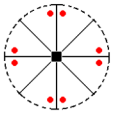
All these symmetry operations form the point group of this crystal.

Of the infinite number of point groups that exist for molecules, only 32 are consistent with one or more Bravais lattices.

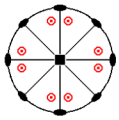
32 point groups that are consistent with one or more Bravais lattices:

http://en.wikipedia.org/wiki/Crystallographic_point_group

Hermann-Mauguin	Schoenflies	Orbifold	Coxeter	Order
1	C_1	11	[ ]$^+$	1
2	C_2	22	[2]$^+$	2
3	C_3	33	[3]$^+$	3
4	C_4	44	[4]$^+$	4
6	C_6	66	[6]$^+$	6
mm2	C_{2v}	*22	[2]	4
3m	C_{3v}	*33	[3]	6
4mm	C_{4v}	*44	[4]	8
6mm	C_{6v}	*66	[6]	12
m	$C_s = C_{1h}$	*11	[ ]	2
2/m	C_{2h}	2*	[2,2$^+$]	4
6	C_{3h}	3*	[2,3$^+$]	6
4/m	C_{4h}	4*	[2,4$^+$]	8
6/m	C_{6h}	6*	[2,6$^+$]	12
1	$C_i = S_2$	1x	[1$^+$,2$^+$]	2
4	S_4	2x	[2$^+$,4$^+$]	4
3	S_6	3x	[2$^+$,6$^+$]	6
222	D_2	222	[2,2]$^+$	4
32	D_3	322	[3,2]$^+$	6
422	D_4	422	[4,2]$^+$	8
622	D_6	622	[6,2]$^+$	12
mmm	D_{2h}	*222	[2,2]	8
62m	D_{3h}	*322	[3,2]	12
4/m mm	D_{4h}	*422	[4,2]	16
6/m mm	D_{6h}	*622	[6,2]	24
42m	D_{2d}	2*2	[2$^+$,4]	8
3m	D_{3d}	2*3	[2$^+$,6]	12
23	T	332	[3,3]$^+$	12
43m	T_d	*332	[3,3]	24
m3	T_h	3*2	[3$^+$,4]	24
432	O	432	[4,3]$^+$	24
m3m	O_h	*432	[4,3]	48



Tasks:
- List all symmetry operations
- Examine how one general point is mapped to all others
- Find a simple geometric shape with this symmetry



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mm2	C_{2v}	*22	[2]	4
3m	C_{3v}	*33	[3]	6
4mm	C_{4v}	***44**	**[4]**	**8**
6mm	C_{6v}	*66	[6]	12
m	$C_s = C_{1h}$	*11	[ ]	2
2/m	C_{2h}	2*	[2,2$^+$]	4
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mmm	D_{2h}	*222	[2,2]	8
62m	D_{3h}	*322	[3,2]	12
4/m mm	**D4h**	***422**	**[4,2]**	**16**
6/m mm	D_{6h}	*622	[6,2]	24
42m	D_{2d}	2*2	[2$^+$,4]	8
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Nice overview of stereographic projections for all 32 point groups:
http://newton.ex.ac.uk/research/qsystems/people/goss/symmetry/Stereographs.html

Idem, but as 3D objects:
http://newton.ex.ac.uk/research/qsystems/people/goss/symmetry/Solids.html

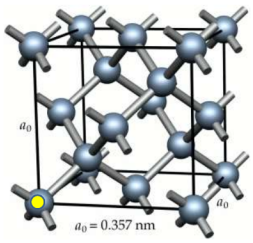
Terminology and definitions

Note: the point group of the crystal depends on the origin choice, i.e. the position in the unit cell where the origin of the lattice vectors is taken.

Example:

Diamond
Origin choice 2: (0, 0, 0)

Does the point group contain inversion symmetry ?



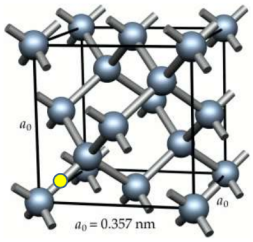
Terminology and definitions

Note: the point group of the crystal depends on the origin choice, i.e. the position in the unit cell where the origin of the lattice vectors is taken.

Example:

Diamond
Origin choice 1: (1/8, 1/8, 1/8)

Does the point group contain inversion symmetry ?

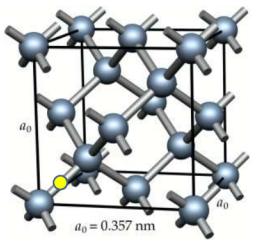


Terminology and definitions

Note: the point group of the crystal depends on the origin choice, i.e. the position in the unit cell where the origin of the lattice vectors is taken.

➔The default origin choice (a.k.a "origin choice 1") is such that the point group contains inversion symmetry.

This simplifies the math, for XRD analysis as well as for DFT calculations.



Group these 32 point groups into sets, called crystal systems: All point groups that are consistent with the same lattice systems (plural !) are in the same set.

Crystal family	Crystal system	Required symmetries of point group	Point groups	Space groups	Bravais lattices	Lattice system
Triclinic		None	2	2	1	Triclinic
Monoclinic		one 2-fold axis or one mirror plane	3	13	2	Monoclinic
Orthorhombic		3 2-fold axes or 1 2-fold axis and 2 mirror planes	3	59	4	Orthorhombic
Tetragonal		one 4-fold axis	7	68	2	Tetragonal
Hexagonal	Trigonal	one 3-fold axis	5	7	1	Rhombohedral
				18	1	Hexagonal
	Hexagonal	one 6-fold axis	7	27		
cubic		four 3-fold axes	5	36	3	Cubic
total = 6	**7**		**32**	**230**	**14**	**7**
		Properties of point groups		Properties of crystals (space groups)		

Point groups can be alternatively divided into crystal families: this is a regrouping of the crystal systems, where two crystal systems that share a lattice system are put into the same crystal family.

Crystal family	Crystal system	Required symmetries of point group	Point groups	Space groups	Bravais lattices	Lattice system
Triclinic		None	2	2	1	Triclinic
Monoclinic		1 2-fold axis or 1 mirror plane	3	13	2	Monoclinic
Orthorhombic		3 2-fold axes or 1 2-fold axis and 2 mirror planes	3	59	4	Orthorhombic
Tetragonal		1 4-fold axis	7	68	2	Tetragonal
Hexagonal	Trigonal	1 3-fold axis	5	7	1	Rhombohedral
				18	1	Hexagonal
	Hexagonal	1 6-fold axis	7	27		
cubic		4 3-fold axes	5	36	3	Cubic
total = 6	**7**		**32**	**230**	**14**	**7**
		Properties of point groups		Properties of crystals (space groups)		

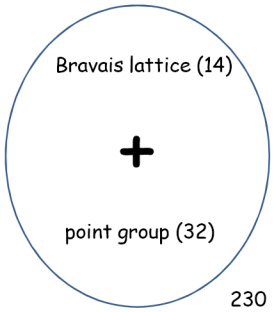
Albeit being often used, a term as

~~rhombohedral crystal system~~

is meaningless !

Terminology and definitions

Space group =



230 combinations possible

Two questions (until next week) :

1) Why 230 and not 32x14=448 ?

2-a) Why 230 and not 66 ? (=number of point groups for each lattice system multiplied by the number of Bravais lattices for this lattice system)

2-b) Search, draw (jmol, vesta,…) and understand an example crystal for space groups 221 and 222, which are both point group m-3m combined with the simple cubic Bravais lattice.

Names and conventions for the 230 space groups: ITA "International Tables for Crystallography, volume A"

List of names:
http://en.wikipedia.org/wiki/Space_group#Table_of_space_groups_in_3_dimensions

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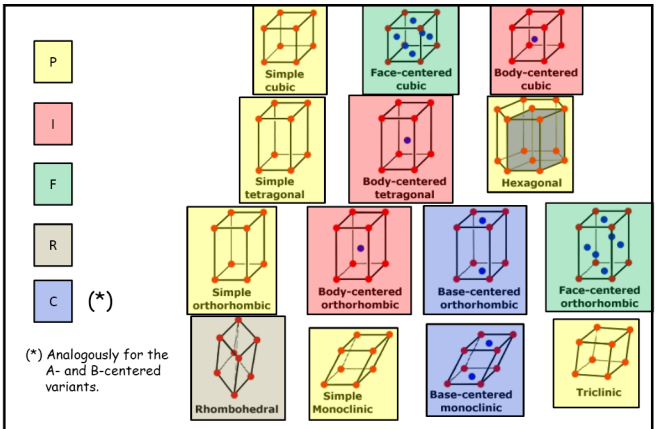
Hermann-Mauguin naming convention:
http://en.wikipedia.org/wiki/Hermann-Mauguin_notation

First letter: partial indication of the Bravais lattice
(not according to lattice type – different classification ! See next slide.)

Then: a sequence that characterizes the main point group symmetry elements (built according to a set of rules – we will treat this as a given name, usually).



Task :

There is no monoclinic I-centered lattice in this list. Show that it is indeed redundant, as you can describe it by a monoclinic C-centered lattice by a different choice of axes.

Most common naming system in materials physics:

Hermann-Mauguin (short version). E.g.: P4/mmm (nr. 123)

More explicit enumeration of symmetry elements in the long version: P 4/m 2/m 2/m.

The Hermann-Maugain symbol does not explicitly indicate the origin, hence different origin choices remain possible.

Hall symbol: naming system that includes the origin choice as well. Fully unambiguous, and often used inside computer programs. (list at http://cci.lbl.gov/sginfo/hall_symbols.html)

Names and conventions for the 230 space groups: ITA "International Tables for Crystallography, volume A"

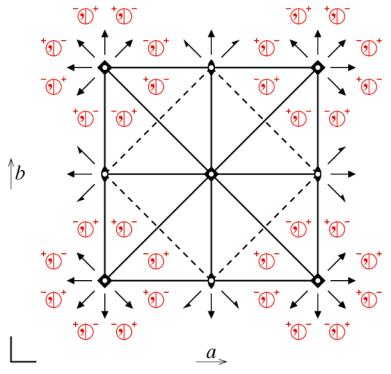
List of names:
http://en.wikipedia.org/wiki/Space_group#Table_of_space_groups_in_3_dimensions

Available in many libraries, or on-line if your institution pays for it.

Legal (?) public version of (part of) this information:
http://img.chem.ucl.ac.uk/sgp/mainmenu.htm

Useful info:
http://img.chem.ucl.ac.uk/sgp/misc/guide.htm

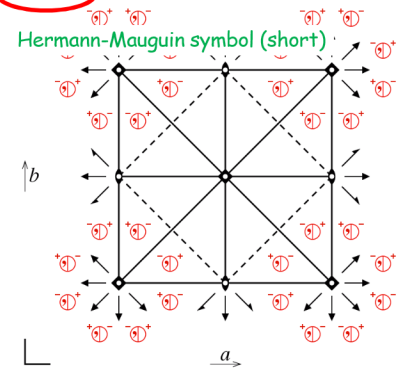
P4/mmm *P 4/m 2/m 2/m* *4/mmm* No. 123



1 x, y, z
2 $\bar{x}, \bar{y}, z$
3 $\bar{y}, x, z$
4 $y, \bar{x}, z$
5 $\bar{x}, y, z$
6 $x, \bar{y}, z$
7 y, x, z
8 $\bar{y}, \bar{x}, z$
9 $\bar{x}, \bar{y}, \bar{z}$
10 $x, y, \bar{z}$
11 $y, \bar{x}, \bar{z}$
12 $\bar{y}, x, \bar{z}$
13 $x, \bar{y}, \bar{z}$
14 $\bar{x}, y, \bar{z}$
15 $\bar{y}, \bar{x}, \bar{z}$
16 $y, x, \bar{z}$

P4/mmm P 4/m 2/m 2/m 4/mmm No. 123

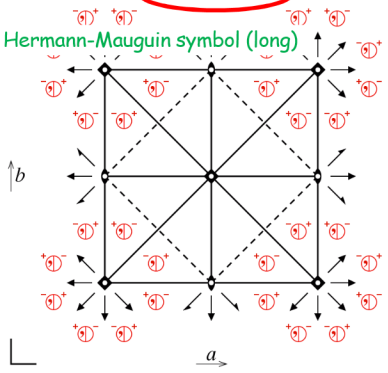
Hermann-Mauguin symbol (short)



1 x, y, z
2 $\bar{x}, \bar{y}, z$
3 $\bar{y}, x, z$
4 $y, \bar{x}, z$
5 $\bar{x}, y, z$
6 $x, \bar{y}, z$
7 y, x, z
8 $\bar{y}, \bar{x}, z$
9 $\bar{x}, \bar{y}, \bar{z}$
10 $x, y, \bar{z}$
11 $y, \bar{x}, \bar{z}$
12 $\bar{y}, x, \bar{z}$
13 $x, \bar{y}, \bar{z}$
14 $\bar{x}, y, \bar{z}$
15 $\bar{y}, \bar{x}, \bar{z}$
16 $y, x, \bar{z}$

P4/mmm P 4/m 2/m 2/m 4/mmm No. 123

Hermann-Mauguin symbol (long)



1 x, y, z
2 $\bar{x}, \bar{y}, z$
3 $\bar{y}, x, z$
4 $y, \bar{x}, z$
5 $\bar{x}, y, z$
6 $x, \bar{y}, z$
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10 $x, y, \bar{z}$
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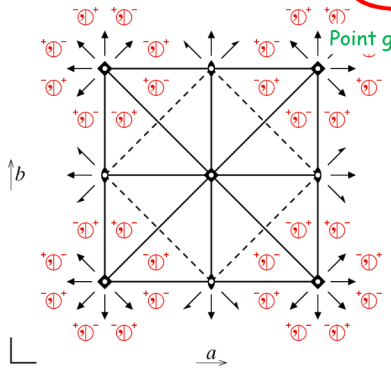
13 $x, \bar{y}, \bar{z}$
14 $\bar{x}, y, \bar{z}$
15 $\bar{y}, \bar{x}, \bar{z}$
16 $y, x, \bar{z}$

P4/mmm P 4/m 2/m 2/m 4/mmm No. 123

Point group of Bravais lattice



3 $\bar{y}, x, z$
4 $y, \bar{x}, z$
5 $\bar{x}, y, z$
6 $x, \bar{y}, z$
7 y, x, z
8 $\bar{y}, \bar{x}, z$
9 $\bar{x}, \bar{y}, \bar{z}$
10 $x, y, \bar{z}$
11 $y, \bar{x}, \bar{z}$
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13 $x, \bar{y}, \bar{z}$
14 $\bar{x}, y, \bar{z}$
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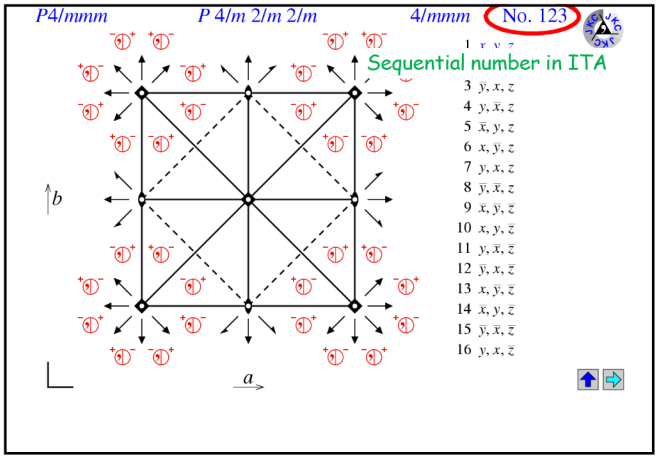
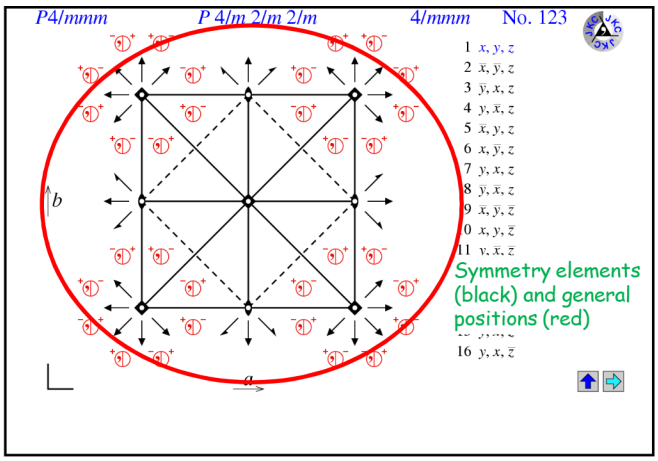
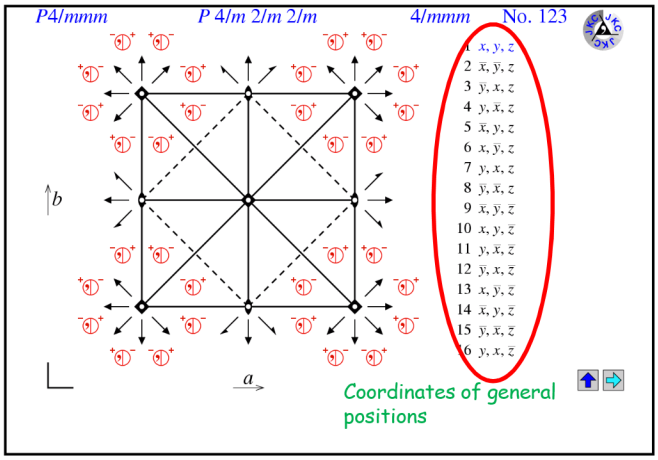
16 $y, x, \bar{z}$


P4/mmm
P 4/m 2/m 2/m
4/mmm
No. 123
Sequential number in ITA
3 $\bar{y}, x, z$
4 $y, \bar{x}, z$
5 $\bar{x}, y, z$
6 $x, \bar{y}, z$
7 y, x, z
8 $\bar{y}, \bar{x}, z$
9 $\bar{x}, \bar{y}, \bar{z}$
10 $x, y, \bar{z}$
11 $y, \bar{x}, \bar{z}$
12 $\bar{y}, x, \bar{z}$
13 $x, \bar{y}, \bar{z}$
14 $\bar{x}, y, \bar{z}$
15 $\bar{y}, \bar{x}, \bar{z}$
16 $y, x, \bar{z}$
b
a


P4/mmm
P 4/m 2/m 2/m
4/mmm
No. 123
1 x, y, z
2 $\bar{x}, \bar{y}, z$
3 $\bar{y}, x, z$
4 $y, \bar{x}, z$
5 $\bar{x}, y, z$
6 $x, \bar{y}, z$
7 y, x, z
8 $\bar{y}, \bar{x}, z$
9 $\bar{x}, \bar{y}, \bar{z}$
10 $x, y, \bar{z}$
11 $y, \bar{x}, \bar{z}$
Symmetry elements (black) and general positions (red)
16 $y, x, \bar{z}$
b
a


P4/mmm
P 4/m 2/m 2/m
4/mmm
No. 123
1 x, y, z
2 $\bar{x}, \bar{y}, z$
3 $\bar{y}, x, z$
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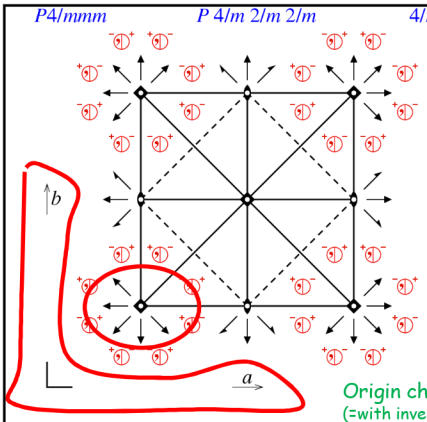
12 $\bar{y}, x, \bar{z}$
13 $x, \bar{y}, \bar{z}$
14 $\bar{x}, y, \bar{z}$
15 $\bar{y}, \bar{x}, \bar{z}$
16 $y, x, \bar{z}$
Coordinates of general positions
b
a

P4/mmm P 4/m 2/m 2/m 4/mmm No. 123



1 x, y, z
2 $\bar{x}, \bar{y}, z$
3 $\bar{y}, x, z$
4 $y, \bar{x}, z$
5 $\bar{x}, y, z$
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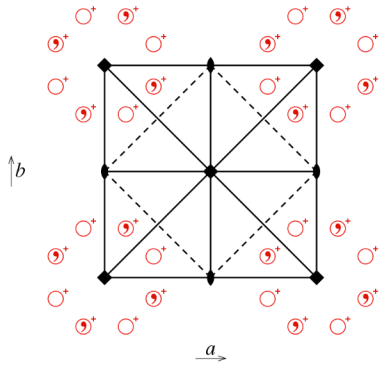
15 $\bar{y}, \bar{x}, \bar{z}$
16 $y, x, \bar{z}$

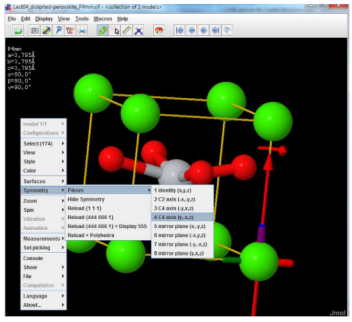
Origin choice 1
(=with inversion whenever possible)

P4mm P 4 m m 4mm No. 99



1 x, y, z
2 $\bar{x}, \bar{y}, z$
3 $\bar{y}, x, z$
4 $y, \bar{x}, z$
5 $\bar{x}, y, z$
6 $x, \bar{y}, z$
7 y, x, z
8 $\bar{y}, \bar{x}, z$

Compare this with similar information in Jmol for nrs. 99 and 123
(if a cif file has been read - see soon) :



Note: 8 items in drop-down menu, corresponds to the 8 general positions on the previous slide.

Task:
Play with this in Jmol, and relate all symmetry information to symbols on the ITA diagram

More extentive web application:
http://chemapps.stolaf.edu/jmol/docs/examples-11/jcse/explore.htm

Wyckoff positions

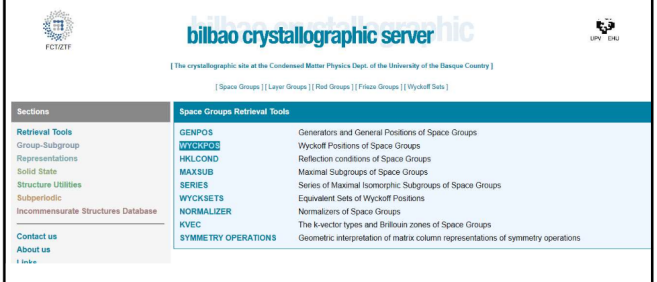
The entire crystal is specified by:

- The space group (in a given setting)
- The occupied wyckoff positions (if needed with values for the free parameters)

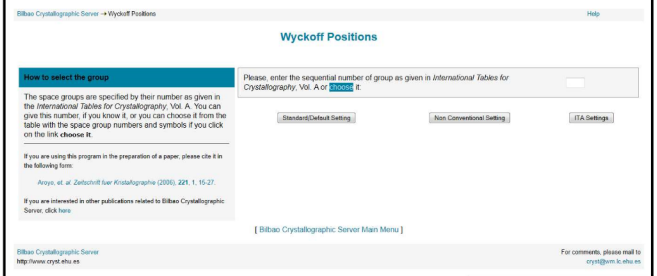
Possible Wyckoff positions for each space group:

Bilbao Crystallographic Server, WYCKPOS program
http://www.cryst.ehu.es/

Wyckoff positions



Wyckoff positions



Wyckoff positions

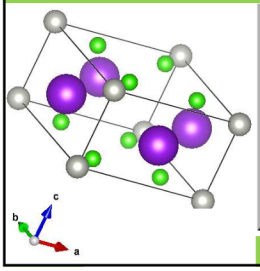
94	$P4_22_12$	95	$P4_322$	96	$P4_32_12$
97	$I422$	98	$I4_122$	99	$P4mm$
100	$P4bm$	101	$P4_2cm$	102	$P4_2nm$
103	$P4cc$	104	$P4nc$	105	$P4_2mc$
106	$P4_2bc$	107	$I4mm$	108	$I4cm$
109	$I4_1md$	110	$I4_1cd$	111	$P\bar{4}2m$
112	$P\bar{4}2c$	113	$P\bar{4}2_1m$	114	$P\bar{4}2_1c$
115	$P\bar{4}m2$	116	$P\bar{4}c2$	117	$P\bar{4}b2$
118	$P\bar{4}n2$	119	$I\bar{4}m2$	120	$I\bar{4}c2$
121	$I\bar{4}2m$	122	$I\bar{4}2d$	123	$P4/mmm$
124	$P4/mcc$	125	$P4/nbm$:origin choice 1 $P4/nbm$:origin choice 2	126	$P4/nnc$:origin choice 1 $P4/nnc$:origin choice 2
127	$P4/mbm$	128	$P4/mnc$	129	$P4/nmm$:origin choice 1 $P4/nmm$:origin choice 2
130	$P4/ncc$:origin choice 1 $P4/ncc$:origin choice 2	131	$P4_2/mmc$	132	$P4_2/mcm$
133	$P4_2/nbc$:origin choice 1 $P4_2/nbc$:origin choice 2	134	$P4_2/nnm$:origin choice 1 $P4_2/nnm$:origin choice 2	135	$P4_2/mbc$
136	$P4_2/mnm$	137	$P4_2/nmc$:origin choice 1 $P4_2/nmc$:origin choice 2	138	$P4_2/ncm$:origin choice 1 $P4_2/ncm$:origin choice 2

Wyckoff Positions of Group 123 (*P4/mmm*)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
16	u	1	(x,y,z) (-x,-y,z) (-y,x,z) (y,-x,z) (-x,y,-z) (x,-y,-z) (y,x,-z) (-y,-x,-z) (-x,-y,-z) (x,y,-z) (y,-x,-z) (-y,x,-z) (x,-y,z) (-x,y,z) (-y,-x,z) (y,x,z)
4	k	m.2 m	(x,x,1/2) (-x,-x,1/2) (-x,x,1/2) (x,-x,1/2)
4	j	m.2 m	(x,x,0) (-x,-x,0) (-x,x,0) (x,-x,0)
4	i	2mm .	(0,1/2,z) (1/2,0,z) (0,1/2,-z) (1/2,0,-z)
2	h	4mm	(1/2,1/2,z) (1/2,1/2,-z)
2	g	4mm	(0,0,z) (0,0,-z)
2	f	mmm .	(0,1/2,0) (1/2,0,0)
2	e	mmm .	(0,1/2,1/2) (1/2,0,1/2)
1	d	4/mmm	(1/2,1/2,1/2)
1	c	4/mmm	(1/2,1/2,0)
1	b	4/mmm	(0,0,1/2)
1	a	4/mmm	(0,0,0)

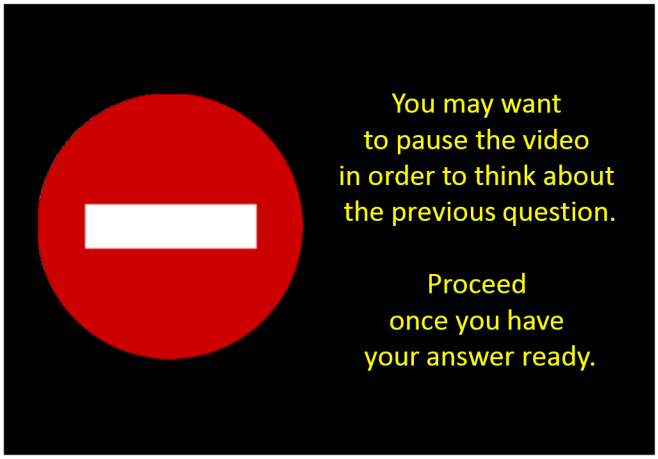
Point group of a Wyckoff position: similar to the point group of a crystal, yet with the atom at this position fixed rather than the origin fixed.

Excercise K_2PdCl_4 : find multiplicity and Wyckoff letter of all sites.



Wyckoff Positions of Group 123 (*P4/mmm*)

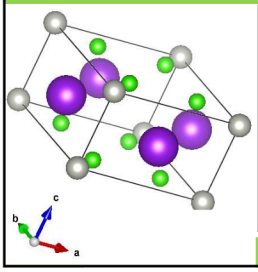
Multiplicity	Wyckoff letter	Site symmetry	Coordinates
16	u	1	(x,y,z) (-x,-y,z) (-y,x,z) (y,-x,z) (-x,y,-z) (x,-y,-z) (y,x,-z) (-y,-x,-z) (-x,-y,-z) (x,y,-z) (y,-x,-z) (-y,x,-z) (x,-y,z) (-x,y,z) (-y,-x,z) (y,x,z)
4	k	m.2 m	(x,x,1/2) (-x,-x,1/2) (-x,x,1/2) (x,-x,1/2)
4	j	m.2 m	(x,x,0) (-x,-x,0) (-x,x,0) (x,-x,0)
4	i	2mm .	(0,1/2,z) (1/2,0,z) (0,1/2,-z) (1/2,0,-z)
2	h	4mm	(1/2,1/2,z) (1/2,1/2,-z)
2	g	4mm	(0,0,z) (0,0,-z)
2	f	mmm .	(0,1/2,0) (1/2,0,0)
2	e	mmm .	(0,1/2,1/2) (1/2,0,1/2)
1	d	4/mmm	(1/2,1/2,1/2)
1	c	4/mmm	(1/2,1/2,0)
1	b	4/mmm	(0,0,1/2)
1	a	4/mmm	(0,0,0)



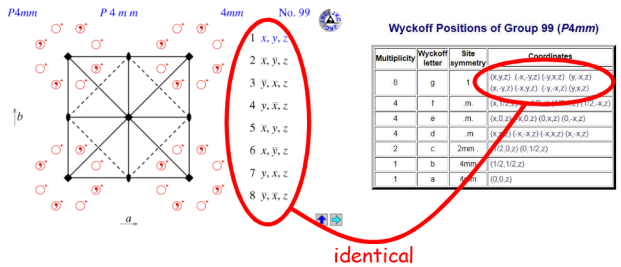
Excercise K_2PdCl_4 : find multiplicity and Wyckoff letter of all sites.

Wyckoff Positions of Group 123 (*P4/mmm*)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
16	u	1	(x,y,z) (-x,-y,z) (-y,x,z) (y,-x,z) (-x,y,-z) (x,-y,-z) (y,x,-z) (-y,-x,-z) (-x,-y,-z) (x,y,-z) (y,-x,-z) (-y,x,-z) (x,-y,z) (-x,y,z) (-y,-x,z) (y,x,z)
4	k	m.2 m	(x,x,1/2) (-x,-x,1/2) (-x,x,1/2) (x,-x,1/2)
4	j	m.2 m	(x,x,0) (-x,-x,0) (-x,x,0) (x,-x,0)
4	i	2mm .	(0,1/2,z) (1/2,0,z) (0,1/2,-z) (1/2,0,-z)
2	h	4mm	(1/2,1/2,z) (1/2,1/2,-z)
2	g	4mm	(0,0,z) (0,0,-z)
2	f	mmm .	(0,1/2,0) (1/2,0,0)
2	e	mmm .	(0,1/2,1/2) (1/2,0,1/2)
1	d	4/mmm	(1/2,1/2,1/2)
1	c	4/mmm	(1/2,1/2,0)
1	b	4/mmm	(0,0,1/2)
1	a	4/mmm	(0,0,0)



Wyckoff positions

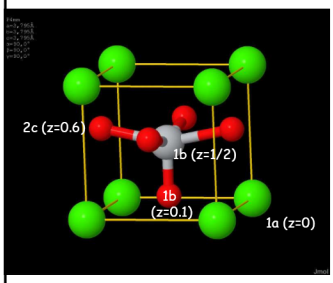


Wyckoff Positions of Group 99 (*P4mm*)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
8	g	1	(x,y,z) (-x,-y,z) (-y,x,z) (y,-x,z) (x,-y,z) (-x,y,z) (-y,-x,z) (y,x,z)
4	f	m.	(x,1/2,z) (-x,1/2,z) (1/2,x,-z) (1/2,-x,-z)
4	e	m.	(x,0,z) (-x,0,z) (0,x,z) (0,-x,z)
4	d	.m	(x,x,z) (-x,-x,z) (-x,x,z) (x,-x,z)
2	c	2mm .	(1/2,0,z) (0,1/2,z)
1	b	4mm	(1/2,1/2,z)
1	a	4/mm	(0,0,z)

identical

Wyckoff positions

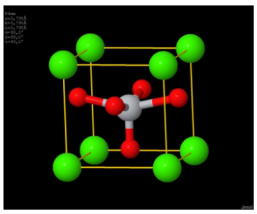


Wyckoff Positions of Group 99 (*P4mm*)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
8	g	1	(x,y,z) (-x,-y,z) (-y,x,z) (y,-x,z) (x,-y,z) (-x,y,z) (-y,-x,z) (y,x,z)
4	f	.m.	(x,1/2,z) (-x,1/2,z) (1/2,x,z) (1/2,-x,z)
4	e	.m.	(x,0,z) (-x,0,z) (0,x,z) (0,-x,z)
4	d	.m	(x,x,z) (-x,-x,z) (-x,x,z) (x,-x,z)
2	c	2mm .	(1/2,0,z) (0,1/2,z)
1	b	4mm	(1/2,1/2,z)
1	a	4mm	(0,0,z)

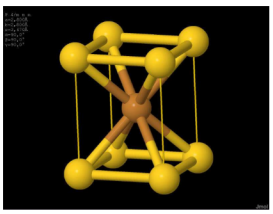
Wigner-Seitz cells

Nr. 99, P4mm



Distorted perovskite

Nr. 123, P4/mmm

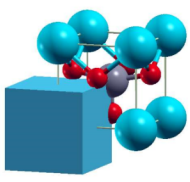


AuCu

Unit cells by jmol

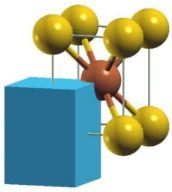
Wigner-Seitz cells

Nr. 99, P4mm



Distorted perovskite

Nr. 123, P4/mmm



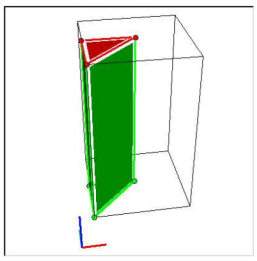
AuCu

Wigner-Seitz cells by Xcrysden

Asymmetric unit

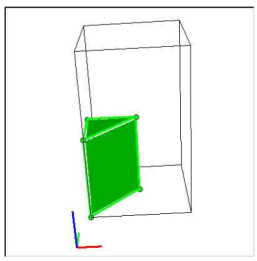
Minimal fraction of the unit cell from which by the symmetry operations the entire unit cell can be reconstructed.
Exhaustive list of pictures at http://cci.lbl.gov/asu_gallery/

Space group: P 4 m m (No. 99)



http://cci.lbl.gov/asu_gallery/asu_099.html

Space group: P 4/m m m (No. 123)



http://cci.lbl.gov/asu_gallery/asu_123.html

Miller indices

- Explained in Kittel.
- Convenient tool in Vesta.